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Statistical Methods in NUCLEAR MATERIAL CONTROL

by

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Prepared for the Division of Nuclear Materials Security
U. S. Atomic Energy Commission

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In monotype	*In linotype*
s_x^2	s_{x^2}
$\chi^2_{1-(\alpha/2)}$	$\chi_{1-(\alpha/2)^2}$

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FOREWORD

A book describing statistical approaches specific to nuclear industry safeguards applications has long been needed. *Statistical Methods in Nuclear Material Control* helps meet this need by presenting selected methods useful for plant safeguards control and evaluation. The discussions in this volume should provide increased industry-wide understanding and guidance that will be instrumental in improving material-unaccounted-for control and evaluation.

The U. S. Atomic Energy Commission, Division of Nuclear Materials Security, in conjunction with the Safeguards Training Program at the Argonne Center for Educational Affairs sponsored the preparation of this book.

Leonard M. Brenner
Acting Director
Division of Nuclear Materials Security
U. S. Atomic Energy Commission

PREFACE

This book grew out of material prepared for several courses on the application of statistics to problems of nuclear control. The courses were conducted as part of the Safeguards Training Program sponsored by the Atomic Energy Commission (AEC) and administered by the Argonne National Laboratory (ANL) through its Center for Educational Affairs. Participants in the courses and others involved with applying statistics to nuclear material control suggested that the course notes be prepared for wider distribution. This general feeling provided the impetus for the project that has resulted in this book.

The project rather forcibly brought to my attention that there is a considerable gap between crudely prepared lecture notes and what, I hope, is a more polished and more nearly complete presentation on the subject. The course material was extended considerably from the original lecture notes. For example, essentially all the material in Chap. 3 dealing with the important topic of estimation of measurement-error variances is new since I touched only very lightly on this subject in my past courses. Because of this and other extensions, all the material presented in this book can scarcely be covered in any detail in a short course.

Although an outgrowth of short courses, this volume is not intended as a textbook. Consequently there is a complete absence of problems that can be assigned. Rather, the book is intended as a personal reference book that the reader would study on an individual basis, applying the methods to his problems. With this in mind I placed heavy emphasis on worked examples, usually with sufficient calculational details to enable the reader to follow the solution step by step.

Some sections can be omitted by the reader whose only interest is in application. The organization of the material is such that the statistical bases for the solutions are in separate sections, which are generally somewhat more mathematical in nature and can be skipped without impairing the usefulness of the book. The material is structured so that each major section in Chaps. 4 to 9 begins with a description of the problem under consideration. If a particular problem is

of little concern, the following sections, which give the solution, worked examples, and basis for the solution, can be omitted. Also, a few topics are quite specialized in nature and may not be of great interest to the reader concerned with applying statistics to his own particular problems. To assist the reader in selecting topics of greatest interest for more intensive study, I included Chap. 10, which summarizes the topics and the examples in an orderly fashion and directs the reader's attention to the parts of the book likely to interest him most.

A bibliography is not included. The only references to other works occur when they are cited in text for specific reasons. This is in no way intended to slight the past writings that touch on this subject. But the time frame of the project was such that a literature survey was out of the question; two complete drafts were written between mid-June and the end of December 1972. Therefore I placed heavy reliance on my personal experience rather than on other works in selecting the material to be presented. Although I hope the end product is mostly self-contained in the essentials, there are, no doubt, inequities in the amount of attention given to certain topics because of my special interest in them. I can only ask your indulgence in this.

I am indebted to many individuals who have contributed in one way or another to this project. In particular, I owe a debt of gratitude to M. A. Kanter, who both conceived of this project and provided financial support through his role as Director of the Safeguards Training Program of the Argonne Center for Educational Affairs. Beyond this, I gratefully acknowledge his personal assistance in providing encouragement and technical comments that resulted in major improvements of the first draft. The project was administered through ANL by T. S. Sherr of the AEC Division of Nuclear Materials Security, whose encouragement and editorial assistance is also appreciated. My thanks to him extend also to others in the AEC and among the AEC contractors who lent their support by reviewing the first draft.

In the examples presented it is apparent that I drew heavily on my years of experience at Hanford. Although I hesitate to mention certain persons by name for fear of omitting others also deserving of mention, it would be a disservice were I to omit expressing gratitude for my pleasant and rewarding associations with R. A. Schneider, K. B. Stewart, and C. A. Bennett, whose collective influence on this book will be noted by the reader. In particular, on numerous occasions while writing the book, I talked by phone with R. A. Schneider to obtain his reactions to certain sentences, paragraphs, examples, etc. His comments and ideas have been most appreciated. Throughout the book I have noted specific contributions from these individuals and

others. In many instances this notation concerns data for the examples. Although acknowledging these data sources, I supplied the solutions and bear full responsibility for any shortcomings in this and other respects.

To continue with the acknowledgments, I am most grateful to the management of Exxon Nuclear Company, and, in particular, to L. P. Bupp, for giving me the time and opportunity to work on this project. I acknowledge a special debt of gratitude to the typist, Marge Groff, who very expertly waded through two complete drafts of the manuscript, and hope that, if nothing else, her knowledge of the Greek alphabet has been enhanced thereby. I would like to thank R. F. Pigeon, AEC Office of Information Services, who handled the administration of the publication of the book. The expert editorial assistance provided by Margaret Givens, Dee Jared, and Joan Roberts at the AEC Technical Information Center is very much appreciated. Finally, for his assistance in indexing, I am grateful to Jonathan Jaech, who was motivated by the opportunity of having his name appear in the preface in lieu of financial rewards.

I dedicate this book to my wife, Lorna, using this means to express the idea that Lorna has been a continuing inspiration to me in all aspects of my life, including the preparation of this book, even though I suspect that she is numbered among those who "don't believe in statistics." Her continuing courage, unwavering faith, and never ending love and concern for others in the face of personal suffering are the sources of this inspiration to me, and to others. Those among my readers who are privileged to know Lorna will understand it when I say that, when judged against what her contributions to mankind have been, this book and all the effort that went into its preparation pale into insignificance. [Prior to the publication of this book, Lorna was called to her eternal rest. This book is lovingly dedicated to her memory.]

I would like to conclude the preface by saying that it is my sincere hope that the end product of these efforts will be useful to you, the reader, in the execution of your work assignments.

John L. Jaech

CONTENTS

Chapter 1

INTRODUCTION

This book is concerned with the application of statistical methods in the solving of problems associated with the control of nuclear materials. The motivation for exercising this control is not the issue here, but it is recognized that more than one motivating factor is at work.

If for no other reason, the operator of a facility is concerned with the control of nuclear materials because of economic incentives. It is good business practice for him to guard against the loss of this economically valuable resource and by being accountable for it to demonstrate to himself and to others that the measures taken to prevent losses have succeeded.

On the other hand, nuclear materials not only have economic value but also strategic value in that they can be harmful if used for illicit purposes. In this connection the operator is responsible to the public to secure nuclear materials entrusted to his care and to demonstrate that his security measures have successfully guarded against the diversion of nuclear materials for illicit purposes. The public is represented in this by a national agency (in the United States, the Atomic Energy Commission) charged with providing credible assurance that each facility operator is exercising responsible stewardship of nuclear materials.

If we take the strategic value of materials one step further, we see that the control of nuclear materials is also an important international issue. The scope of the problem differs, but the essential ingredients are the same. In this instance the international agency (namely, the International Atomic Energy Agency) is charged with providing assurance to the member states that a given state has not diverted nuclear materials from peaceful endeavors to the production of nuclear weapons.

In viewing these different situations, we see two quite distinct aspects of the problem. First, and quite clearly more important, is the problem of guarding against losses. This is accomplished (1) by plant design and operation to minimize the amount of nuclear materials that is lost in the sense that it exits from the facility without having been measured, or perhaps it remains within the facility unbeknownst to anyone and is therefore

unaccountable, and (2) by a physical security system that guards against theft of such materials. With respect to the first point, the operator of a facility strives to keep the yield high and to guard against all losses, measured or unmeasured. From a control viewpoint, it does not matter in principle how small the yield is as long as scrap and waste materials can be measured adequately. However, experience indicates that scrap and waste materials are difficult to measure, and, as a general rule, the smaller the amount of such materials created, the better the control that is exercised.

The second aspect of nuclear materials control is the ability to demonstrate that the amount of material lost is below some specified amount, i.e., that the steps taken to guard against losses have been effective. Clearly, if the preventive measures have not been effective, the control cannot be demonstrated. (This assumes that the system of accounting provides an honest reflection of the true state of affairs.) Thus the problem of guarding against losses is the more important one. On the other hand, it is not comforting if the steps taken to physically control the materials have been effective but the control system cannot demonstrate this with any credible assurance. Therefore the importance of this aspect cannot be minimized either.

How is adequate control demonstrated? In its simplest form, adequate control requires only proper accounting for all the nuclear materials entering and leaving a facility. In addition, at specified times there must be the ability to measure the materials in inventory. This process is referred to in broad terms as nuclear materials accountability.

Thus far in the discussion there has been no mention of statistics. If the problem of accounting for materials were as simple as indicated in the previous paragraph, there would, in fact, be little need for statistical methods to effect and/or to demonstrate control. But the problem is not that simple—it is difficult to count atoms! It is never known for certain how much material enters or leaves a facility or how much is really there when an inventory is taken. Because of measurement errors, these quantities can only be estimated, and effective control is limited by the ability to measure.

This problem is not different in principle from problems associated with control of other materials. The operator of a grocery store, for example, also makes errors when taking an inventory, and he also has unmeasured losses. The problems are more serious for nuclear materials, however, for two reasons. First, the control must be very tight because of the high value (economic and strategic) of these materials; and second, the measurement problems can be very complex.

This, then, is where statistics enters in. The role of statistical methods in this field of application is twofold: (1) to obtain objective measures of the effectiveness of the control system and (2) to indicate how the effectiveness can be improved.

This book is aimed at providing the practitioner with the tools needed to apply statistical methods profitably in nuclear materials control problems. Although statistics is a universal discipline that can be applied in any field, a specialized book for nuclear materials control is considered profitable because each field of application presents unique problems, whose solutions may not be adequately covered in readily accessible sources. Such appears to be the case in nuclear materials control, where the dominant problems are associated with such topics as

- estimation of many different measurement-error variances
- existence of (and often the dominance of) systematic-error variances
- propagation of error variances in complex systems
- problems associated with measuring and verifying an inventory
- paired data, which occur in shipper–receiver differences, in inventory verification activities, and when an item is measured simultaneously by two methods of measurement

This book is intended to present a unified approach to the preceding problems and to other problems of primary concern to the practitioner in the field of nuclear materials control.

Chapters 2 and 3 are introductory chapters, with Chap. 2 covering essential topics in probability and statistics and Chap. 3 concerned with the sources of measurement errors in this particular field of application. Chapters 4 to 9 follow a format that, I hope, will be helpful to the reader. Each section is divided into four parts: (1) a statement of the problem and the assumptions; (2) the solution; (3) worked numerical examples; and (4) the basis for the solution. The intent is that the book be usable even if the bases for the solutions are not studied or even read. In this sense the book is similar in nature to a cookbook, but at the same time, by including the bases for the solutions, it creates the opportunity for the reader to understand better the various topics.

Chapter 10 is, in a sense, a summary chapter. All the examples, except those in Chap. 2, are indexed by type of problem and type of facility to permit easy reference. Further, brief descriptions are given of these problems to convey their substance with respect to both technical and statistical content.

Chapter 2

PROBABILITY AND STATISTICS

OVERVIEW

"Probability and Statistics" is an ambitious title for a single chapter. In a specialized book of this nature, there are those who might question the need for including material that is readily available from a large number of other sources of varying difficulty. Most potential users of this book will be likely to have at least one book on probability and statistics in their own personal libraries or, if not, to have ready access to one. Why then is this chapter included? There are a number of reasons.

First, as mentioned in the Preface, this book is largely based on material from several short courses presented as part of the Safeguards Training Program conducted at the Argonne Center for Educational Affairs. Even though most students were familiar with the basic ideas of probability and statistics, the instructor considered it helpful to spend some time reviewing this basic material as a preliminary to discussing special topics of interest in nuclear material control. The review served the twofold purpose of refreshing memories on topics that might not have been reviewed for several years and of providing a common base of usage and terminology to aid in later presentations. I hope that the material in this chapter will fulfill the same role in this book.

Second, in spite of the ready availability of reference books, I considered it worthwhile to make this book self-contained so that the user does not need a battery of reference books to use the material presented here. Although complete success is not possible, I hope that this chapter will minimize the number of occasions in which the user must look elsewhere for help and clarification.

Third, even introductory books on probability and statistics are often lengthy and contain material of little direct value for statistical problems of nuclear material control. This chapter is an attempt to emphasize the topics of greatest value and interest to the specialized reader who will have occasion to use this book. Additional emphasis is gained by the presen-

tation of examples that largely relate to the application of probability and statistics to problems of nuclear material control.

There is no attempt to be mathematically rigorous in the presentation; such rigor is sacrificed for clarity in exposition. Further, many basic topics may be conspicuous by their absence, because completeness is not the aim. Rather, the intent is to focus on the topics considered to be most useful in understanding the material in subsequent chapters.

Chapter 2 is divided into nine major sections. Section 2.1 deals with descriptive statistics. In Sec. 2.2 some basic ideas and results in probability are presented. This leads to a discussion of random variables and probability distributions in Sec. 2.3, with some specific distributions considered in Sec. 2.4. Bivariate distributions involving two random variables are discussed in Sec. 2.5. The remaining sections deal with statistical inference, with sampling distributions covered in Sec. 2.6, parameter estimation in Sec. 2.7, and hypothesis testing in Sec. 2.8. The final section, Sec. 2.9, presents some particular tests for testing the validity of distributional assumptions.

2.1 DESCRIPTIVE STATISTICS

This section is concerned with the presentation of data. How can a number of data points, or observations, be presented to summarize them best? The practitioner faces this problem when making oral or written presentations involving data. No attempt is made to make inferences from the data; the problem is simply to present the data in such a way that the listener, or reader, can visualize the entire set of data. The ways in which this can be accomplished are best shown by an example.

Example 2.A

Table 2.1 lists 144 consecutive months of diffusion plant MUF* experience data.† These data have been coded to disassociate the MUF experience from any specific production period and from any relation to throughput.

First, the need for some kind of data summarization is evident. The data as tabulated are not very meaningful. One approach might be to retabulate the data in increasing magnitude. This would be helpful, but still not too instructive, and would involve considerable effort if done by hand. One can achieve the same result and provide additional information at the same time with a frequency table, or frequency distribution.

* The term "MUF" is an acronym for material unaccounted for, which is the algebraic difference between a book inventory and a physical inventory. A negative MUF represents a "gain" of material.

† These data were supplied by Charles A. Keller of the Oak Ridge Operations Office, U.S. Atomic Energy Commission.

TABLE 2.1 DIFFUSION PLANT MUF DATA

Month	Year 1	2	3	4	5	6
1	−358	−10,771	−1,524	4,518	−7,461	4,526
2	−3,287	−1,416	906	292	−202	−4,055
3	5,798	−889	4,410	−2,160	346	2,678
4	−4,115	134	645	−433	4,338	−1,132
5	616	1,555	−684	418	−3,182	517
6	−2,825	−19	3,056	336	−117	−2,689
7	1,287	144	−635	−140	−460	−1,895
8	−1,619	−932	−624	1,225	−248	1,592
9	394	4,462	−164	212	−1,759	1,956
10	1,930	854	491	179	−1,440	2,081
11	3,701	4,612	2,225	−2,716	1,911	1,481
12	6,254	−5,593	198	13,859	737	−5,317

Month	Year 7	8	9	10	11	12
1	−694	−345	15	1,604	−3,690	−3,476
2	933	1,344	529	324	299	2,736
3	−1,350	−1,508	−59	−725	−580	−4,147
4	637	1,501	1,701	−493	201	58
5	−1,305	1,782	−447	264	−336	447
6	1,318	−2,542	767	1,520	−2,436	−418
7	−779	1,018	1,421	−1,120	4,364	−2,100
8	−351	−436	−85	−352	−3,634	−47
9	2,354	1,055	−248	2,263	−3,014	−667
10	11,311	277	434	−3,615	3,835	4,525
11	−13,775	234	820	4,002	−3,094	−376
12	1,384	928	144	2,155	617	3,618

In the construction of a frequency distribution, the first step consists in dividing the total range of values into a number of classes, or cells, of equal width. Experience shows that 12 to 20 such cells will result in a good picture of the distribution of values. To accomplish this, note the smallest and largest values in the table. The smallest is −13,775 (observation for year 7, month 11), while the largest is 13,859 (year 4, month 12). Thus the data range from 13,859 to −13,775 for a total of 27,634 units. A cell width of 2000 units gives about the right number of cells.

In the formation of the cells, it is helpful to select the cell boundaries or limits such that there is no question as to which cell each observation belongs. This is accomplished by defining cell boundaries to be halfway

between any two potential observations. For example, if observations are rounded to the nearest unit, as in this example, the cell boundaries are rounded to the nearest half unit.

For the data under consideration, the cell boundaries can be defined as follows, in descending order:

14,000.5
12,000.5
10,000.5
etc.

A frequency table, or a frequency distribution, is then formed from the data by tallying each observation in its appropriate cell. Table 2.2 gives the results for the data being discussed The first observation falls in cell 8, the second in cell 9, the third in cell 5, etc.

TABLE 2.2 FREQUENCY DISTRIBUTION OF MUF DATA

Cell	Cell boundaries	Frequency
1	12,000 5–14,000 5	1
2	10,000 5–12,000 5	1
3	8,000 5–10,000 5	
4	6,000 5–8,000 5	1
5	4,000 5–6,000 5	𝍸 𝍸
6	2,000 5–4,000 5	𝍸 𝍸 1
7	0 5–2,000 5	𝍸 𝍸 𝍸 𝍸 𝍸 𝍸 𝍸 𝍸 𝍸 𝍸 1111
8	−1,999 5–0 5	𝍸 𝍸 𝍸 𝍸 𝍸 𝍸 𝍸 𝍸 11
9	−3,999 5–(−1,999 5)	𝍸 𝍸 𝍸 1
10	−5,999 5–(−3,999 5)	𝍸
11	−7,999 5–(−5,999 5)	1
12	−9,999 5–(−7,999 5)	
13	−11,999 5–(−9,999 5)	1
14	−13,999 5–(−11,999 5)	1

This frequency distribution gives a much clearer picture of the historical MUF data than does Table 2.1. We can see immediately where the bulk of the data lies and can readily observe that most of the monthly MUF's lie between −6000 and +6000 units.

A frequency distribution or frequency table can be presented as a histogram or bar graph. This is simply a representation of the frequency distribution by rectangles of equal width, corresponding to the cell width, in which the height of the rectangle is proportional to the number of observations. If one is careful to make the tally marks of equal size, then the histogram does not really carry much additional visual impact. The histogram for the preceding frequency distribution is shown in Fig. 2 1.

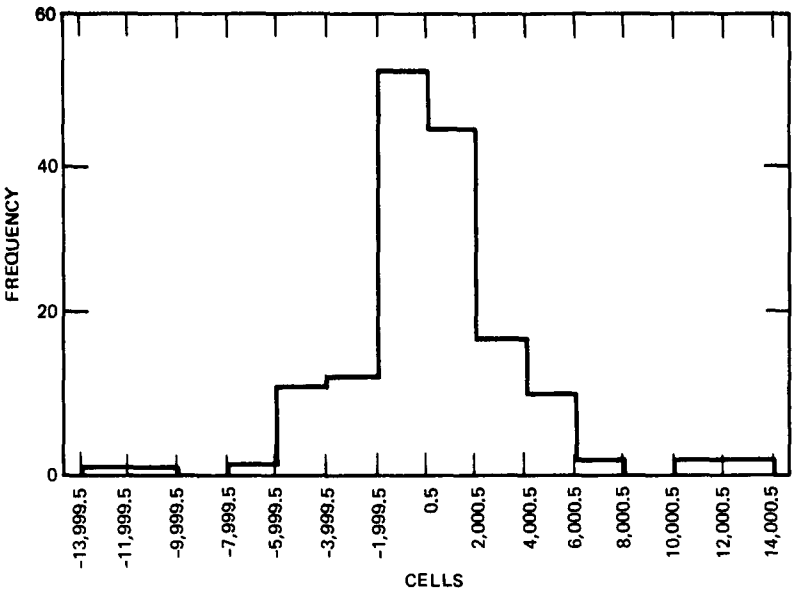

FIGURE 2.1 Histogram of MUF data.

Although the frequency distribution and the histogram serve to summarize the data as a group, they fail to provide any information about time trends that may appear in the data. This problem is discussed in more detail in Sec. 2.8. It is worthwhile to indicate here, however, that for this particular set of data, where the observations are ordered in time, a plot of the monthly MUF data versus time would be an instructive companion plot to present along with the histogram. In more general terms, when data are ordered with respect to some variable or variables, a plot of the data versus each such variable is helpful not only in summarizing the data but also as a prelude in using the data for making inferences. The importance of simple data plots should not be minimized. One danger of the use of high-speed computers is that this plotting step is often not included.

To continue with descriptive statistics, the data described by the histogram in Fig. 2.1 can be characterized quite well by two kinds of numbers, one describing *central tendency* and the other describing spread, or *dispersion*. Measures of central tendency most often used are the mean, the median, and, less frequently, the mode. Dispersion is usually described by the range and the variance (or its square root, the standard deviation).

The mean is the arithmetic average of the observations. The observations are summed, and the sum is divided by the total number of observa-

tions. The reader can verify that the mean of the MUF data is 22508/144 = 156 units.

When the data are grouped as in the frequency distribution, the mean is more easily calculated (by hand). The mean calculated for the grouped data will not agree exactly with the value calculated from the original ungrouped data, because all observations in a given cell are assumed to have the same value. This value is halfway between the cell boundaries and is called the class mark.

The frequency distribution for the MUF data of Table 2.1 is shown in Table 2.3, where x_i denotes the class mark for cell i and f_i is the frequency. The mean is then denoted by $\bar{x}$ and is calculated by the following steps:

Instructions for Eq. 2.1

1. Multiply each class mark, x_i, by the class frequency, f_i.
2. Sum these products over the k classes.
3. Sum the class frequencies, f_i, over the k classes.
4. Divide the sum in instruction 2 by the sum in instruction 3. The resulting value is $\bar{x}$.

In algebraic form, $\bar{x}$ is given by

$$\bar{x} = \frac{f_1x_1 + f_2x_2 + \cdots + f_kx_k}{f_1 + f_2 + \cdots + f_k} = \sum_{i=1}^{k} f_ix_i \Big/ \sum_{i=1}^{k} f_i \tag{2.1}$$

where there are k cells.

This calculation can be done without the aid of a calculator if a simple transformation is made on the data. This is done by defining a new quantity, u_i, and setting it equal to zero in some central cell, to ± 1 in the cells on either side of this middle cell, to ± 2 in the next cells, etc. (The answer does not depend on which cell is chosen as the central cell.) The mean of u is then calculated from Eq. 2.1 with u_i replacing x_i. The relation between the mean of x, $\bar{x}$, and the mean of u, $\bar{u}$, is

$$\bar{x} = w\bar{u} + x_0 \tag{2.2}$$

where w is the class width and x_0 is the value of x_i in the cell chosen as the central cell corresponding to $u_i = 0$. In Table 2.3, $w = 2000$ and $x_0 = 1000.5$. (At this point in the discussion of the example, ignore the last column of the table.)

TABLE 2.3 FREQUENCY DISTRIBUTION FOR MUF DATA

Class mark (x_i)	Frequency (f_i)	u_i	u_i^2
13,000.5	1	6	36
11,000.5	1	5	25
9,000.5	0	4	16
7,000.5	1	3	9
5,000.5	10	2	4
3,000.5	11	1	1
1,000.5	54	0	0
−999.5	42	−1	1
−2,999.5	16	−2	4
−4,999.5	5	−3	9
−6,999.5	1	−4	16
−8,999.5	0	−5	25
−10,999.5	1	−6	36
−12,999.5	1	−7	49
	$\sum_{i=1}^{14} f_i = 144$		

From Eq. 2.1, with u_i replacing x_i,

$$\bar{u} = \frac{(1)(6)+(1)(5)+\ \ldots\ +(1)(-7)}{144}$$

$$= -61/144 = -0.4236$$

Then, the mean of x is, from Eq. 2.2,

$$\bar{x} = (2000)(-0.4236)+1000.5$$

$$= 153 \text{ units}$$

which compares with the value of 156 units found for the ungrouped data. This comparison gives some indication of the size of the computational error that might be introduced by grouping.

Consider the median as another measure of central tendency. The median is defined as the middle observation, half the values being larger than the median and half being smaller. If the total number of observations is odd, the median is a unique value; if the total number is even, the median is the average of the two middle values. For the MUF data of Table 2.1, we can verify that the two middle values are 179 and 198; thus the median is 188. This value is in fair agreement with the mean, $\bar{x}$, in this example because the frequency distribution appears to be quite symmetric about the central values. The median is a useful alternate measure of central tendency especially when unsymmetric or skewed

distributions are encountered. Since this does not occur often in nuclear material control applications, the median receives little attention in this book as a descriptive statistic.

The final measure of central tendency is the mode. The mode is the observation that occurs the most frequently and is meaningful only for grouped data. The mode for the grouped MUF data is 1000.5. No further mention is made of the mode in this book.

Next, consider measures of dispersion, or spread. The two common measures are (1) the range and (2) the variance or the square root of the variance, which is the standard deviation.

The range is the difference between the largest and the smallest observations. For the MUF data the range was shown previously to be 27,634 units. The range sets bounds on the observed values and has the advantage of being very simple to calculate. One disadvantage is that the size of the range depends on the number of observations. It is clear that, if additional MUF data were to be presented, the calculated range for all the data could never become smaller than the value based on the original 144 observations; it could only become larger. Another disadvantage is that one or two spurious observations have a great effect on the range and can result in a misleading picture of dispersion.

The more commonly used measure of dispersion is the variance, or its square root, the standard deviation. The variance is the second moment about the mean. When the variance is used as a descriptive statistic, a word of caution is in order. The use of the variance requires a certain knowledge on the part of the reader or listener as to how to make the translation from the standard deviation to data spread. He may know, for example, that for certain commonly encountered symmetric distributions, the mean plus or minus twice the standard deviation encompasses most of the data whereas the mean plus or minus three times the standard deviation encompasses virtually all the data. The danger is that the standard deviation may always be interpreted in this way, even when calculated for unsymmetric distributions. Fortunately most applications in this book deal with distributions for which this interpretation of the standard deviation is reasonably valid.

The calculation of the variance and the standard deviation requires more effort than does the calculation of the range. For ungrouped data, $y_1, y_2, \ldots, y_n$, the variance is conveniently defined as

$$s^2 = \frac{\sum_{i=1}^{n} (y_i - \bar{y})^2}{n-1} \tag{2.3}$$

where $\bar{y}$ is the mean of the y values. The divisor is $(n-1)$ rather than n for reasons that will become clear in Sec. 2.7.

An equivalent form of Eq. 2.3 that is more convenient from a computational viewpoint is

$$s^2 = \frac{\sum_{i=1}^{n} y_i^2 - \left[\left(\sum_{i=1}^{n} y_i\right)^2 / n\right]}{n-1} \tag{2.4}$$

If one prefers instructions rather than formulas, the following steps are performed.

Instructions for Eq. 2.4

1. Square each value, and sum over all the n values.
2. Sum the n values, and square this sum.
3. Divide the sum in instruction 2 by n.
4. Subtract the result in instruction 3 from that in instruction 1.
5. Divide the result in instruction 4 by $(n-1)$. The result is s^2.

When the data are grouped as in Table 2.3, the formula for the variance is

$$s^2 = \frac{\sum_{i=1}^{k} f_i x_i^2 - \left[\left(\sum_{i=1}^{k} f_i x_i\right)^2 / \sum_{i=1}^{k} f_i\right]}{\sum_{i=1}^{k} f_i - 1} \tag{2.5}$$

where the x_i are the class marks and the f_i the class frequencies.

As was true in calculating $\bar{x}$, it is again much simpler to use transformed u_i values. The variance of the u_i values is found from Eq. 2.5, with u_i replacing x_i. Then the variance of the x_i values, denoted by s_x^2, is related to the variance of the u_i values, denoted by s_u^2, by

$$s_x^2 = w^2 s_u^2 \tag{2.6}$$

where w is the class width.

For the MUF data under discussion,

$$\sum_{i=1}^{14} f_i u_i = -61$$

$$\sum_{i=1}^{14} f_i u_i^2 = 373 \qquad \text{(sum of cross products of columns 2 and 4 of Table 2.3)}$$

Then, from Eq. 2.5, with u_i in place of x_i,

$$s_u^2 = \frac{373 - [(-61)^2/144]}{143}$$
$$= 2.4277$$

The variance of the x values is then found from Eq. 2.6:

$$s_x^2 = (2000)^2\ (2.4277) = 9.7108 \times 10^6$$

The standard deviation, s_x, is

$$s_x = \sqrt{9.7108 \times 10^6} = 3116$$

In this example, note that

$$\bar{x} \pm 2s_x = 153 \pm 2(3116)$$
$$= -6079 \text{ to } 6385$$

does, in fact, embrace "most of the data," and s_x is reasonably descriptive in this sense.

2.2 PROBABILITY

Probability is a measure of the likelihood that some chance event will occur. The calculus of probabilities is basic to statistical inference. Most modern texts develop the concept of probability on a purely axiomatic basis, making use of set theory. This purist approach, although logically much more satisfactory, is not considered essential for purposes of this book. Rather, the laws of probability are stated for the more easily understandable classical definition of probability. The empirical and subjective concepts of probability are then treated briefly.

2.2.1 Classical Interpretation of Probability

With the classical approach to probability, an experiment can have N equally likely and mutually exclusive outcomes, of which n have some attribute E. Two outcomes are said to be mutually exclusive if the occurrence of one precludes the occurrence of the other. Then the probability that the event with attribute E will occur (or, more simply, the probability that the event E will occur) is written Pr (E) and is defined as

$$\Pr(E) = \frac{n}{N} \tag{2.7}$$

For example, let an experiment consist in tossing a fair coin. There are two equally likely and mutually exclusive outcomes: a head (H) or a tail (T). Thus $N = 2$. Let the event E be the occurrence of a head. This can occur in $n = 1$ way. Then, from Eq. 2.7,

$$\Pr(E) = \Pr(\text{head}) = \frac{1}{2}$$

As another example, let the experiment now consist in tossing three coins. There are now $\mathcal{N}=8$ equally likely and mutually exclusive outcomes, as shown in Table 2.4.

TABLE 2.4 COIN-TOSSING EXPERIMENT

Outcome*	Coin number 1	2	3
1	H	H	H
2	H	H	T
3	H	T	H
4	H	T	T
5	T	H	H
6	T	H	T
7	T	T	H
8	T	T	T

* Clearly the ordering of these outcomes is immaterial.

In the three-coin experiment, let the event E be the occurrence of exactly two heads. Note that this event happens with outcomes 2, 3, and 5. Thus, $n=3$ and, from Eq. 2.7,

$$\Pr(E) = \Pr(2 \text{ heads}) = \frac{3}{8}$$

With this classical definition of probability, it follows that:

1. For any event E,

$$0 \leq \Pr(E) \leq 1 \tag{2.8}$$

since $0 \leq n \leq \mathcal{N}$. Further, as Pr (E) approaches 1, the event is more likely to occur, but, as Pr (E) nears 0, E is less likely to occur. When Pr $(E)=1$, the event is sure to occur, and Pr $(E)=0$ means it cannot occur.

2. Then,

$$\sum \Pr(E_i) = 1 \tag{2.9}$$

The probabilities of all events E_i must sum to 1. This is true since $\Sigma_i\, n_i = \mathcal{N}$.

3. For any two mutually exclusive events, E and F,

$$\Pr(E \text{ or } F) = \Pr(E) + \Pr(F) \tag{2.10}$$

where this notation means that either E will occur or F will occur. The

left-hand side of Eq. 2.10 may also be written as Pr $(E + F)$ or, with set-theory notation, Pr $(E \cup F)$.

4. If E and F are not mutually exclusive, then

$$\Pr(E \text{ or } F) = \Pr(E) + \Pr(F) - \Pr(EF) \tag{2.11}$$

where the event "EF" means that both E and F occur. This is also written Pr (E,F), Pr $(E \times F)$, or Pr $(E \cap F)$. In Eq. 2.11 the event "E or F" means that E occurs, F occurs, or both occur.

To illustrate Eqs. 2.10 and 2.11, let us again consider the coin-tossing experiment involving the three coins. Let the event E be the occurrence of exactly two heads and let F be the occurrence of three heads. Clearly E and F are mutually exclusive because both cannot occur simultaneously. From Eq. 2.7,

$\Pr(E) = \frac{3}{8}$ (corresponding to outcomes 2, 3, and 5 in Table 2.4)

$\Pr(F) = \frac{1}{8}$ (corresponding to outcome 1 in Table 2.4)

From Eq. 2.10,

$$\Pr(E \text{ or } F) = \frac{3}{8} + \frac{1}{8} = \frac{1}{2}$$

which is the probability that exactly two or three heads will occur. This corresponds to outcomes 1, 2, 3, and 5 in Table 2.4.

If E were again defined as the occurrence of exactly two heads but if F were the event *second coin is a tail*, then E and F are not mutually exclusive, and Eq. 2.11 is applied.

$\Pr(E) = \frac{3}{8}$ (outcomes 2, 3, and 5 in Table 2.4)

$\Pr(F) = \frac{4}{8}$ (outcomes 3, 4, 7, and 8)

$\Pr(EF) = \frac{1}{8}$ (outcome 3: two heads and second coin a tail)

Then from Eq. 2.11,

$$\Pr(E \text{ or } F) = \frac{3}{8} + \frac{4}{8} - \frac{1}{8} = \frac{3}{4}$$

This corresponds to outcomes 2, 3, 4, 5, 7, and 8.

5. If E and F are independent events in the sense that the occurrence or nonoccurrence of one event in no way affects the probability of occurrence for the other, then

$$\Pr(EF) = \Pr(E) \times \Pr(F) \tag{2.12}$$

If E and F are not independent, then

$$\Pr(EF) = \Pr(F) \times \Pr(E|F) \tag{2.13}$$

$$= \Pr(E) \times \Pr(F|E) \tag{2.14}$$

where $\Pr(E|F)$ is the conditional probability that E will occur, given that the event F has occurred, and $\Pr(F|E)$ is the conditional probability that F will occur, given that the event E has occurred.

To illustrate, consider the three-coin experiment. If E is the occurrence of two heads and F is the event *second coin is a head*, then E occurs in outcomes 2, 3, and 5. Given that E has occurred, i.e., that outcome 2, 3, or 5 has occurred, then $\Pr(F|E) = 2/3$, i.e., F occurs in outcomes 2 and 5. Therefore, from Eq. 2.14,

$$\Pr(EF) = \left(\frac{3}{8}\right)\left(\frac{2}{3}\right) = \frac{2}{8} = \frac{1}{4}$$

gives the probability that there are two heads and that the second coin is a head. This event corresponds to outcomes 2 and 5.

2.2.2 Other Interpretations of Probability

Although the classical interpretation of probability is attractive because of its simplicity and because it creates an understanding of the laws of probability, some troublesome difficulties are associated with this approach. For example, what if the total number of possible outcomes, N, is infinite? Or, suppose the coins used in the previous section are biased so that the N events are not equally likely? Also, how could one use the classical definition of probability to answer a question such as "What is the probability a given fuel pellet will have a density exceeding 93% of theoretical density?" Here N is not defined, nor are the outcomes equally likely.

Handling of such problems requires other interpretations of probability, different from the classical interpretation but still retaining the basic idea that probability is a measure of the likelihood that some event will occur. Two such interpretations are called the empirical and the subjective definitions of probability.

(a) Empirical Interpretation

If an experiment is conducted N times and some event, E, occurs n times, then the limit of n/N as N becomes large is defined as the probability of E, Pr (E).

The experiment in question need not actually be conducted to define or interpret Pr (E). However, to evaluate Pr (E), one would have to experiment.

This interpretation does not cover all situations since in some instances it is difficult to conceptualize the preceding experiment. What is the probability of an accidental process spill of a given size? Of a process holdup in excess of k kilograms of uranium? Of an attempted diversion of nuclear material? A third interpretation is given for such situations.

(b) Subjective Interpretation

In this interpretation, Pr (E) is a measure of the degree of belief one holds that the event E will occur.

This interpretation gets back to the basic idea of probability. Clearly the interpretation is a much broader definition and is deficient because of its subjectivity. Nevertheless, in some situations it is the only interpretation that is adequate.

No matter which concept of probability is used, the basic laws of probability given in Sec. 2.2.1 remain the same. The different concepts should therefore present no practical difficulty in application.

2.2.3 Examples of Probability*

Ten cans are listed on an inventory as containing UO_2 powder. Actually, two cans contain marijuana. If an audit team opens one can at random, what is the probability it contains marijuana? Suppose two cans are opened. Then what is the probability that marijuana is found in one or both of the cans?

To answer the first question, apply Eq. 2.7. There are $N = 10$ possible outcomes of the experiment, corresponding to the 10 cans that may appear in the inspector's sample. The number of outcomes, n, which correspond to the event, E (marijuana in the can selected), is 2. Therefore

$$\Pr(E) = \frac{n}{N} = \frac{2}{10}$$

Working from basic principles, we can find the solution to the second question with different but equally valid approaches, the specific approach

* Further examples of probability are given in Sec. 2.4.

depending upon how the problem is structured. Different approaches are discussed in the following paragraphs.

Approach 1: Assign (conceptually) the numbers 1 to 10 to the 10 cans. If we keep a record of which can is drawn first and which is drawn second, then there are 10 cans (outcomes) corresponding to the first drawing and 9 corresponding to the second. Thus the total number of outcomes, N, is $10 \times 9 = 90$. These could be listed as in Table 2.5.

TABLE 2.5 POSSIBLE OUTCOMES

Outcome	Can number	
	In first drawing	In second drawing
1	1	2
2	1	3
3	1	4
10	2	1
11	2	3
12	2	4
88	10	7
89	10	8
90	10	9

Consider the outcomes that correspond to the event *one or both cans contain marijuana*. Let the two marijuana cans be numbered 1 and 2 (clearly, it makes no difference which numbers are selected). Then the outcomes that contain can 1 or can 2 or both are outcomes numbered 1 to 18 (which have either can 1 or can 2 as the first can drawn), 19–20 (which have either can 1 or can 2 as the second can drawn), 28–29, 37–38, 46–47, 55–56, 64–65, 73–74, and 82–83. Thus in this approach n is $18+2+2+2+2+2+2+2+2+2=34$, and, by Eq. 2.7,

$$\Pr(E) = \frac{n}{N} = \frac{34}{90} = \frac{17}{45}$$

Approach 2: This is similar to approach 1, but now the order in which the cans are drawn is ignored. The N possible outcomes now correspond to the number of ways in which two cans can be selected from the total cans. In this instance outcomes 1 and 10 in Table 2.5 are identical

since both outcomes consist of cans 1 and 2. This is true of all pairs of cans, and the number of outcomes becomes $90/2=45$. Similarly the number of outcomes corresponding to the event E is also halved, and Eq. 2.7 then gives

$$\Pr(E)=\frac{17}{45}$$

which is the same result as for approach 1.

Approach 3: In the previous two approaches, we made recourse to the basic definition of classical probability. We can also structure the solution by applying the laws of probability. To do this, we define two events, E and F, where E relates to the outcome of the first drawing and F to the outcome of the second.

First, note that the overall event G *one or two cans of marijuana in the sample of two cans* can occur in three ways:

1. First can contains marijuana; second does not. $(E_1; F_1)$
2. First can does not contain marijuana; second does. $(E_2; F_2)$
3. Both cans contain marijuana. $(E_3; F_3)$

These three outcomes are mutually exclusive so that the probability of each can be found and then summed by Eq. 2.10 to give the probability of interest.

Consider case 1.

$$\Pr(E_1)=\frac{2}{10} \qquad \text{(by Eq. 2.7)}$$

$$\Pr(F_1 \mid E_1)=\frac{8}{9} \qquad \text{(also by Eq. 2.7)}$$

because after a can of marijuana was drawn in the first sample, nine cans are now left, eight of which do not contain marijuana. Then, by application of Eq. 2.14 to case 1,

$$\Pr(E_1F_1)=\frac{2}{10}\frac{8}{9}=\frac{16}{90} \tag{2.15}$$

Consider case 2. By similar reasoning,

$$\Pr(E_2)=\frac{8}{10}$$

$$\Pr(F_2 \mid E_2)=\frac{2}{9}$$

$$\Pr(E_2F_2) = \frac{8}{10}\frac{2}{9} = \frac{16}{90} \tag{2.16}$$

Consider case 3. Again, by similar reasoning,

$$\Pr(E_3) = \frac{2}{10} \qquad \text{(first can contains marijuana)}$$

$$\Pr(F_3 | E_3) = \frac{1}{9} \qquad \text{(second can also contains marijuana)}$$

$$\Pr(E_3F_3) = \frac{2}{10}\frac{1}{9} = \frac{2}{90} \tag{2.17}$$

Then, sum Eqs. 2.15, 2.16, and 2.17:

$$\Pr(G) = \frac{16}{90} + \frac{16}{90} + \frac{2}{90} = \frac{34}{90} = \frac{17}{45}$$

the same result as in the other two approaches.

This example has been belabored a bit. It shows that we can solve problems of this nature by applying first principles, although even this small example gives an indication that the enumeration of all possible outcomes can be onerous. For a way to avoid this enumeration, a fourth approach to the same problem is given in Sec. 2.4.

2.3 RANDOM VARIABLES AND PROBABILITY DISTRIBUTIONS

In the previous section the concept of an outcome of an experiment was introduced. It is usually convenient to assign numbers to the possible outcomes. Usually this occurs quite naturally. For example, outcomes can be the percent ^{235}U measured in a sample, the number of gross discrepancies between the facility and an audit team in an inspection situation, or the amount of plutonium in a barrel of solid waste. When a number is not assigned naturally, it can be assigned somewhat arbitrarily without difficulty. Thus, for example, if we speak of an attempted diversion, either there will be an attempt of some kind in a given instance or there will not be. To the two possible outcomes, we can arbitrarily assign the values 0 and 1 (or 1 and 0, if we prefer) for convenience.

This assignment of numbers is described by defining a *random variable*. By definition a random variable is a numerical-valued function defined over the elements of a sample space (outcomes of an experiment). By convention, a capital letter is used to designate the random variable and a small letter to designate a particular value taken on by the random variable.

To illustrate, X may be the percent ^{235}U in a sample of UO_2 powder. In a given sample, x may be 3.912%, for example. Alternately, if X is the number of gross discrepancies of some kind between a facility and audit team in a sample of N containers, then it may take on the values $x = 0, 1, 2, \ldots, N$.

This distinction becomes clearer if it is related to the previous section on probability. We speak of

$$\Pr\ (x = x_0)$$

which is the probability that the random variable, X, takes on a particular value, x_0. In a given instance this probability can be evaluated, and, if we could enumerate all the k possible values that X may take on and calculate the associated probabilities of occurrence, a table such as Table 2.6 could be prepared.

TABLE 2.6 PROBABILITY DENSITY FUNCTION IN TABULAR FORM

x	$\Pr\ (x = x_i) = f(x_i)$
x_1	$f(x_1)$
x_2	$f(x_2)$
	.
	.
x_k	$f(x_k)$
	$\sum_{i=1}^{k} f(x_i) = 1$ by Eq. 2.9

Table 2.6 is an example of a *probability density function*, which assigns a probability to each possible value of the random variable.

It is generally possible, and more convenient, to express the probability density function in functional form, i.e., with an equation rather than a table. By convention the density function is denoted by $f(x)$; so the following relation holds:

$$\Pr\ (x = x_i) = f(x_i) \tag{2.18}$$

Examples of some specific density functions are given in Sec. 2.4. We can verify at this point, however, that in the three-coin experiment, if the random variable X is defined as the number of heads that appears among the three coins, its density function can be written

$$f(x) = \frac{3!}{x!(3-x)!}\,(0.5)^3 \qquad (x = 0, 1, 2, 3)$$

Keep in mind that $0! = 1$ by definition.

Since X is numerically valued, it is ordered. Thus we can also speak of the probability that X takes on values equal to or less than x. By convention, this is written as

$$\Pr\ (x \leq x_0) = F(x_0) \tag{2.19}$$

$F(x)$ is called a cumulative distribution function or, more simply, a *distribution function.*

Again with reference to the three-coin experiment,

$$\begin{aligned}\Pr\ (x \leq 1) &= F(1) = f(o) + f(1) \\ &= \frac{3!}{0!3!}(0.5)^3 + \frac{3!}{1!2!}(0.5)^3 \\ &= \frac{1}{8} + \frac{3}{8} = \frac{1}{2}\end{aligned}$$

Also note that, by Eqs. 2.19 and 2.9,

$$\Pr\ (x > x_0) = 1 - F(x_0) \tag{2.20}$$

Thus far in the discussion, attention has been restricted to *discrete* random variables. A random variable, X, is discrete if its distribution function, $F(x)$, is a step function when plotted against x. If the random variable is not discrete, it is continuous, and $F(x)$ is then plotted as a monotonically nondecreasing curve. Stated alternately, discrete random variables are associated with *counted data*, whereas continuous random variables are associated with *measured data.*

A continuous random variable also has a density function and a distribution function associated with it, but the interpretation is slightly different from that for a discrete random variable. This difference is seen in Fig. 2.2, which shows examples of $f(x)$ for both a discrete and a continuous random variable. If X is discrete, the density function, $f(x)$, has the appearance of a bar graph, or a histogram (Fig. 2.2(a)); the area of a given rectangle is proportional to $f(x)$, and these areas sum to one. If X is continuous, $f(x)$ is a smooth curve (Fig. 2.2 (b)); the total area under the curve equals one.

In the continuous case it is not possible theoretically to speak of the probability that x is any given value, since probability is proportional to area. At any given value, x, the area under the curve is zero. However, the density function is converted to a probability upon multiplication by some incremental quantity, dx, so that $f(x)\,dx$ represents an area and hence describes a probability.

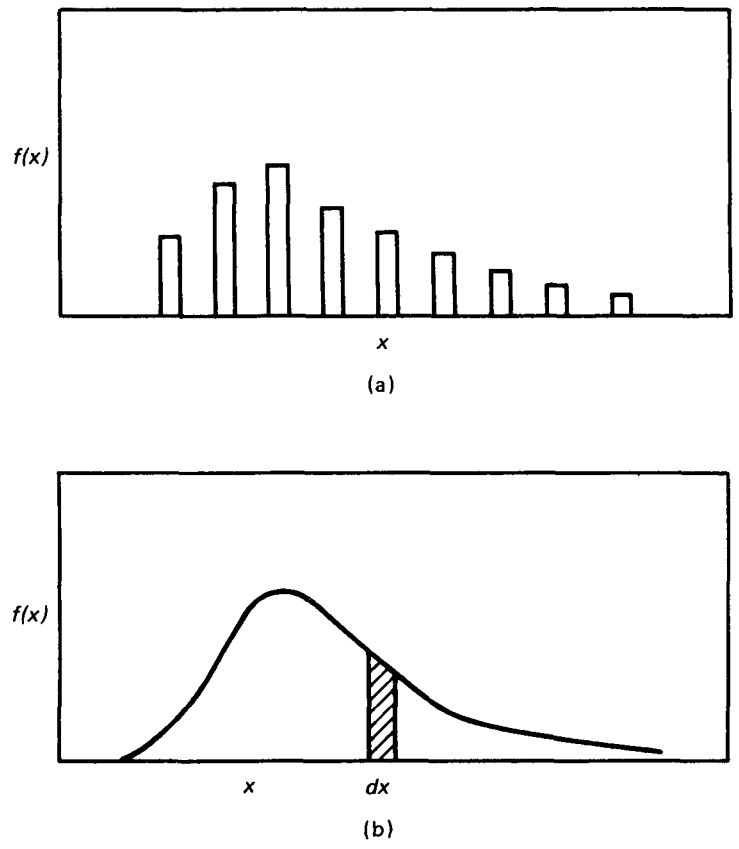

FIGURE 2.2 Example of (a) discrete density function and (b) continuous density function.

In the discrete case the distribution function, $F(x)$, is obtained from the density function, $f(x)$, by the summation process. Thus

$$F(x_k) = \sum_{i=1}^{k} f(x_i) \tag{2.21}$$

where $x_1 < x_2 < \ldots < x_k$.

In the continuous case this summation process is replaced by integration and gives the relation

$$F(x_0) = \int_{-\infty}^{x_0} f(x)\, dx \tag{2.22}$$

In this instance the probability that x lies between two values, x_1 and x_2, with $x_1 < x_2$, is

$$\Pr\ (x_1 < x < x_2) = F(x_2) - F(x_1) = \int_{x_1}^{x_2} f(x)\ dx \tag{2.23}$$

It was remarked earlier that, for a continuous random variable, there is zero probability of observing any given value of the random variable. Mathematically this is a true statement, but it is not very helpful for such a question as, "What is the probability that the measured percent uranium in a given fuel pellet is 88.1%?" Clearly this answer cannot be zero. To answer this, we must recognize that, because of rounding, the question should really be phrased, "What is the probability that the measured percent uranium in a given fuel pellet lies between 88.05% and 88.15%, i.e., that it equals 88.1% when rounded?" This question can now be answered with Eq. 2.23:

$$\Pr\ (88.05\% < x < 88.15\%) = \int_{88.05}^{88.15} f(x)\ dx$$

2.3.1 Mean and Variance of a Random Variable

In the discussion of descriptive statistics, it was pointed out that there are two kinds of numbers which can be quite descriptive of the entire frequency distribution: numbers which describe central tendency and those which describe dispersion. The same is true for random variables; one would like to define quantities that are descriptive of the density function, at least with respect to its central tendency and its dispersion.

These descriptive measures are usually based on *moments*. The first moment about the origin (zero) describes central tendency and is called the mean of x, or its expected value. Conventionally this quantity is denoted by the Greek letter mu, μ. For a discrete random variable,

$$\mu = E(x) = \sum_{\text{all } x} xf(x)\ ^* \tag{2.24}$$

where $E(x)$ is the expected value of x.

For a continuous random variable,

$$\mu = \int_{-\infty}^{\infty} xf(x)\ dx \tag{2.25}$$

Note the similarity between Eq. 2.24 and the definition of the mean for a group of data in Eq. 2.1.

To illustrate Eq. 2.24, again consider the density function in the three-coin experiment of Sec. 2.2. This density function was written

---

* In general, the expected value of a constant times some function of x, e g , $ag(x)$, is

$$E[ag(x)] = a\,E[g(x)] = a \sum_{\text{all } x} g(x)\ f(x)$$

$$f(x)=\frac{3!}{x!(3-x)!}(0.5)^3 \qquad (x=0,\ 1,\ 2,\ 3)$$

By Eq. 2.24, the mean of x is

$$\mu=0+(1)(3)(0.5)^3+(2)(3)(0.5)^3+(3)(0.5)^3$$

$$=0+\frac{3}{8}+\frac{6}{8}+\frac{3}{8}=1.5$$

Note that in this example the mean is a fractional value and cannot occur. Yet it does describe central tendency.

The dispersion can be measured with moments by using the second moment about the mean. This moment is called the variance and is conventionally denoted by the square of the Greek letter sigma, σ^2. The square root of the variance is called the standard deviation and is denoted by σ.

For a discrete random variable,

$$\sigma^2=E(x-\mu)^2=\sum_{\text{all } x}(x-\mu)^2 f(x) \tag{2.26}$$

Equivalently* this may be written

$$\sigma^2=E(x^2)-\mu^2=\sum_{\text{all } x}x^2 f(x)-\mu^2 \tag{2.27}$$

For a continuous random variable, the corresponding equations are

$$\sigma^2=\int_{-\infty}^{\infty}(x-\mu)^2 f(x)\,dx \tag{2.28}$$

and

$$\sigma^2=\int_{-\infty}^{\infty}x^2 f(x)\,dx-\mu^2 \tag{2.29}$$

In the three-coin experiments, on application of Eq. 2.26, with $\mu=1.5$, as already determined,

$$\sigma^2=E(x-\mu)^2=(0-1.5)^2(0.5)^3+(1-1.5)^2(3)(0.5)^3+(2-1.5)^2(3)(0.5)^3$$
$$+(3-1.5)^2(0.5)^3$$

$$=\frac{2.25}{8}+\frac{0.75}{8}+\frac{0.75}{8}+\frac{2.25}{8}=0.75$$

and

$$\sigma=\sqrt{\sigma^2}=\sqrt{0.75}=0.866$$

* The definitions in Eqs 2.26 and 2.27 are identically the same but are simply expressed in different forms The same is true of Eqs 2.28 and 2.29

Alternatively, by Eq. 2.27,

$$\sigma^2 = (0)^2(0.5)^3 + (1)^2(3)(0.05)^3 + (2)^2(3)(0.5)^3 + (3)^2(1)(0.5)^3 - (1.5)^2$$
$$= 0 + \frac{3}{8} + \frac{12}{8} + \frac{9}{8} - \frac{9}{4} = \frac{6}{8} = 0.75$$

an identical result.

Consider another example. Assume that, of a large number of containers in inventory, 30% of them weigh 10 kg, 20% weigh 15 kg, 15% weigh 20 kg, and 35% weigh 30 kg. The random variable, X, is the weight of the given container. What is its mean, μ, and its variance, σ^2?

This is a discrete density function that can be written in tabular form as follows:

x_i	Pr $(x = x_i)$
10	0 30
15	0 20
20	0 15
30	0 35
	1 00

Then, from Eq. 2.24,

$$\mu = (10)(0.30) + (15)(0.20) + (20)(0.15) + (30)(0.35)$$
$$= 3.0 + 3.0 + 3.0 + 10.5 = 19.5 \text{ units}$$

From Eq. 2.26,

$$\sigma^2 = (10 - 19.5)^2(0.30) + (15 - 19.5)^2(0.20) + (20 - 19.5)^2(0.15) + (30 - 19.5)^2(0.35)$$
$$= 27.0750 + 4.0500 + 0.0375 + 38.5875$$
$$= 69.75 \text{ kg}^2$$

(These results are used later in example 4.B of Sec. 4 1.3.)

Although attention is focused on these two moments, let us briefly discuss two higher moments. The third moment about the mean, $E(x-\mu)^3$ is a measure of the skewness, or lack of symmetry of a density function. (For a symmetric density function, it is intuitively obvious that this quantity is zero because of cancellation of positive and negative values.) The fourth moment, $E(x-\mu)^4$, is a measure of kurtosis, or peakedness. No further use is made of these higher moments in this book.

Finally, although moments are most commonly used to describe central tendency and dispersion, there are other measures of these charac-

teristics. For central tendency, the median and mode are defined in a manner completely analogous to their definitions when used as descriptive statistics. The range, as a measure of dispersion of a density function, is obviously meaningful only if it is finite. There are other measures of dispersion. As far as density functions are concerned, however, the mean and variance (or standard deviation) are used exclusively in this book.

2.4 SOME SPECIFIC POPULATION DENSITY FUNCTIONS

A large number of specific density functions have been used in the various applications of statistics. Some common discrete functions include (in alphabetical order) the binomial, geometric, hypergeometric, multinomial, negative binomial, and Poisson functions. Commonly encountered continuous density functions include the beta, Cauchy, exponential, gamma, log–normal, normal, uniform (or rectangular), and Weibull functions. The foregoing are population density functions. In addition, derived sampling density functions are discussed in Sec. 2.6 (Student's t, chi-square, F distribution), where the distinction between population and derived sampling density functions is covered.

This section is limited to population density functions, of which four have particular application in this book: the binomial and hypergeometic density functions for discrete random variables and the normal and uniform densities for continuous random variables.

2.4.1 Binomial Density Function

The binomial density function is applicable to certain audit inspection activities. It arises under the following conditions:

Condition 1: A single observation is classified as being either a "success" or a "failure."

Condition 2. The parameter p is the probability that any given observation is a success, and it is a constant.

Condition 3: The occurrence of a success or a failure for any given observation in no way affects the probability of success or failure for other observations (i.e., there is independence).

Condition 4: There are n total observations.

Condition 5: The random variable, X, is the number of successes among the n observations.

In inspection, a success may correspond to the occurrence of a "defect," which might be described as a well-defined discrepancy between the operator's statement of what is in the container and what the audit team finds. Alternatively, one could choose to label this a failure, and the problem

would then be restructured. Of course, there is no essential difference in the two choices as long as one assigns the appropriate value to p.

The binomial density function is

$$f(x) = \frac{n!}{x!(n-x)!} p^x (1-p)^{n-x} \qquad (x = 0, 1, 2, \ldots, n) \qquad (2.30)$$

We immediately recognize that the three-coin experiment previously considered is an example of the binomial density function with $n = 3$ and $p = 0.5$. Also, consider the following example.

Assume that $\mathcal{N}$ items are in inventory, $\mathcal{N}$ being a "large" number. (The question of how large is "large" is deferred until Sec. 2.4.2.) Twenty-five of these are selected at random and classified as either being a defect (in some sense) or not being a defect. The inventory is accepted as having been verified if there are ≤ 1 defects among the 25 selected. What is the probability of accepting the inventory if p, the probability that any item is a defect, is 0.05? 0.10? 0.20?

The solution is based on the binomial density function. This function is applicable because $\mathcal{N}$ is large. Strictly speaking, with finite $\mathcal{N}$, the binomial density function cannot apply, because the occurrence of a defect on any trial does affect the probability of occurrence of a defect on the subsequent trial and thus violates condition 3. However, for large $\mathcal{N}$, this is not a practical concern.

To find the probability of accepting the inventory, find the probabilities that $x = 0$ and that $x = 1$, and sum. The summation of the two probabilities gives the probability that either 0 or 1 defect will be found, by Eq. 2.10, and corresponds to the situation in which the inventory is accepted.

Therefore, applying Eq. 2.30 gives the following solutions.

For $p = 0.05$,

$$f(0) = \frac{25!}{0!25!}(0.05)^0(0.95)^{25} = 0.277$$

$$f(1) = \frac{25!}{1!24!}(0.05)^1(0.95)^{24} = 0.365$$

Therefore

$$F(1) = f(0) + f(1) = 0.642 = \Pr(\text{inventory is accepted} \mid \text{given that } p = 0.05)$$

For $p = 0.10$,

$$f(0) = \frac{25!}{0!25!}(0.10)^0(0.90)^{25} = 0.072$$

$$f(1) = 0.199$$

Therefore

$$F(1) = 0.072 + 0.199 = 0.271 = \Pr(\text{inventory is accepted} \mid \text{given that } p = 0.10)$$

For $p = 0.20$,

$$f(0) = 0.004$$

$$f(1) = 0.024$$

Therefore

$$F(1) = 0.028 = \Pr(\text{inventory is accepted} \mid \text{given that } p = 0.20)$$

By these calculations the inspection plan has been characterized for its adequacy. If the inspector is not happy with a probability of 0.271 of accepting an inventory with $p = 0.10$, i.e., with 10% defects, he should alter his plan to reduce this probability.

Chapter 9 is devoted entirely to inventory-verification activities and contains rather complete characterizations of inspection plans. This example was introduced here to illustrate the application of the binomial density function.

The mean and variance of the binomial distribution are given by the following formulas:

$$\mu = E(x) = np \tag{2.31}$$

$$\sigma^2 = E(x-\mu)^2 = np(1-p) \tag{2.32}$$

Of more interest in many situations are the mean and variance of x/n, the ratio between the number of successes and the total number of observations. These quantities are

$$E\left(\frac{x}{n}\right) = p \tag{2.33}$$

$$E\left(\frac{x}{n} - p\right)^2 = \frac{p(1-p)}{n} \tag{2.34}$$

To illustrate, for $n = 25$ and $p = 0.2$:

$$E(x) = (25)(0.2) = 5.0^* \qquad \text{(from Eq. 2.31)}$$

$$\sigma^2 = E(x-\mu)^2 = (25)(0.2)(0.8) = 4.0 \qquad \text{(from Eq. 2.32)}$$

$$\sigma = \sqrt{4.0} = 2.0$$

$$E\left(\frac{x}{n}\right) = 0.2^* \qquad \text{(from Eq. 2.33)}$$

* Thus, on average, we would expect to find 5 defects in a sample of size 25 drawn from a large population containing 20% defects. Since $x/n = 5/25 = 0.20$, the expected probability of finding a defect in this sample is the same as that of finding a defect in the population.

$$E\left(\frac{x}{n}-p\right)^2=\frac{(0.2)(0.8)}{25}=0.0064 \qquad \text{(from Eq. 2.34)}$$

$$\sqrt{0.0064}=0.08$$

2.4.2 Hypergeometric Density Function

In the audit inspection example of the previous section, 25 items were selected from a total inventory of N items, N being large, and the probability of finding zero or one defect in the sample of 25 was found for different values of p, the probability that any given item is defective. Suppose now that N is not large, i.e., that N is so small that the random variable cannot be validly assumed to follow the binomial distribution. In this situation the hypergeometric probability density function applies.

Let N = total number of items (in population, lot, inventory, etc.)
D = number of items which are defects (or successes, in a more general discussion)
n = number of items in sample
x = number of defects in the sample of size n

Then, the density function is

$$f(x)=\frac{\binom{D}{x}\binom{N-D}{n-x}}{\binom{N}{n}} \tag{2.35}$$

This is called the hypergeometric probability density function. The notation

$$\binom{a}{b}=\frac{a!}{b!(a-b)!} \tag{2.36}$$

which some readers will recognize as the number of combinations of a things taken b at a time in combinatorial theory.

Equation 2.35 is applied to the inspection problem of the preceding section. Evaluate the probabilities of obtaining 0 or 1 defect in a sample of size 25 for $N=40$ and $N=100$. The values of D corresponding to $p=0.05$, 0.10, and 0.20 are 2, 4, and 8 for $N=40$ (i.e., $2/40=0.05$, $4/40=0.10$, etc.) and 5, 10, and 20 for $N=100$.

Equation 2.35 is applied to calculate the various probabilities. For $N=40$:

At $p=0.05$ or $D=2$,

$$f(0)=\frac{\binom{2}{0}\binom{38}{25}}{\binom{40}{25}}=\frac{2!38!25!15!}{0!2!25!13!40!}=\frac{(15)(14)}{(40)(39)}=0.135^*$$

$$f(1)=\frac{\binom{2}{1}\binom{38}{24}}{\binom{40}{25}}=\frac{2!38!25!15!}{1!1!24!14!40!}=\frac{(2)(25)(15)}{(40)(39)}=0.481$$

At $p=0.10$ or $D=4$,

$$f(0)=\frac{\binom{4}{0}\binom{36}{25}}{\binom{40}{25}}=0.015$$

$$f(1)=\frac{\binom{4}{1}\binom{36}{24}}{\binom{40}{25}}=0.124$$

At $p=0.20$ or $D=8$,

$$f(0)=\frac{\binom{8}{0}\binom{32}{25}}{\binom{40}{25}}=0.000$$

$$f(1)=\frac{\binom{8}{1}\binom{32}{24}}{\binom{40}{25}}=0.002$$

For $N=100$:

At $p=0.05$ or $D=5$,

* The evaluation of hypergeometric probabilities is simplified if we recognize that, for a>b,

$$a!/b! = a(a-1)(a-2) \quad (a-b+1)$$

For example, $15!/13!=(15)(14)$

$$f(0) = \frac{\binom{5}{0}\binom{95}{25}}{\binom{100}{25}} = 0.229$$

$$f(1) = \frac{\binom{5}{1}\binom{95}{24}}{\binom{100}{25}} = 0.404$$

At $p = 0.10$ or $D = 10$,

$$f(0) = \frac{\binom{10}{0}\binom{90}{25}}{\binom{100}{25}} = 0.048$$

$$f(1) = \frac{\binom{10}{1}\binom{90}{24}}{\binom{100}{25}} = 0.181$$

At $p = 0.20$ or $D = 20$,

$$f(0) = \frac{\binom{20}{0}\binom{80}{25}}{\binom{100}{25}} = 0.001$$

$$f(1) = \frac{\binom{20}{1}\binom{80}{24}}{\binom{100}{25}} = 0.013$$

The results of this example plus those of the corresponding example in the previous section for large N are summarized in Table 2.7, which is instructive in visualizing how large is "large."

A comparison of the ∞ columns (binomial) with the $N = 40$ and $N = 100$ columns (hypergeometric) makes it evident that ignoring the fact that the population is of finite size and applying the binomial density to this particular inspection problem can lead to grossly incorrect probabilities. Thus it would appear that a population of size 100 is not sufficiently large to permit valid application of the binomial density function, at least for the sample of size 25.

TABLE 2.7 PROBABILITIES OF OBSERVING ZERO OR ONE DEFECT

	$\frac{f(0)}{N}$			$\frac{f(1)}{N}$		
Percent defect	40	100	∞	40	100	∞
5%	0.135	0.229	0.277	0.481	0.404	0.365
10%	0.015	0.048	0.072	0.125	0.181	0.199
20%	0.000	0.001	0.004	0.002	0.013	0.024

There can be no precise answer to the question of how large is "large" in more general terms, because it is a question of how close an approximation is required. However, a rule of thumb given by many authors is that the binomial density function provides an acceptable approximation to the hypergeometric if the sample size is less than 10% of the population size. This is a reasonable rule to apply. Note that this criterion was not met in the numerical example just concluded.

The rule of thumb can be given some basis if the moments of the hypergeometric are examined and compared with the moments of the binomial. The mean is

$$\mu = E(x) = \frac{nD}{N} \tag{2.37}$$

This mean is identical with the mean for the binomial if D/N is written as p, its equivalent. (See Eq. 2.31.)

The variance for the hypergeometric is

$$\sigma^2 = \frac{(N-n)nD(N-D)}{N^2(N-1)} \tag{2.38}$$

Again, if D/N is replaced by p to relate it to the binomial variance, Eq. 2.38 may be written in its equivalent form,

$$\sigma^2 = \frac{(N-n)np(1-p)}{(N-1)} \tag{2.39}$$

In comparing this with Eq. 2.32, note that the equations differ only by the factor $(N-n)/(N-1)$. This is commonly called the finite population correction factor. As N gets large, this factor approaches one, and the variances are identical. Also note that, if $n = 0.10N$, corresponding to the rule-of-thumb criterion, this finite population correction factor is about 0.9, which means that the variance of x found by using the binomial density is inflated by about 10% or the standard deviation by about 5%. This is not generally considered to be a serious inflation.

For another application of the hypergeometric density function, see the example in Sec. 2.2.3. The same problem was solved previously by three different methods by the use of the basic laws of probability. It is handled more easily by the hypergeometric function.

The problem of Sec. 2.2.3 is not restated here. If the hypergeometric notation is used,

$N=10$	(ten cans in inventory)
$D=2$	(two "defects", i.e., cans containing marijuana)
$n=2$	(sample size)
$x=1, 2$	(values of the random variable corresponding to detection of the defects)

Then from Eq. 2.35,

$$f(1)=\frac{\binom{2}{1}\binom{8}{1}}{\binom{10}{2}}=\frac{2!8!2!8!}{1!1!1!7!10!}=\frac{16}{45}$$

$$f(2)=\frac{\binom{2}{2}\binom{8}{0}}{\binom{10}{2}}=\frac{2!8!2!8!}{0!2!0!8!10!}=\frac{1}{45}$$

$$f(0)+f(1)=\frac{17}{45}$$

which is in agreement with the results found by the other three approaches.

Further detailed consideration is given the hypergeometric density function in Chap. 9 dealing with inventory verification. This is a most important topic in nuclear materials control applications. However, before leaving this topic, let us make an interesting and somewhat more challenging application which (it is hoped) is primarily of academic interest in nuclear materials control. Although this particular example is unrealistic, the problem suggests an inspection situation in which the strategy is to inspect until x defects are found (x being specified), with the random variable being the sample size corresponding to the x defects. This is contrasted with the more common approach of fixing the sample size and counting the number of defects.

Example 2.B

Ten cylinders of UF_6 are received. Four are known to be at one ^{235}U enrichment and the other six at quite a different enrichment. Unfortunately the identifying labels were removed by some prankster, and the cylinders appear indistinguishable. A cylinder is selected at random,

analyzed, and identified with respect to enrichment. What is the probability that the identification will require sampling exactly five cylinders before all cylinders are correctly identified? eight cylinders? ten cylinders?

Immediately it is known that the probability of sampling ten cylinders must be zero since once the first nine are identified there is no need to identify the tenth.

To find the probability that exactly five cylinders will require sampling, note that this possibility occurs only if exactly three of the first four cylinders sampled are at the first enrichment and, further, if the fifth cylinder is also at this enrichment. The probability that both these events will occur is found by using Eqs. 2.35 and 2.13, where the event E is three of first four cylinders at enrichment one and F is fifth cylinder at enrichment one.

From Eq. 2.35,

$$\Pr(E) = \frac{\binom{4}{3}\binom{6}{1}}{\binom{10}{4}} = \frac{4!6!4!6!}{3!1!1!5!10!} = \frac{4}{35}$$

and, from Eq. 2.7,

$$\Pr(F|E) = \frac{1}{6}$$

since of the six cylinders remaining only one is at the first enrichment.

Then, from Eq. 2.13,

$$\Pr(EF) = \left(\frac{4}{35}\right)\left(\frac{1}{6}\right) = \frac{4}{210} = 0.019$$

which is the probability that exactly five cylinders must be sampled.

To find the probability that exactly eight must be sampled is a bit more complicated because this can occur by two routes: (1) either all the cylinders of enrichment one are identified, which occurs if exactly three of the first seven are identified as enrichment one, as is the eighth, or (2) all the cylinders of enrichment two are identified, which occurs if exactly five of the first seven are identified as enrichment two, as is the eighth. The probabilities are calculated as previously.

Route 1:

$$\Pr(E_1) = \frac{\binom{4}{3}\binom{6}{4}}{\binom{10}{7}} = \frac{4!6!3!7!}{1!3!2!4!10!} = \frac{1}{2}$$

$$\Pr(F_1|E_1) = \frac{1}{3}$$

$$\Pr(E_1F_1) = \left(\frac{1}{2}\right)\left(\frac{1}{3}\right) = \frac{1}{6}$$

Route 2:

$$\Pr(E_2) = \frac{\binom{4}{2}\binom{6}{5}}{\binom{10}{7}} = \frac{4!6!3!7!}{2!2!1!5!10!} = \frac{3}{10}$$

$$\Pr(F_2 | E_2) = \frac{1}{3}$$

$$\Pr(E_2F_2) = \left(\frac{3}{10}\right)\left(\frac{1}{3}\right) = \frac{1}{10}$$

Then by Eq. 2.10 the probability that exactly eight cylinders must be sampled is

$$\frac{1}{6} + \frac{1}{10} = \frac{4}{15} = 0.267$$

It is interesting to calculate this probability for all possible values of the random variable. Table 2.8 summarizes the results.

TABLE 2.8 PROBABILITY FOR ALL POSSIBLE VALUES OF THE RANDOM VARIABLE

Number of cylinders that must be inspected (x)	$f(x)$
4	1/210
5	4/210
6	11/210
7	26/210
8	56/210
9	112/210
	$\sum = 1$

Note that the highest probability is associated with nine cylinders, and, in fact, the probability exceeds 0.5 that this many cylinders must be tested.

2.4.3 Normal Density Function

Contrary to what at times appears to be popular belief, it is not true that all continuous random variables are normally distributed, i.e., have density functions of the form

$$f(x) = \frac{1}{\sqrt{2\pi}\, a} \exp\left[-\frac{(x-b)^2}{2a^2}\right] \qquad (-\infty < x < \infty) \qquad (2.40)$$

Nevertheless, the normal density function is one of great importance because:

1. In fact, many random variables are normally distributed or can be made normal by some simple data transformation.
2. It is a limiting distribution in sampling situations (see Sec. 2.6).
3. Much statistical inference assumes that the random variable is normally distributed.

Reason 3 is not a justifiable reason in itself, of course. However, fortunately many statistical-inference procedures are quite "robust," a term used to indicate that slight-to-moderate departures from normality for the random variable in question will have small effect on the validity of the statistical procedure in question. Thus the assumption that a random variable is normally distributed can often be violated to some moderate degree without affecting the validity of conclusions reached on the basis of data.

With respect to reason 1, in the great majority of problems of interest in nuclear materials control, we deal with random variables that relate to errors of measurement. In this type of situation, the normal density function is generally applicable, although some transformation may be required in certain instances.

Let us note here, however, that we cannot simply assume that the normal distribution assumption is always valid without giving the question further thought. Section 2.9 deals with the problem of how this assumption can be verified for a given set of data if there is some concern as to its validity.

The normal density function, Eq. 2.40, involves the parameters a and b. However, since it can be shown that $E(x)=b$ and $E(x-b)^2=a^2$, i.e., since x has mean b and standard deviation a, and since, as was pointed out earlier, the Greek letters μ and σ are conventionally used to denote the mean and standard deviation for any random variable, the normal density function is generally written

$$f(x)=\frac{1}{\sqrt{2\pi}\,\sigma}\exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] \qquad (-\infty<x<\infty) \tag{2.41}$$

From Eq. 2.22 the distribution function $F(x)$ is

$$F(x)=\frac{1}{\sqrt{2\pi}\,\sigma}\int_{-\infty}^{x}\exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]dx \tag{2.42}$$

This integral cannot be evaluated in closed form, and numerical integration is required. Clearly it would be an impossible task to tabulate $F(x)$ for all conceivable combinations of the two parameters μ and σ.

Fortunately this is not required, because the random variable is "standardized" by (1) subtraction of the mean, μ, and (2) division of this difference by the standard deviation, σ.

In mathematical terms this means that the random variable, X, is replaced by a new random variable, Z, by means of the transformation

$$z=\frac{x-\mu}{\sigma} \tag{2.43}$$

in which μ and σ are the mean and the standard deviation of x. This transformation being made, the mean and the standard deviation of z become 0 and 1, respectively. This then permits tabulation of the normal distribution function in standard form.

A table of

$$F(z_p)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{z_p} e^{-z^2/2}\,dz \tag{2.44}$$

is given as Appendix A, where $P=F(z_p)$.

In Appendix A the values of z_p are given only for positive values of z_p. Symmetry makes this possible. If z_p is negative, then $F(z_p)$ is 1 minus the tabulated value. The sketch at the top of Appendix A should help us understand this. In fact, when we read values from a table such as this without complete confidence in our ability to read the table, we should make a rough sketch similar to that at the top of Appendix A to make sure that we are using the table properly.

As a very simple example on the use of Appendix A, assume that a random variable, X has mean $\mu=2$ units and standard deviation $\sigma=5$ units. Find the probability that a given x value is less than 3 units; i.e., find Pr $(x<3)$.

Operate on both sides of the inequality to standardize the random variable. Using the transformation Eq. 2.43, proceed as follows:

$$\Pr\,(x<3)=\Pr\left(\frac{x-2}{5}<\frac{3-2}{5}\right)=\Pr\,(z<0.20)$$

From Appendix A this probability is 0.5793.

Suppose now that the probability that x will fall between -4 and 3 is to be determined; i.e., find Pr $(-4<x<3)$.

By Eq. 2.23 this is

$$\begin{aligned}F(3)-F(-4)&=\Pr\,(x<3)-\Pr\,(x<-4)\\&=\Pr\left(\frac{x-2}{5}<\frac{3-2}{5}\right)-\Pr\left(\frac{x-2}{5}<\frac{-4-2}{5}\right)\\&=\Pr\,(z<0.20)-\Pr\,(z<-1.20)\\&=0.5793-(1-0.8849)=0.4642\qquad\text{(from Appendix A)}\end{aligned}$$

Note that Pr $(z < -1\ 20)$ is 1 minus the entry tabled at $z = +1\ 20$ However, rather than trying to remember this rule by rote and applying it when negative values of the standardized normal random variable are encountered, it is preferable to create a better understanding by drawing a rough sketch similar to Fig 2 3 to identify the probabilities, or areas, of interest The shaded area corresponds to the probability of interest

2.4.4 Uniform (Rectangular) Density Function

Another continuous density function that has application to nuclear materials control problems is the uniform or rectangular density function This very simple function also has two parameters and is written as

$$F(x) = \frac{1}{b-a} \qquad (a < x < b) \tag{2 45}$$

The function does not involve x Its plot is of equal height throughout the entire finite range of the random variable This means that the probability that a given observation, x, will lie between any two specified quantities, x_1 and x_2, is dependent only on the difference, $x_2 - x_1$, and not on the values x_1 and x_2

It is easy to see that the distribution function, $F(x)$, is

$$F(x) = \frac{x-a}{b-a} \tag{2 46}$$

The mean of x, μ, is

$$\mu = \frac{a+b}{2} \tag{2 47}$$

which is the value halfway between a and b

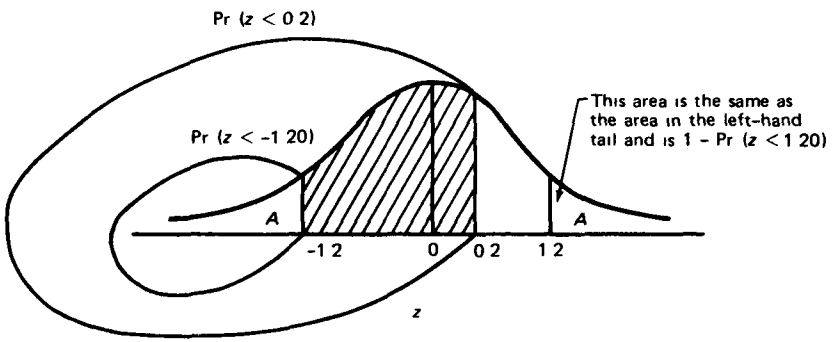

FIGURE 2 3 Identification of probabilities in Appendix A

The variance is

$$\sigma^2 = \frac{(b-a)^2}{12} \tag{2.48}$$

or one-twelfth the square of the range.

The density function has application in nuclear materials control because it describes "rounding" error. If a recorded weight, for example, is always rounded to the nearest 50 g and if no other weighing errors are made, then the true weight of the item may be regarded as a random variable. This true weight lies somewhere in the interval within 25 g on either side of the reported weight and is equally likely to occur anywhere in this interval. Thus from Eq. 2.45, the density function of X, the true weight is

$$f(x) = \frac{1}{50} \qquad [(W-25) < x < (25+W)]$$

where W is the reported weight in grams.

From Eq. 2.47, the mean of x, μ, is

$$\mu = \frac{(W-25)+(25+W)}{2} = W$$

and from Eq. 2.48, the variance is

$$\sigma^2 = \frac{(25+W-W+25)^2}{12} = \frac{(50)^2}{12} = 208.33 \text{ g}^2$$

$$\sigma = 14.4 \text{ g}$$

The variance σ^2 is that due to rounding. In nuclear materials control applications, this may be a dominant source of variation due to weighing for some types of items.

It is instructive to note the effects of different rounding rules on the standard deviation due to rounding, as given by Table 2.9.

TABLE 2.9 EFFECT OF ROUNDING ON VARIANCE DUE TO ROUNDING

Round to nearest G, g*	σ^2, g^2	σ, g
G = 1	0.0833	0.29
5	2.0833	1.44
10	8.3333	2.89
25	52.08333	7.22
50	208.3333	14.43
100	833.3333	28.87

* Or kg, lb, or other unit of weight.

This topic will be discussed further in Chap. 3.

2.5 BIVARIATE DISTRIBUTIONS

Thus far in the discussion, only a single random variable has been considered. The single random variable receives almost exclusive attention in this book because most problems of interest in the control of nuclear materials can be dealt with on this basis. This is not to say that certain quantities may not, in turn, be functions of several random variables. But, if all the random variables are defined over different sample spaces, the resulting function of random variables is itself regarded as a single random variable, and there is no need to speak of other than the univariate situation.

However, in some instances this simple modeling may not apply, and it is necessary to introduce the multivariate case. In particular, let us consider the bivariate case involving two random variables, X and Y, both defined on the same sample space.

Restricting interest to the continuous case, we say that two random variables, X and Y, have the bivariate probability density function $f(x,y)$ if, for two pairs of values (x_1,x_2) and (y_1,y_2),

$$\Pr\ (x_1<x<x_2;\ y_1<y<y_2)=\int_{y_1}^{y_2}\int_{x_1}^{x_2} f(x,y)\ dx\ dy \tag{2.49}$$

The expression $f(x,y)$ is also referred to as the joint probability density function for the random variables X and Y. In extending the principle expressed in Eq. 2.12, we say that two random variables are independent if and only if their joint probability density function is the product of their marginal density functions, where the marginal density function of x, for example, is represented by $g(x)$, given by

$$g(x)=\int_{-\infty}^{\infty} f(x,y)\ dy \tag{2.50}$$

i.e., $g(x)$ is the density function of x without regard to the value of y.

Also, with reference to Eq. 2.13 or Eq. 2.14, x and y have conditional density functions. For x,

$$h(x\,|y)=\frac{f(x,y)}{g(y)} \tag{2.51}$$

with $h(y\,|x)$ similarly defined.

For the bivariate case we can also define the means and variances of x and y. For example,

$$\mu_x=E(x)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} x f(x,y)\ dx\ dy \tag{2.52}$$

with μ_y similarly defined. The variances are the second moments about the means, as before.

Of particular interest in the bivariate case is a quantity called the covariance between x and y, defined as

$$\text{cov } (x,y) = E[(x-\mu_x)(y-\mu_y)] \tag{2.53}$$

or, alternately and equivalently, as

$$\text{cov } (x,y) = E(xy) - \mu_x\mu_y \tag{2.54}$$

If x and y are independently distributed, it follows immediately that $E(xy) = (\mu_x)(\mu_y)$ and, from Eq. 2.54, the covariance is zero.

Finally, it is often convenient to use a standardized measure of the dependence between x and y. This is called the correlation coefficient, generally denoted by the Greek letter rho, ρ, and is simply the covariance divided by the product of the standard deviations.

$$\rho_{x,y} = \frac{\text{cov } (x,y)}{\sigma_x\sigma_y} \tag{2.55}$$

Later in the book as the need arises, we will refer to the results presented here.

2.6 SAMPLING DISTRIBUTIONS

The problem of statistical inference is one of drawing conclusions about a population of possible events on the basis of a given random sample of the events. Thus far, it has been tacitly assumed that the population is known or completely specified and, in the continuous case, that the sample size is one.

The idea of sampling from a known population is consistent with certain aspects of statistical inference. For example, in the formulation of the tests in Sec. 2.8 dealing with hypothesis testing, this situation obtains, either wholly or in part. In other facets of inference and, in particular, those dealing with estimation discussed in Sec. 2.7, the population is only partially specified, and the problem is to use the sample results to complete the specification as well as possible.

In either situation we deal with the idea of sampling and of making inferences about the population from the results of the sampling, which may be called the data. This is the subject of this section.

Before proceeding further, let us consider the term "random" sampling. Random sampling can be defined in rigorous terms, but here we shall sacrifice unneeded rigor for clarity of meaning and define a random sample as a selection of items from a population such that every item in that population has a fixed and known probability of being selected.

Some objective means should be used to achieve randomness, e.g., with random number tables, because individuals left to their own devices are simply not capable of making a random selection in the true sense of the word.

To continue with the ideas of sampling, let the random variable be denoted by X, and let it have the density function $f(x)$. Draw a random sample of n items from the population, and designate the sample values by $x_1, x_2, \ldots, x_n$. The problem is to use the sample values, or data points, to make inferences about $f(x)$. Specific types of inferences to be made are discussed in Secs. 2.7 and 2.8. The problem in this section is to provide the additional necessary tools that will permit making these inferences.

In the case of the discrete distributions, binomial and hypergeometric, the tools have already been provided in Secs. 2.4.1 and 2.4.2, and the results will be applied to statistical inference problems later. In this section, therefore, attention is restricted to the problem of sampling from continuous distributions.

There are two statistics of primary interest in many problems of statistical inference: the sample mean and the sample variance. These quantities were introduced in Sec. 2.1 on descriptive statistics. At that point their function was simply to summarize a set of data. There was no intent to make inferences about some population from which these data might have been sampled. Now they are to be used for this purpose. In this connection we must recognize that the sample mean and variance are also random variables and, as such, have their own probability density functions and corresponding moments. These and the density functions for certain functions of means and variances are discussed in this section.

The sample mean, $\bar{x}$, is given by

$$\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n} \tag{2.56}$$

The x_i are observations on a random variable. Assume that each x_i has mean μ and variance σ^2. Since $\bar{x}$ is also an observation on a random variable, this random variable has its own probability density function, and we can speak of the mean and variance of $\bar{x}$. It will be shown in Sec. 4.1.2 that

$$E(\bar{x}) = \mu \tag{2.57}$$

The variance of $\bar{x}$ is also derived in Sec. 4.1.2. Assume initially that the population being sampled is of infinite size. This assumption has the effect of making the individual observations, x_i, statistically independent; i.e., the covariance between x_i and x_j is zero. Under this assumption, the variance of $\bar{x}$, denoted by $\sigma_{\bar{x}}^2$, is

$$\sigma_{\bar{x}}^2=\frac{\sigma^2}{n} \tag{2.58}$$

If the population is finite in size, containing N items, then x_i and x_j have a nonzero covariance. As shown in Sec. 4.1.2, this leads to the result

$$\sigma_{\bar{x}}^2=\frac{(N-n)\sigma^2}{(N-1)n} \tag{2.59}$$

where the factor $(N-n)/(N-1)$ is called the finite population correction factor. This factor has been introduced before in connection with the hypergeometric density function (see Eq. 2.39). In nuclear materials control applications in which one deals with measurements, it is generally true that the population sizes may be regarded as infinite so that Eq. 2.58 is applicable. Unless specifically stated otherwise, we shall assume in what follows that this is the case.

Although Eqs. 2.57 and 2.58 give, respectively, the mean and variance of $\bar{x}$, they shed no light on its probability density function. However, the following two points are made:

1. If the x_i are normally distributed, then $\bar{x}$ is also normally distributed.

2. As a consequence of the important Central Limit Theorem, the sum of a "sufficient number" of random variables having finite variances will be approximately normally distributed, regardless of how the individual random variables are distributed. Roughly speaking, this says with respect to a sample mean that, if a population has finite variance, then the distribution of the sample mean approaches normality as the sample size increases.

Thus in many instances we can say that the sample mean, $\bar{x}$, is normally distributed with mean, μ, and variance, σ^2/n. It should be pointed out that in some instances some data transformation is desirable to achieve a closer approximation to normality. One common transformation applied is the logarithmic transformation. Further, such transformations are sometimes made for other reasons, and the closer approximation to normality that results is a desirable by-product. If data are transformed by the use of logarithms, we say that the original untransformed random variable has the log normal probability density function, or, simply, is log normal.

Return to the data: $x_1, x_2, \ldots, x_n$. The other statistic of interest is the sample variance, s^2, defined by

$$s^2=\frac{\sum_{i=1}^{n}(x_i-\bar{x})^2}{n-1} \tag{2.60}$$

An equivalent form of s^2, more convenient for calculation purposes, is

$$s^2 = \frac{\sum_{i=1}^{n} x_i^2 - \left[\left(\sum_{i=1}^{n} x_i\right)^2 / n\right]}{n-1} \tag{2.61}$$

The reason for division by $(n-1)$, called the degrees of freedom, rather than by n is explained in Sec. 2.7. [If we should happen to know the population mean, μ, then $\bar{x}$ in the preceding equations would be replaced by μ and the $(n-1)$ divisor by n.]

The sample variance, s^2, is also a random variable. Its expected value is

$$E(s^2) = \sigma^2 \tag{2.62}$$

The variance of s^2 is not too important for purposes of this book but is given for completeness:

$$\sigma_{s^2}^2 = \frac{\mu_4 - [(n-3)\sigma^4/(n-1)]}{n} \tag{2.63}$$

where μ_4 is the fourth moment about the mean, i.e., $\mu_4 = E(x-\mu)^4$.

When sampling is from a normal population, μ_4 is $3\sigma^4$, and so Eq. 2.63 reduces to

$$\sigma_{s^2}^2 = \frac{2\sigma^4}{n-1} \tag{2.64}$$

In practice we wish to use $\bar{x}$ and/or s^2 to make inferences about the corresponding population parameters, μ and/or σ^2. The specific inferences to be made are the subjects of Secs. 2.7 and 2.8. However, to make the

TABLE 2.10 COMMON SAMPLING DISTRIBUTIONS

	Statistic	Distribution
1.	$\frac{\bar{x}-\mu}{\sigma/\sqrt{n}}$	Standardized normal; mean 0 and standard deviation 1
2.	$\frac{(n-1)s^2}{\sigma^2}$	Chi-square; $(n-1)$ degrees of freedom
3.	$\frac{\bar{x}-\mu}{s/\sqrt{n}}$	Student's t; $(n-1)$ degrees of freedom
4.	$\frac{s_1^2}{s_2^2}$ (Two sample variances drawn from populations with the same variances)	F distribution; (n_1-1) and (n_2-1) degrees of freedom

inferences, we must know the density functions for $\bar{x}$ and s^2 and for certain of their functions, i.e., knowing only their moments is not sufficient. To that end, we speak of the sampling distributions of certain statistics. These are summarized in Table 2.10, and each of the four functions is briefly discussed in the following sections. It is assumed that the population random variable is normally distributed with mean, μ, and variance, σ^2, and that the population is of infinite size.

Other statistics of interest are introduced later.

2.6.1 Standardized Normal

Since $\bar{x}$ is normally distributed with mean, μ, and variance, σ^2/n, it follows from Eq. 2.43 that $(\bar{x}-\mu)\sqrt{n}/\sigma$ is normally distributed with mean 0 and standard deviation 1. This density function is used to make inferences about μ when the population standard deviation is assumed known.

2.6.2 Chi-Square

If $t_1, t_2, \ldots, t_\nu$ are independently distributed standardized normal variables, then the sum of their squares, denoted by χ^2, has a density function:

$$f(\chi^2) = C_1 e^{-\chi^2/2} (\chi^2)^{(\nu/2)-1} \tag{2.65}$$

where C_1 is a constant. This is known as the χ^2 density function with the single parameter ν, called the degrees of freedom.

The result of Eq. 2.65 is used to develop the density function for

$$\chi^2 = \frac{(n-1)s^2}{\sigma^2} \tag{2.66}$$

and the resulting density function is given by Eq. 2.65 with parameter $(n-1)$ in place of ν.

A table of the cumulative distribution function,

$$F(\chi_P^2) = \int_0^{\chi_P^2} f(\chi^2)\, d\chi^2 \tag{2.67}$$

is given as Appendix B, where $P = F(\chi_P^2)$. The column headed "*df*" is the degrees of freedom, $(n-1)$.

Example 2.C

If $\sigma^2 = 5$ (units)^2, what is the probability that the sample variance, s^2, based on $n = 17$ observations will exceed 10 (units)^2?

For an answer, s^2 must be standardized by Eq. 2.66; i.e., it must be multiplied by $(n-1)$ and divided by the population variance, σ^2.

$$\begin{aligned}\Pr\,(s^2>10) &= \Pr\left[\frac{(n-1)s^2}{\sigma^2}>\frac{(n-1)10}{\sigma^2}\right]\\ &= \Pr\left[\frac{(n-1)s^2}{\sigma^2}>\frac{(16)(10)}{5}\right]\\ &= \Pr\,(\chi^2>32.00)\\ &= 1-0.99 \qquad \text{(from Appendix B with 16 } df\text{)}\\ &= 0.01\end{aligned}$$

2.6.3 Student's *t*

When σ is not known and we wish to make inferences on μ using $\bar{x}$, it is intuitively reasonable to replace σ in the standardized normal random variable by s, giving the statistic, t,

$$t=\frac{\bar{x}-\mu}{s/\sqrt{n}} \tag{2.68}$$

Because s is in itself a random variable and introduces additional uncertainty, we would not expect t to be normally distributed but, rather, to have a broader distribution to account for the added uncertainty. It turns out that the density function for t is of the form

$$f(t)=C_3\left[1+\frac{t^2}{\nu}\right]^{-(\nu+1)/2} \tag{2.69}$$

where C_3 is a constant and $\nu=(n-1)$ is the single parameter called the degrees of freedom.

The t statistic can be described in more-general terms. If two random variables, w and y, are independently distributed and if w is normally distributed with zero mean and unit variance while y is distributed as chi-square with ν degrees of freedom, then the random variable

$$t=\frac{w}{\sqrt{y/\nu}} \tag{2.70}$$

is distributed as Student's t with ν degrees of freedom. In the application leading to Eq. 2.68, identify

$$w=\frac{\bar{x}-\mu}{\sigma/\sqrt{n}} \qquad \text{and} \qquad y=\frac{(n-1)s^2}{\sigma^2}$$

Then

$$t=\frac{w}{\sqrt{y/\nu}}=\frac{(\bar{x}-\mu)\sqrt{n}\,\sigma}{\sigma s}=\frac{\bar{x}-\mu}{s/\sqrt{n}}$$

consistent with the definition in Eq. 2.68, since $\nu=(n-1)$. Notice that the degrees of freedom in the t-statistic are those associated with the determination of s^2 and the sample size used to determine $\bar{x}$ does not enter in.

A table of the cumulative distribution function,

$$F(t_p)=\int_{-\infty}^{t_p} f(t)\,dt \tag{2.71}$$

is given as Appendix C, where $P=F(t_p)$. The column headed "*df*" is the degrees of freedom, $(n-1)$.

Example 2.D

Nine observations are drawn from a normal population. What is the probability that the sample mean, $\bar{x}$, is greater than $0.62s$ units removed from the true mean, μ, where s is the observed sample standard deviation? This occurs either when $\bar{x}$ is too small or too large, and the desired probability is the sum of two probabilities, p_1 and p_2, where

$$p_1=\Pr\ [(\bar{x}-\mu)>0.62s]$$
$$p_2=\Pr\ [(\mu-\bar{x})>0.62s]=\Pr\ [(\bar{x}-\mu)<-0.62s]$$

p_1 will be evaluated, and p_2 equals p_1 by symmetry. Standardize the random variable, $(\bar{x}-\mu)$, by dividing it by its estimated standard deviation, $s/\sqrt{n}=s/\sqrt{9}=s/3$. Then

$$p_1=\Pr\ [(\bar{x}-\mu)>0.62s]=\Pr\left[\frac{(\bar{x}-\mu)}{s/\sqrt{n}}>\frac{0.62s}{s/3}\right]$$
$$=\Pr\qquad (t>1.86)$$

From Appendix C, with 8 degrees of freedom, this probability is 1—0.95 or 0.05. Therefore, since $p_1=p_2$ by symmetry, $p_1+p_2=0.10$, which is the desired probability.

2.6.4 F Distribution

The final sampling distribution of particular note introduced at this time is that used in comparing two independent sample variances, s_1^2 and s_2^2, based on samples drawn from populations having variances σ_1^2 and σ_2^2 and with ν_1 and ν_2 degrees of freedom, respectively. The statistic called the F ratio is introduced.

$$F=\frac{s_1^2/\sigma_1^2}{s_2^2/\sigma_2^2} \tag{2.72}$$

The density function for F is given as

$$f(F)=C_4F^{(\nu_1/2)-1}\left[1+\frac{\nu_1F}{\nu_2}\right]^{-(\nu_1+\nu_2)/2} \tag{2.73}$$

where C_4 is a constant.

This is a two-parameter density function with parameters ν_1 and ν_2, the degrees of freedom for the numerator and denominator, respectively, in the F ratio.

It is also possible to describe the F ratio in more-general terms as the ratio of two independently distributed chi-square variables, each divided by its degrees of freedom.

A table of the cumulative distribution function,

$$F(F_p)=\int_0^{F_p} f(F)\,dF \tag{2.74}$$

is given as Appendix D, where $P=F(F_p)$. In this table the degrees of freedom for the numerator and denominator are given as n_1 and n_2, respectively. These are not sample sizes but degrees of freedom.

Example 2.E

A random sample of size 7 is drawn from a normal population, and s_1^2 is computed. A second sample of size 5 is then drawn from the same population, and s_2^2 is computed. What is the probability that the first variance, s_1^2, is at least four times as large as the second variance, s_2^2?

To answer this, recognize that $\sigma_1^2=\sigma_2^2$ since both samples are drawn from the same population. Then, the F statistic given in Eq. 2.72 is simply

$$F=\frac{s_1^2}{s_2^2}$$

with $(7-1)=6$ and $(5-1)=4$ degrees of freedom for the numerator and denominator, respectively. The probability required is

$$\Pr\left(\frac{s_1^2}{s_2^2}>4\right)=\Pr\,(F>4)=1-0.90=0.10 \qquad \text{(from Appendix D)}$$

(The tabular entry corresponding to $n_1=6$ and $n_2=4$ at $P=0.90$ is 4.01, rounded to 4.)

2.7 PARAMETER ESTIMATION

The introductory remarks to the preceding section stated that the problem of statistical inference was that of using sample results to draw conclusions about the population. These conclusions fall in two broad categories:

1. Parameter estimation, in which we obtain estimates of the parameters of the density function for the population random variable and indicate how "good" these estimates are.
2. Hypothesis testing, in which we make a priori statements (hypotheses) about the population parameters and use the sample results to verify or refute these statements.

Both types of inference are of interest in nuclear materials control applications. Parameter estimation is described in this section; hypothesis testing is covered in Sec. 2.8 and is extended to other more general hypotheses in Sec. 2.9.

In parameter estimation we distinguish between the "point" estimates of the parameters and their "interval" estimates. Point estimation is discussed first.

2.7.1 Point Estimation

The principle of maximum likelihood is often used to estimate parameters. Under this principle the parameter values are chosen to maximize the likelihood, or probability, of obtaining the sample results. That is, for all other possible values that could be assigned the parameter in question, the probability of observing the given set of sampled data is smaller than for the maximum-likelihood estimate of the parameter.

This principle is best understood with an illustration. Consider the binomial density function. For n observations, let X be the number of observed successes. Then, the likelihood, or probability, that x will take on a given value is given by Eq. 2.30, which is repeated here:

$$f(x) = \frac{n!}{x!(n-x)!} p^x (1-p)^{n-x} \tag{2.30}$$

The maximum-likelihood estimation principle says that the parameter, p, should be chosen to maximize $f(x)$. It is a simpler mathematical exercise to maximize the logarithm of $f(x)$, which is clearly maximized at the same value of p as is $f(x)$.

Write the logarithm of $f(x)$ as

$$L = \ln f(x) = \ln n! - \ln x! - \ln(n-x)! + x \ln p + (n-x) \ln (1-p)$$

This is a simple function that can be maximized by applying basic results from calculus.

The partial derivative of L is taken with respect to p, equated to zero, and solved for p. The solution is the maximum-likelihood estimate of p.

$$\frac{\partial L}{\partial p}=\frac{x}{p}-\frac{n-x}{1-p}=0$$

which gives

$$\hat{p}=\frac{x}{n} \tag{2.75}$$

where the caret ($\hat{}$) is used to denote that x/n is an estimate of the parameter p.

Thus the maximum-likelihood estimate of the binomial parameter, p, is the number of successes divided by the number of observations.

Reference to Eq. 2.33 shows that $\hat{p}$, or x/n, has expected value p. When the expected value of an estimate is equal to the parameter being estimated, this estimate is said to be unbiased. This is a desirable property because it indicates that, by use of the estimating procedure that produces the unbiased estimate, the estimate will equal the parameter being estimated "on the average."

There are other important properties of estimators that are not discussed here. It suffices to say that the maximum-likelihood method results in estimators with desirable qualities. (It is noted that maximum-likelihood estimators are not, in general, unbiased. They can be made unbiased, however, very simply, and this is not a serious criticism of the method.)

The hypergeometric, normal, and uniform density functions have been discussed previously. The following point estimates are maximum-likelihood estimates of the parameters, the notation being consistent with that in Sec. 2.4.

(a) *Hypergeometric Density Function*

$$\hat{D}=\left\{\frac{x(N+1)}{n}\right\} \tag{2.76}$$

where $\{\ \}$ denote "the integer just less than . . .". Clearly $\hat{D}$ must be an integer.

(b) *Normal Density Function*

The maximum-likelihood estimate of μ is

$$\hat{\mu}=\bar{x} \tag{2.77}$$

Since $E(\bar{x})=\mu$ for any distribution, including the normal, from Eq. 2.57, $\bar{x}$ is an unbiased estimate of μ.

The maximum-likelihood estimate of σ^2 is

$$\hat{\sigma}^2 = \sum_{i=1}^{n} \frac{(x_i - \bar{x})^2}{n} \tag{2.78}$$

However, it can be shown that $E(\hat{\sigma}^2) \neq \hat{\sigma}^2$, and the estimate is biased. This can be remedied if n in Eq. 2.78 is replaced by $(n-1)$ to give the estimate

$$s^2 = \sum_{i=1}^{n} \frac{(x_i - \bar{x})^2}{n-1} \tag{2.79}$$

By Eq. 2.62 since $E(s^2) = \sigma^2$, s^2 is an unbiased estimate of σ^2. This is the motivation for division by $(n-1)$ rather than by n.

We noted earlier in Sec. 2.1 that other measures of central tendency and dispersion might be used as descriptive statistics. The question arises as to whether or not the median, for example, could be used to estimate the population mean, μ, and some function of the range, say, to estimate σ^2. This is possible. The resulting estimates are not as good in a statistical sense as $\bar{x}$ and s^2, but this may not be a serious drawback if simplicity is thereby introduced. For example, we can find the range of 5 numbers by inspection, but determining the variance, s^2, requires calculation. However, the author's experience is that in most nuclear materials control applications there is little occasion to use estimates other than $\bar{x}$ and s^2, and therefore we shall drop the subject at this point without further mention. Those interested in pursuing it further can find the subject discussed in many textbooks.

(c) *Uniform Density Function*

The maximum-likelihood estimates for the parameters of the uniform density are found by letting x' be the smallest of the n x_i values and x'' be the largest. Then the parameters a and b of the density function (Eq. 2.45) are estimated by

$$\hat{a} = x' \qquad \hat{b} = x'' \tag{2.80}$$

Since there will be no occasion to estimate the parameters of the uniform density function in this book, no more will be said on this subject.

2.7.2 Interval Estimation

After an estimate of some given parameter is obtained, the next obvious question is "How good is the estimate?" To rephrase this more precisely, we might ask, "What is the probability that the estimate of a

parameter differs from the true value of that parameter by more than u units?" * This question is answered by the construction of a *confidence interval.*

Roughly speaking, a confidence interval is an interval within which the true parameter value lies with some specified degree of confidence, or with some specified probability. This may bother some readers because it seems to imply that the parameter has a distribution and hence is a random variable. However, this is not the case. Rather, the interval is the random variable. A 95% confidence interval, say, on some arbitrary parameter, θ, is interpreted as follows: If the experiment were to be repeated over and over again and the interval were always constructed in the given manner, then 95% of these intervals will be expected to include the true parameter θ. This is often freely translated as "With 95% confidence, θ is included within the interval in question."

Confidence intervals (the end points of a confidence interval are called confidence limits) are constructed for the parameters of the density functions of greatest interest in this book. The normal density function is considered first.

(a) *Normal Density Function*

Three cases are considered. In the first two cases, a confidence interval is to be constructed on the population mean, μ, first with σ known and second with σ not known. In the third case a confidence interval is constructed on the population variance, σ^2.

Case 1: Confidence limits (CL) on μ, known σ.

Since

$$z=\frac{\bar{x}-\mu}{\sigma/\sqrt{n}}$$

is standardized normal, with zero mean and unit standard deviation, the following "equal-tailed" probability statement can be made if we wish to construct a confidence interval within which μ lies with $100(1-\alpha)\%$ confidence.

$$\Pr\left(z_{\alpha/2}<\frac{\bar{x}-\mu}{\sigma/\sqrt{n}}<z_{1-\alpha/2}\right)=1-\alpha \tag{2.81}$$

where

$$\int_{z_{\alpha/2}}^{z_{1-\alpha/2}} f(z)\,dz=1-\alpha \tag{2.82}$$

defines $z_{\alpha/2}$ and $z_{1-\alpha/2}$. Because of symmetry, $z_{\alpha/2}$ may also be written as $-z_{1-\alpha/2}$.

* Or, possibly, by more than p %?

Equation 2.81 is solved for μ to give the equivalent probability statement,

$$\Pr\left(\bar{x}-z_{1-\alpha/2}\frac{\sigma}{\sqrt{n}}<\mu<\bar{x}+z_{1-\alpha/2}\frac{\sigma}{\sqrt{n}}\right)=1-\alpha \tag{2.83}$$

This is the desired confidence interval for μ, with known σ. It may also be written as

$$\mu=\bar{x}\pm z_{1-\alpha/2}\frac{\sigma}{\sqrt{n}} \tag{2.84}$$

Case 2: Confidence limits on μ, unknown σ.

An approach similar to that of case 1 is used. Now the z statistic is replaced by t defined by Eq. 2.68. The quantities $t_{\alpha/2}$ and $t_{1-\alpha/2}$ are defined as in Eq. 2.82 with the density function being Student's t rather than the standardized normal. Again, with the use of the symmetry of the t density function, the resulting $100(1-\alpha)\%$ confidence interval is

$$\mu=\bar{x}\pm t_{1-\alpha/2}\frac{s}{\sqrt{n}} \tag{2.85}$$

Case 3: Confidence limits on σ^2.

The confidence interval on σ^2 is constructed by using the χ^2 variable given by Eq. 2.66. The probability statement is

$$\Pr\left(\chi^2_{\alpha/2}<(n-1)\frac{s^2}{\sigma^2}<\chi^2_{1-\alpha/2}\right)=1-\alpha \tag{2.86}$$

with $\chi^2_{\alpha/2}$ and $\chi^2_{1-\alpha/2}$ defined by Eq. 2.67. This interval is constructed on σ^2 to give

$$\Pr\left(\frac{(n-1)s^2}{\chi^2_{1-\alpha/2}}<\sigma^2<\frac{(n-1)s^2}{\chi^2_{\alpha/2}}\right)=1-\alpha \tag{2.87}$$

Note that the confidence intervals constructed in the preceding paragraphs are all symmetric in the sense that equal probabilities are assigned to each tail. This is common practice when two-sided intervals are used. However, there is nothing in the definition of a confidence interval which requires this.

In some applications one is interested in constructing a one-sided interval, i.e., in making a statement to the effect that some arbitrary parameter θ is less than (or greater than) some value with a given stated degree of confidence. This is a limiting case of an unsymmetrical two-sided interval in the sense that either the subscript $\alpha/2$ for z, t, or χ^2 for the three cases just studied is replaced by α and the subscript $(1-\alpha/2)$ is replaced

by 1 or $(1-\alpha/2)$ is replaced by $\alpha/2$ and $\alpha/2$ by 0. One-sided intervals are discussed more fully when the parameters of the binomial and hypergeometric density functions are treated in Secs. b and c.

Example 2.F

Five samples of UO_2 powder are measured for percent uranium with the following results:

$$x_1 = 87.627 \qquad x_4 = 87.571$$
$$x_2 = 87.649 \qquad x_5 = 87.637$$
$$x_3 = 87.642$$

Construct a 95% two-sided confidence interval on the mean, μ, for the population from which the samples were drawn and a 90% two-sided confidence interval on the variance.

To construct the CL for the mean, apply Eq. 2.85. For 95% confidence, $\alpha = 0.05$ and $\alpha/2 = 0.025$. Therefore, from Appendix C with $df = 4$,

$$t_{1-\alpha/2} = t_{0.975} = 2.776$$

Next, $\bar{x}$, s^2, and s are calculated from the data. By Eq. 2.56, $\bar{x}$ is found by summing the five values and dividing by 5:

$$\bar{x} = \frac{(87.627 + \ldots + 87.637)}{5}$$

$$= 87.625$$

By Eq. 2.61,

$$s^2 = \frac{(87.627)^2 + \ldots + (87.637)^2 - [(87.627 + \ldots + 87.637)^2/5]}{4}$$

$$= 0.000982$$

and

$$s = \sqrt{0.000982} = 0.0313^*$$

Instructions for Eq. 2.4 (Sec. 2.1) may be used if the reader prefers instructions to equations.

From Eq. 2.85, the 95% confidence limits for the mean, μ, are

$$\mu = 87.625 \pm \frac{(2.776)(0.0313)}{\sqrt{5}}$$

$$= 87.625 \pm 0.039$$

* In the actual calculation, 87 may be subtracted from all the numbers to permit working with small values. Then 87 is added to the calculated mean to give $\bar{x}$. The terms s^2 and s are unaffected by addition of, or subtraction of, the same quantity to (from) all the observations.

Thus the mean, μ, lies in the interval from 87.586 to 87.664 with 95% confidence.

To construct the 90% confidence interval on the variance, σ^2, apply Eq. 2.87. For the 90% confidence level, $\alpha = 0.10$ and, from Appendix B with 4 *df*,

$$\chi^2_{1-\alpha/2} = \chi^2_{0.95} = 9.49 \qquad \text{and} \qquad \chi^2_{\alpha/2} = \chi^2_{0.05} = 0.711$$

Thus the confidence interval is

$$\frac{(4)(0.000982)}{9.49} < \sigma^2 < \frac{(4)(0.000982)}{0.711}$$

$$0.000414 < \sigma^2 < 0.005525$$

The corresponding interval for the standard deviation, σ, is found by extracting the square roots of these limit values:

$$0.0203 < \sigma < 0.0743$$

Example 2.G

In example 2.F, suppose it is known from previous data that $\sigma = 0.05\%$ (absolute percentage units). Then what is the 95% confidence interval on μ?

Equation 2.85 is applied. From Appendix A,

$$z_{1-\alpha/2} = z_{0.975} = 1.96$$

Then the interval is

$$\mu = 87.625 \pm \frac{(1.96)(0.05)}{\sqrt{5}}$$

$$= 87.625 \pm 0.044$$

(b) *Binomial Density Function*

The problem of constructing confidence limits for the binomial parameter, p, is more complex. This reduces to finding the largest value of p, say p_1, such that, for that value of p,

$$\sum_{x=x_0}^{n} \frac{n!}{x!(n-x)!} p^x (1-p)^{n-x} \leq \frac{\alpha}{2} \tag{2.88}$$

and the smallest value of p, say p_2, such that

$$\sum_{x=0}^{x_0} \frac{n!}{x!(n-x)!} p^x (1-p)^{n-x} \leq \frac{\alpha}{2} \tag{2.89}$$

where x_0 is the number of observed successes in n total observations and $100(1-\alpha)\%$ is the confidence coefficient.

With the binomial and hypergeometric density functions, we are often interested in a "one-sided" interval, i.e., an upper limit on the parameter only. This is accomplished by solving Eq. 2.89 with $\alpha/2$ replaced by α and by ignoring Eq. 2.88. If a lower limit is required, $\alpha/2$ is replaced by α in Eq. 2.88, and Eq. 2.89 is ignored.

Equations 2.88 and 2.89 can be solved by trial and error, but this is a laborious process unless x_0 is very small. Fortunately, in the most common nuclear materials control applications that are related to inspection activities, x_0 will be quite small, and it is reasonable to proceed on that basis.

For larger x_0, we must resort to tables or approximate formulas. This is not discussed further here, however, because (1) it is felt that Eqs. 2.88 and 2.89 can be solved rather easily in most applications likely to be encountered in this particular field of application and (2) owing to the finite population sizes often encountered, more attention should be given the hypergeometric density function, which is the next subject.

Example 2.H

Fifty fuel rods are selected at random and scanned to verify the ^{235}U enrichment. All are verified as having the correct enrichment, i.e., as stated on the inventory listing. If we assume that the total population of fuel rods is very large, what is the upper 99% confidence limit on the proportion of fuel rods that might have the wrong enrichment, based solely on this inspection activity?

Here n equals 50, and x_0, the number of defects or successes, is 0. Since an upper limit is desired, Eq. 2.89 is solved for p, with $\alpha/2$ replaced by $\alpha = 0.01$. There is only one term in the sum, namely, that corresponding to $x = 0$. This term is very simply $(1-p)^n$ or $(1-p)^{50}$. Equate this to 0.01 and solve for p.

$$(1-p)^{50} = 0.01$$

$$(1-p) = (0.01)^{1/50} = 0.912$$

so that

$$p = 1 - 0.912 = 0.088$$

Thus with 99% confidence the true proportion of fuel rods that might have the wrong enrichment is 0.088, or 8.8%, based on the results of the inspection activity.

Suppose now that 120 rods were scanned and one defect were found. What is the 99% upper limit based on these data?

Here n equals 120 and x_0 equals 1. Equation 2.89 is again solved for p, but this time there are two terms in the sum, namely,

$$(1-p)^{120}+120p(1-p)^{119}$$

Factoring out $(1-p)^{119}$ and equating to $\alpha=0.01$, we must solve the following equation for p.

$$(1-p)^{119}(1-p+120p)=0.01$$

or

$$(1-p)^{119}(1+119p)=0.01$$

This equation is most easily solved by trial and error. In the following table, values are assigned to p, and the quantity on the left-hand side of the preceding equation is evaluated. The solution for p occurs at the point where this quantity is equal to 0.01.

p	$(1-p)^{119}(1+119p)$	p	$(1-p)^{119}(1+119p)$
0 08	0 0005	0 055	0.0090
0 05	0 0156	0 053	0 0112
0 06	0 0052	0 054	0 0100

Thus $p=0.054$ is the required solution. With 99% confidence the true proportion of fuel rods that might have the wrong enrichment is 0.054, or 5.4%, based on the results of the inspection activity (i.e., one defect discovered in 120 rods scanned).

(c) *Hypergeometric Density Function*

Attention is restricted to construction of an upper confidence limit on D, the number of defective items in the population of size N. For 100 $(1-\alpha)$% confidence, this requires finding the smallest value of D such that

$$\sum_{x=0}^{x_0} \frac{\binom{D}{x}\binom{N-D}{n-x}}{\binom{N}{n}} \leq \alpha \tag{2.90}$$

where x_0 is the number of observed defects in n total observations.

Again, in most instances of practical concern, x_0 is very small, and it is possible to replace the left-hand side of Eq. 2.90 by approximations that yield solutions for D with very little effort. In particular, solutions are

found for $x_0=0$ and for $x_0=1$. For $x_0=0$, i.e. ,no observed defects, Eq. 2.90 is replaced by

$$\left(1-\frac{2n}{2N-D+1}\right)^D \leq \alpha \tag{2.91}$$

For $x_0=1$, it becomes

$$\left(1-\frac{2n}{2N-D+1}\right)^D \left(1+\frac{nD}{N-D-n+1}\right) \leq \alpha \tag{2.92}$$

The basis for these equations is given in Sec. 9.1.4. Further discussion and applications of the hypergeometric density function as it pertains to the important inspection applications in nuclear materials control are also contained in Chap. 9, which deals with inspection.

Example 2.I

In the examples considered for the binomial case, let the total number of rods in inventory be $N=300$. Then, for $x_0=0$ defects, apply Eq. 2.91 to find the upper 99% confidence limit on D. For $n=50$, find the smallest value of D such that

$$\left(1-\frac{100}{601-D}\right)^D \leq 0.01$$

This is solved by trial and error. The left-hand side of the equation is evaluated for different values of D, and the solution is the largest integral value of D such that this quantity is less than 0.01.

D	$\left(1-\frac{100}{601-D}\right)^D$
25	0.0085
22	0.0154
24	0.0104

Therefore the upper limit on D is 25, since this is the smallest value of D that produces an α smaller than 0.01. Note that $D/N=25/300=0.083$, whereas the corresponding upper limit in the binomial case was 0.088.

If $n=120$ and $x_0=1$, then Eq. 2.92 is solved for D.

$$H(D)=\left(1-\frac{240}{601-D}\right)^D \left(1+\frac{120D}{181-D}\right) \leq 0.01$$

This equation is a bit more formidable than when $x_0=0$ but can still be solved rather easily by trial and error on a desk calculator.

D	$H(D)$
15	0.0044
14	0.0070
13	0.0112

Thus $D=14$ is the upper limit. By comparing this with the result based on the binomial distribution, note that $D/N=14/300=0.047$ whereas the corresponding upper limit in the binomial case was 0.054.

Some comment is in order on the choice of α in constructing confidence intervals. This topic has been avoided thus far except that, in the various examples, confidence intervals of 90%, 95%, and 99% were constructed and thereby left the impression by implication that they are reasonable choices for $100(1-\alpha)\%$.

It is important to note that the choice of α is not a statistical problem; however, the construction of the confidence interval once α is selected is a problem in statistics. In addition, the user who selects a value for α in a given application must be made aware of the implications of this choice. For example, if the user wants to construct a 90% confidence interval, he should recognize that there is one chance in ten that the parameter he has estimated is not contained within the interval. It that good enough? Is it perhaps too good? This is for the user to decide. Of course, there is nothing to prevent the construction of several intervals corresponding to different values for α in a given instance. This gives a more complete picture of just how well the parameter in question has been estimated.

Before we leave the subject of parameter estimation, and, in particular, interval estimation, it is worthwhile to make the distinction between a confidence interval and other statistical intervals, particularly, a tolerance interval and prediction interval. This distinction is as follows:

Confidence interval: An interval that includes a *given parameter* with a specified degree of confidence.

Tolerance interval: An interval that includes *a specified proportion of all population values* with a specified degree of confidence.

Prediction interval: An interval that includes some *specified function of k future observations* from some population with a specified degree of confidence.

Attention in this book is restricted to confidence interval estimation, which is the kind of interval of most interest in nuclear materials control applications.

2.8 HYPOTHESIS TESTING

This aspect of statistical inference plays an important role in nuclear materials control applications. Hypothesis testing involves the following steps:

Step 1. A statement is made about some parameter. This is called the null hypothesis and is denoted by H_0. Examples of null hypotheses include:

a. The true amount of material unaccounted for (MUF, or M) during a given material balance period is zero units. This is written as $H_0: M = 0$ or, possibly, $M \leq 0$.

b. The true shipper–receiver difference, R, for a given shipment of materials is zero units. (H_0: $R = 0$)

c. The true discrepancy, D, between the operator's statement of his inventory and the corresponding statement of an audit team is zero. (H_0: $D = 0$)

d. The true proportion, p, of incorrectly labeled containers in some segment of an inventory is below some amount, p_0. (H_0: $p \leq p_0$)

Step 2. Decisions are made as to how the validity of a given hypothesis will be tested. This involves specifying the data to be collected, the test statistic to be computed, and the range of values for the test statistic which will result in the conclusion that the stated hypothesis is not a valid one.

Step 3. The data are collected, the test statistic is calculated, and the decision is made to reject or not to reject the hypothesis.

A misapplication of hypothesis testing occurs when the hypotheses are formulated after the data are collected. This practice of using data to suggest hypotheses is at variance with the whole idea of hypothesis testing. Once the data have been collected, anyone with an ounce of brains and a lesser amount of integrity, or more charitably stated, "any misguided individual," can formulate hypotheses that will be rejected when tested against the data. The statement is then made that "the data prove that such and such . . .". It is an acceptable practice, of course, to formulate hypotheses based on given data sets, but it is simply not acceptable to test their validity with the same set of data that provided the basis for formulating the hypotheses in the first place.

2.8.1 Definitions of Terms in Hypothesis Testing

In its formal structure, hypothesis testing involves such terms as null and alternative hypotheses, type I and type II errors, α and β probabilities, significance level, critical region, power curve, and one-sided tests. These terms are defined in this section.

A *null hypothesis*, H_0, is established. This is a statement about the value of some population parameter or some function of several parameters either from the same or from different populations. If the hypothesis involves a single value, e.g., H_0: $\mu = \mu_0$, it is called a *simple hypothesis*. If it involves a range of values, e.g., H_0: $\mu \leq \mu_0$, it is called a *composite hypothesis*.

After the data have been collected, the test statistic has been calculated, and a decision has been reached either to reject or to accept H_0, the following possibilities exist:

1. The null hypothesis is actually true, but it has been rejected.
2. The null hypothesis is actually false, but it has been accepted.
3. The null hypothesis is actually true, and it has been accepted.
4. The null hypothesis is actually false, and it has been rejected.

With possibilities 3 and 4, the correct conclusions are reached. If possibility 1 occurs, a *type I error* has been committed, i.e., the null hypothesis has been rejected even though it is true. If possibility 2 occurs, a *type II error* has been committed, i.e., the null hypothesis has been accepted even though it is false.

For a given situation the probability of committing a type I error can be computed. This is designated by α. The α probability is controlled by the experimenter in the sense that the range of values that the test statistic must take on to result in the rejection of the null hypothesis, called the *critical region*, is defined so as to achieve the desired value for α. (What value should be chosen for α? In many applications, α is chosen to be 0.05, and the reader may have formed the impression that this is a magic value. It is not. See the closing comments in Sec. 2.7 dealing with the choice of α in constructing confidence limits. The same sort of comments might well be made here.) The α is also called the *significance level* of the test. The type I error is sometimes loosely referred to as the α error. This is poor practice; α is a probability, not an error.

The probability of committing a type II error is designated by β. A value for β is meaningful only when it is related to an *alternative hypothesis*, which is a value outside the region designated by H_0 for the parameter in question. A specified alternative hypothesis is usually designated by H_1 or H_A. Because of the relation between β and H_1, it is instructive to calculate β for various values of H_1. This evaluates the ability of the test in question to reject a given hypothesis when it is false for a range of such alternative hypotheses. The plot of $(1-\beta)$ versus H_1 is called a *power curve*. If the range

of the alternative hypothesis includes values of the parameter on both sides of the null hypothesis, the hypothesis test is a *two-sided* test. This occurs, for example, if H_0: $\mu=\mu_0$ against the range of values for H_1: $\mu\neq\mu_0$. If, in this example, H_0: $\mu\leq\mu_0$, then the range of values for H_1 is $\mu>\mu_0$, and the corresponding test is called a *one-sided* test. Figure 2.4, a sketch related to a one-sided test is helpful in clarifying some of the preceding ideas.

For the two-sided test with a simple hypothesis, the sketch is similar except that the power curve reaches the minimum value of α at H_0. Examples of statistical hypothesis testing are contained throughout the book, particularly in the next section, Sec. 2.9. Although the main purpose of this section is to introduce the concepts and terminology, a simple example at this point can help fix the ideas discussed. The example also shows how the test design is influenced by the values assigned the various test parameters.

Example 2.J

A number of samples of UO_2 powder from a given batch are to be measured for percent uranium. In practice a standard factor of 87.60% is used for UO_2 powder, but, if the true factor for a given batch of powder is as low as 87.55%, this must be detected with a probability of 0.80 and the new factor must be used for the batch in question. On the other hand, if the true factor for the batch in question does not differ from 87.60%, it

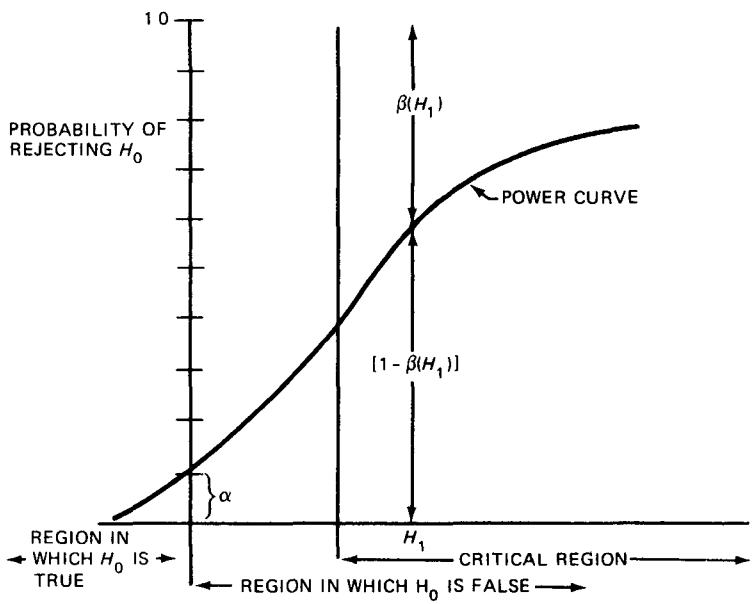

FIGURE 2.4 Power curve.

is desired to use the standard factor of 87.60%; the new estimated factor should be used with a probability of <0.02 in this instance. It is known that the standard deviation of a given observation is 0.04 percentage points. Design the test procedure to accomplish this, i.e., find the sample size and the critical region Assume that the random variable is normally distributed.

With μ the true concentration factor for the batch in question and $\bar{x}$ the estimated factor based on n samples, the various test parameters are identified as follows:

H_0: $\mu \geq 87\ 60$*	The true percent uranium for the batch equals or exceeds 87.60%.
H_1: $\mu = 87.55$	The true percent uranium corresponding to the stated alternative hypothesis.
$\alpha = 0.02$	When $\mu = 87.60\%$, H_0 should be rejected with a probability of 0.02.
$\beta = 1 - 0.80 = 0.20$	When $\mu = 87.55\%$, H_0 should be rejected with a probability of 0.80 or accepted with a probability of 0.20.
$\sigma = 0.04$	The known standard deviation of a single observation.

This is a one-sided test. The null hypothesis is rejected if $\bar{x} < c$, where c defines the critical region and $\bar{x}$ is the sample mean which estimates the true mean, μ.

Since $\alpha = 0.02$, c must be chosen to satisfy the equation

$$\Pr(\bar{x} < c \mid \mu = 87.60) = 0.02$$

i.e., when the true batch mean is 87.60%, the probability that H_0 is rejected is 0.02; H_0 is rejected when $\bar{x} < c$.

Also, to satisfy the requirements on β,

$$\Pr(\bar{x} < c \mid \mu = 87.55) = 0.80$$

i.e., when the true batch mean is 87.55%, the probability that H_0 is rejected is 0.80.

These two equations are solved simultaneously for c and n (which appears implicitly in $\bar{x}$) by standardizing each and using Eq. 2.43. To standardize, we subtract the mean and divide by the standard deviation. The mean of $\bar{x}$ is 87.60 in the first equation and 87.55 in the second. The standard deviation of $\bar{x}$ is $\sigma/\sqrt{n} = 0.04/\sqrt{n}$ (by Eq. 2 58).

* In practice a two sided test would be more reasonable in this example. However, a one-sided test is used at this point in the discussion to avoid unnecessary complications in the arithmetic

The first equation is

$$\Pr\left(\frac{\bar{x}-87.60}{0.04/\sqrt{n}}<\frac{c-87.60}{0.04/\sqrt{n}}\right)=0.02$$

or

$$\Pr\left[z<\frac{(c-87.60)\sqrt{n}}{0.04}\right]=0.02$$

where z is a standardized normal random variable. From Appendix A,

$$\frac{(c-87.60)\sqrt{n}}{0.04}=-2.054$$

since the area from $-\infty$ to -2.054 under the standardized normal density curve is 0.02.

The second equation is handled similarly:

$$\Pr\,(\bar{x}<c\,|\,\mu=87.55)=\Pr\left[z<\frac{(c-87.55)\sqrt{n}}{0.04}\right]=0.80$$

From Appendix A,

$$\frac{(c-87.55)\sqrt{n}}{0.04}=0.842$$

since the area from $-\infty$ to 0.842 under the standardized normal density curve is 0.80.

The two equations are solved simultaneously for c and n. The first becomes

$$\sqrt{n}=\frac{(0.04)(-2.054)}{c-87.60}=\frac{-0.08216}{c-87.60}$$

and the second becomes

$$\sqrt{n}=\frac{(0.04)(0.842)}{c-87.55}=\frac{0.03368}{c-87.55}$$

After equating the right-hand sides of these equations to eliminate n, the equation in c becomes

$$-0.08216\,(c-87.55)=0.03368\,(c-87.60)$$

or

$$c=\frac{10.14348}{0.11584}=87.565$$

from which

$$n=\left(\frac{0.03368}{0.015}\right)^2=5.04 \qquad \text{(or 5)}$$

Thus the test procedure is to draw a sample of 5 observations and compute the mean, $\bar{x}$. If $\bar{x} < 87.565\%$, reject H_0; i.e., conclude that the standard factor of 87.60% should not be used for the batch in question.

2.8.2 Control Charts

In the example just concluded, a test was made of the hypothesis that the percent uranium in a given batch of UO_2 powder is not different from some standard value, where the standard value is presumably based on past experience. This is a situation in which the test would be performed for each batch. That is, a series of hypothesis tests would be made corresponding to the batches as they are created.

In this instance the successive hypothesis tests are related to one another in the sense that the sample size is constant from batch to batch, as is the critical region. This suggests that the hypothesis testing procedure can be simplified since the critical region need not be determined for each test. When the simplification is accomplished by plotting the successive batch means as a function of time and noting whether or not each mean falls in the critical region, the resulting plot is called a control chart. (This discussion on control charts is very limited. Once the reader understands, however, that a control chart and a test of hypothesis are equivalent, he can construct control charts of many kinds, e.g., on sample variances.)

A standard control chart on sample means is simple to construct. The construction involves determining the null hypothesis value, μ (the standard factor of 87.60% in the preceding example), the known standard deviation of a sample average, σ, and the critical region, defined by what are called control limits in control chart terminology.

The proper value to use for σ is covered in detail in Chap. 3. At this point in the development, it suffices to say that σ is the standard deviation that describes the dispersion of successive $\bar{x}$ values when a state of control exists, i.e., when the true batch means are constant.

The control limits are of the form $(\mu \pm k\sigma)$ for a two-sided test, with either the plus or minus sign disregarded in a one-sided test. The constant, k, depends on the significance level of the test. In the previous example, it was seen that at a significance level of 0.02, or 2%, and with a one-sided test, k is 2.054. For other significance levels, the appropriate value for k may be read from Appendix A. For a one-sided test, k is read directly from the table corresponding to a given α. For a two-sided test, the significance level, α, must be divided by two before finding k. For example, if the significance level for a two-sided test is $\alpha = 0.05$, k is found from Appendix A as the value that corresponds to 0.025 (i.e., a tabular entry of 0.975), which is 1.96.

Although the appropriate k may be read from Appendix A, this degree of refinement is often not used in the practical application of control charts.

Rather, it is customary in many occasions to simply choose $k=3$ and use $(\mu \pm 3\sigma)$ as the control limits. This procedure has the advantage of simplicity in construction and ensures that a plotted point that is out of control (i.e., falls in the critical region defined by the control lines) constitutes rather strong evidence that the true mean for the batch in question is really different from μ. (At $k=3$, with a two-sided test, the α value is only 0.0026, which means that only 0.26% of the time will a point fall out of control because of chance alone.) Although each application of control charts should be examined to see if the use of $k=3$ is appropriate or if a different value should be used, a choice of $k=3$ should prove to be satisfactory in many nuclear materials control applications.

Example 2.K

Construct a control chart for the average percent uranium in batches of UO_2 powder. Assume that the standard factor, μ, is 87.60%, and use $\sigma=0.06\%$ (absolute percent). Then plot the batch averages for the following 19 batches and determine whether there is any significant shift from the standard factor.

87.54	87.56	87.47	87.72
87.56	87.71	87.60	87.77
87.50	87.61	87.69	87.79
87.47	87.60	87.78	87.78
87.64	87.60	87.69	

The two-sided control limits are of the form $(\mu \pm k\sigma)$. With a k value of 3, these limits are

$$87.60 \pm 3(0.06) = 87.42 - 87.78$$

The control chart, Fig. 2.5, shows the plotted batch averages. The circled points fall on or beyond the upper control limit; this indicates that the true means for the batches in question are greater than 87.60%. In fact, it appears that the means for all the last few batches have shifted, even though not all the individual batch means are out of control.

It should be evident from this example that an out-of-control situation can occur for more than one reason. For example, it may be that the mean for only a single batch is high (or low) for some reason. Or it may be (as appears to be the case in this example) that the mean of several successive batches has shifted, although the shift might be small enough that it is not detected for several batches.

Although a moderate shift in the overall mean will be detected eventually by a standard control chart, other means for detecting such a shift also have some appeal. One such means is the cusum chart, or cusum plot.

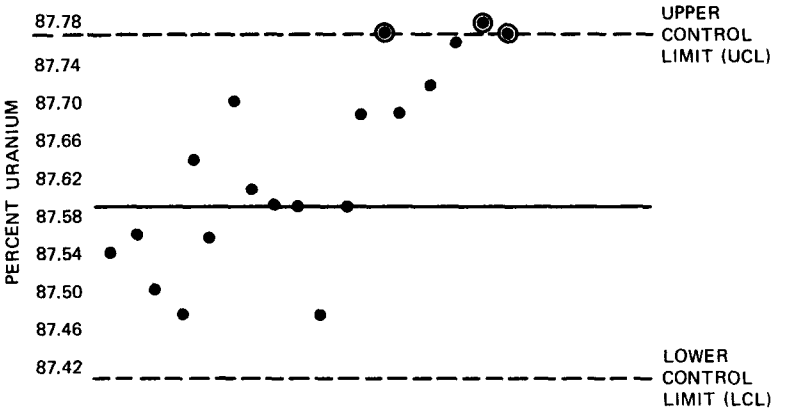

FIGURE 2.5 Control chart on batch average percent uranium values.

2.8.3 Cusum Plot

The cusum plot is ideally suited for detecting shifts. Although formal means exist for constructing control limits for use with cusum plots, their formal construction is beyond the scope of this book. Rather, the cusum plot is introduced very briefly here as a method of plotting data. This is especially useful because of the visual impact created by shifts in the mean. With such a plot, just where the mean may have changed in value can be pinpointed rather precisely.

This is best illustrated by presenting the data of the previous example as a cusum plot. "Cusum" stands for "cumulative sum". The values plotted are the successive sums of $(\bar{x}-\mu)$ values. The calculations for the cusum

TABLE 2.11 CUSUM VALUES FOR BATCH AVERAGE PERCENT URANIUM

Batch	$\bar{x}$	$(\bar{x}-87.60)$	Cusum	Batch	$\bar{x}$	$(\bar{x}-87.60)$	Cusum
1	87.54	−0.06	−0.06	11	87.47	−0.13	−0.34
2	87.56	−0.04	−0.10	12	87.60	0.00	−0.34
3	87.50	−0.10	−0.20	13	87.69	0.09	−0.25
4	87.47	−0.13	−0.33	14	87.78	0.18	−0.07
5	87.64	0.04	−0.29	15	87.69	0.09	0.02
6	87.56	−0.04	−0.33	16	87.72	0.12	0.14
7	87.71	0.11	−0.22	17	87.77	0.17	0.31
8	87.61	0.01	−0.21	18	87.79	0.19	0.50
9	87.60	0.00	−0.21	19	87.78	0.18	0.68
10	87.60	0.00	−0.21				

FIGURE 2.6 Cusum plot.

plot are shown in Table 2.11, and the cusum values are plotted in Fig. 2.6. A shift in an overall mean is reflected by a change in the slope of the plotted points. Although a formal test of significance has not been made, it is evident from this plot that a shift in the mean occurred with the last 7 to 8 batches. This indication of a shift is often all that is required in practice; i.e., formal tests of significance may not contribute much additional justification for taking some kind of action, such as changing the value for a standard factor in this instance.

2.9 TESTING DISTRIBUTIONAL ASSUMPTIONS

The final topic in this chapter deals with a few specific techniques for testing the validity of certain assumptions made in using sampled data to make inferences about the corresponding population. The following types of perturbations may occur and hence invalidate the results of the statistical analysis:

1. One or more of the sample values may be an "outlier" in the sense that it is questionable whether or not it can be considered to be a member of the population it is represented to be.

2. There may be a lack of "randomness" in the data; this suggests either that the population parameter(s) are shifting or that the sample selection method is creating nonrandomness.

3. A random variable may be assumed to be normally distributed when, in actual fact, the density function differs from the normal function in some respect or respects.

Each of these three situations is a major topic in itself and can be treated only rather briefly. The main purposes are to warn the reader to be aware of the possible discrepancies between assumptions that are made and the actual situation that may obtain and to call attention to some statistical tests that may be used profitably.

2.9.1 Test for Outliers

Much has been written on this subject. There are two quite distinct aspects to the problem: how to detect outliers objectively and how to treat them, once detected. Only the first problem is covered here, even though the second is equally, if not more, important. (A detected outlier is evidence of some difficulty and should, at least, be investigated to determine the cause or causes. When an experimenter is too zealous in indiscriminately ignoring "discrepant" observations, this results in a biased picture of reality.)

A number of statistical tests have been suggested to identify outliers. Only the simplest situation is considered here, namely, that in which there is a single random variable and one population density function. Further, it is assumed that this population density function is the normal function with variance not known and that only a single observation is suspect. Although this is a simple situation, it is commonly encountered.

The so-called "T_n test" is applicable in this instance. To perform this test, order the sample values so that $x_1 < x_2 \ldots < x_n$, where n is the size of the sample. Then, calculate $\bar{x}$ and s^2 by Eqs. 2.56 and 2.60 or Eq. 2.61, using *all* the data, including the suspect observation. Let the suspect observation be the largest one. The T_n statistic is computed.

$$T_n = \frac{x_n - \bar{x}}{s} \tag{2.93}$$

The hypothesis is that x_n *is* from the population. If T_n exceeds the critical value given in Appendix E at the α significance level, this hypothesis is rejected; i.e., x_n is labeled an outlier.

The table is constructed so that critical values are shown for a one-sided test, i.e., in the case where suspect observations are always either on the high side or on the low side. For the more common situation in which an outlier may be either too large or too small, the column headings should be multiplied by two. Thus, in this instance, for $\alpha = 0.10$, the column for the 5% significance level in Appendix E should be used; for $\alpha = 0.05$, the column for the 2.5% significance level is applicable; and for $\alpha = 0.02$, the column for the 1% significance level applies.

If the suspect observation is on the low side, the test statistic is

$$T_1 = \frac{\bar{x} - x_1}{s} \tag{2.94}$$

Example 2.L

For the data of example 2.F in Sec. 2.7.2, assume that the fourth observation is suspect. Perform the outlier test at the $\alpha = 0.02$ level (two-sided test).

For this example, from the previous calculations,

$$\bar{x} = 87.625 \qquad \text{and} \qquad s = 0.0313$$

Also, for the ordered data, $x_1 = 87.571$ (the smallest value) so that the test statistic, T_1, is given by Eq. 2.94. This observation will be detected as an outlier if $T_1 > 1.75$, from Appendix E ($n = 5$; 1% significance level).

$$T_1 = \frac{87.625 - 87.571}{0.0313}$$

$$= 1.725$$

Since $T_1 < 1.75$, the critical value, the observation in question is not detected as an outlier.

2.9.2 Tests for Randomness

Any set of data is ordered with respect to time, i.e., x_1 is the first observation drawn, x_2 is the second, etc. If the population from which the samples are drawn is not stable over time, or if the sample selection method does not produce a random sample, there may be significant evidences of nonrandomness in the data. It is important to have some means of detecting nonrandomness because all statistical inference is built on the idea of a random sample.

As with tests for outliers, there are a large number of available statistical tests that can be used to test for nonrandomness. One difficulty here is that the alternative hypothesis is not a simple one; i.e., there are many ways in which data could be nonrandom. The best test to use in any instance depends partly on the kind of nonrandomness that might be present. It is not possible to discuss all such tests that have been proposed. Only two very simple ones are covered here, both of which are "runs" tests.

Before discussing the tests, however, we should note that a simple plot of the ordered data can be very instructive in identifying nonrandomness. The cusum plot of Sec. 2.8.3 might also be used profitably. On occasion, a plot will be so revealing that more objective tests are not needed.

If the plot is not conclusive, however, we can resort to one of the following tests or to others that have been proposed.

(a) *Runs Above and Below Median*

The median is calculated for the data in question. The number of runs, r, above and below the median is counted. (If the data are plotted and the data points connected by straight-line segments, then r is one more than the number of times the median line is intersected.) Under the hypothesis that the data are random, r has mean and variance given by

$$E(r) = 0.5n + 1 \tag{2.95}$$

$$\sigma_r^2 = \frac{n(n-2)}{4(n-1)} \tag{2.96}$$

where n is the total number of data points. For $n > 25$, it can be assumed with validity that r is normally distributed.

The significance test is two-sided, since either too few or too many runs give evidence of nonrandomness. For given α, the critical values c_1 and c_2 can be found from

$$\Pr\,(r < c_1 \mid H_0 \text{ true}) = \frac{\alpha}{2} \tag{2.97}$$

$$\Pr\,(r > c_2 \mid H_0 \text{ true}) = \frac{\alpha}{2} \tag{2.98}$$

where "H_0 true" means that $E(r)$ and σ_r^2 are given by Eqs. 2.95 and 2.96, respectively. Thus c_2 is that value which is exceeded by the observed number of runs with a probability of $\alpha/2$ when, in fact, the data are random, and c_1 is similarly defined.

Example 2.M

Diffusion plant monthly MUF data are given in Table 2.1. Apply the *Runs Above and Below Median* test to these data to test for nonrandomness. Use $\alpha = 0.05$.

Here $n = 144$ so that under the hypothesis, H_0, we compute $E(r)$ and σ_r^2. From Eq. 2.95,

$$E(r) = (0.5)(144) + 1 = 73$$

and from Eq. 2.96,

$$\sigma_r^2 = \frac{(144)(142)}{(4)(143)} = 35.75$$

so that

$$\sigma_r = \sqrt{35.75} = 5.98$$

The value of c_1 is determined from Eq. 2.97. Once again the random variable is transformed to the standardized normal by subtracting the mean and dividing the difference by the standard deviation.

$$\Pr\left[r<c_1 \mid E(r)=73 \text{ and } \sigma_r=5.98\right]=\Pr\left(\frac{r-73}{5.98}<\frac{c_1-73}{5.98}\right)=\frac{\alpha}{2}=0.025$$

From Appendix A,

$$\frac{c_1-73}{5.98}=-1.96$$

This last equation follows since the area under the standardized normal curve from $-\infty$ to -1.96 is 0.025.

The solution for c_1 is

$$c_1=73-(1.96)(5.98)=61.28$$

Similarly,

$$c_2=73+(1.96)(5.98)=84.72$$

The decision rule then is to reject H_0 (conclude the data are nonrandom) if $r\leq 61$ or if $r\geq 85$ runs.

The number of runs, r, is counted. From Sec. 2.1, it was found earlier that the median for this set of data is 188.5. This median line is crossed 87 times, as the reader can verify, so the observed r is 88. Since this exceeds the critical value of 85, it is concluded that the MUF data are nonrandom. The reason for this in this example is discussed in Chap. 7.

(b) Runs Up and Down

The second run test discussed does not require determining the median. Rather, for the ordered data, if $x_{i+1}>x_i$, a "+" is recorded, and, if $x_{i+1}<x_i$, a "−" is recorded. A run then consists of a sequence of +'s or −'s.

Let the number of runs of this type be denoted by U. Then, under the hypothesis of randomness,

$$E(u)=\frac{2n-1}{3} \tag{2.99}$$

and

$$\sigma_u^2=\frac{16n-29}{90} \tag{2.100}$$

Again, normality may be assumed for large n, say $n>25$, and the test is set up as for the other run test. The test is again two-sided.

Example 2.N

Consider the diffusion plant MUF data. With this run test,

$$E(u) = \frac{288-1}{3} = 95.67 \qquad \text{(from Eq. 2.99)}$$

and

$$\sigma_u^2 = \frac{(16)(144)-29}{90} = 25.28 \qquad \text{(from Eq. 2.100)}$$

Therefore

$$\sigma_u = \sqrt{25.28} = 5.03$$

The lower critical value, c_1, is determined. Again, setting $\alpha = 0.05$, this gives

$$\frac{c_1 - 95.67}{5.03} = -1.96$$

or

$$c_1 = 95.67 - (1.96)(5.03) = 85.81$$

Similarly,

$$c_2 = 95.67 + (1.96)(5.03) = 105.53$$

The decision rule is to reject H_0 if $u \leq 85$ or if $u \geq 106$ runs.

The number of runs is now counted. The first few counts are shown to demonstrate the procedure.

MUF	Sign of successive difference
− 358	
−3287	−
5798	+
−4115	−
616	+
−2825	−
1287	+
−1619	−
394	+
.	.
.	.
.	.

(There are 8 runs for these observations.)

For the entire data set, the number of runs is 104, as we can verify. Since $104 < 106$, the hypothesis of randomness is not rejected with this particular run test.

Although the two run tests are similar with respect to the types of nonrandomness they detect, they are not identical. It is not surprising, therefore, that one test should reject the hypothesis, while the other fails to reject it, although with these data the critical value was just barely exceeded in the first instance and was almost exceeded in the second.

In actual application, more than one test of randomness can be used. This introduces the problem of what is the actual significance level of the test procedure. It is difficult to calculate this since the various tests are not independent. Since the significance level is somewhat arbitrary in many instances anyway, this concern is not usually a major practical one.

2.9.3 Test for Normality

Again, a large number of tests have been suggested to test whether or not the population in question is normal. As with other tests of validity of distributional assumptions, the best test to use depends in part on the nature of the alternative hypothesis, i.e., on the type of nonnormality that may exist.

One test is discussed here, the "W test" for normality. This test is chosen because it is effective against different types of nonnormality. The W test may be used for sample sizes less than 50.

The W test is applied as follows:

Step 1. Order the data so that $x_1 < x_2 \ldots < x_n$.

Step 2. Compute $(n-1)s^2$ with s^2 given by Eq. 2.53 or Eq. 2.61, and where n is the sample size.

Step 3. Compute

$$b = a_n(x_n - x_1) + a_{n-1}(x_{n-1} - x_2) + \ldots + a_{n-k+1}(x_{n-k+1} - x_k) \tag{2.101}$$

where $k = n/2$ for even n and $k = (n-1)/2$ for odd n and where the a_i coefficients are given in Appendix F.

Step 4. Compute the test statistic

$$W = \frac{b^2}{(n-1)s^2} \tag{2.102}$$

Step 5. Reject the hypothesis of normality if W is less than the critical value given in Appendix G at a given $\alpha(=P)$ level.

Example 2.O

Percent uranium values for 17 cans of ADU (ammonium diuranate) scrap are as follow:

35.5	78.2	29.4
79.4	37.1	29.8
35.2	48.4	28.4
40.1	28.6	23.4
25.0	75.5	77.0
78.5	34.3	

Is there evidence of nonnormality for these data? Use a significance level of $\alpha = 0.01$.

Let us follow the five previously mentioned steps:

Step 1. The ordered data are

23.4	34.3	75.5
25.0	35.2	77.0
28.4	35.5	78.2
28.6	37.1	78.5
29.4	40.1	79.4
29.8	48.4	

Step 2. $$(n-1)s^2 = (23.4)^2 + \ldots + (79.4)^2 - \frac{(23.4 + \ldots + 79.4)^2}{17}$$
$$= 7625.55$$

Step 3. $$b = 0.4968(79.4 - 23.4) + 0.3273(78.5 - 25.0)$$
$$+ 0.2540(78.2 - 28.4) + 0.1988(77.0 - 28.6)$$
$$+ 0.1524(75.5 - 29.4) + 0.1109(48.4 - 29.8)$$
$$+ 0.0725(40.1 - 34.3) + 0.0359(37.1 - 35.2)$$
$$= 77.1796$$

Step 4. $$W = \frac{(77.1796)^2}{7625.55}$$
$$= 0.781$$

Step 5. At $\alpha = P = 0.01$, for $n = 17$, the critical value is 0.851. Since $0.781 < 0.851$, reject the hypothesis and conclude that there is evidence of nonnormality.

Chapter 3

SOURCES OF UNCERTAINTY IN NUCLEAR MATERIALS CONTROL

OVERVIEW

Measurements form the backbone of a nuclear materials control system. For example, when material is transferred from one responsible custodian to another, it is measured; when material is inventoried, it is measured; and when an audit inspection is made, measurements are performed.

If a measured value were always equal to the true value of the item being measured, there would be no need for a book such as this. This is not to say that the problems associated with the control of nuclear materials would disappear, because decisions would still be required, for example, on the part of management or a regulating agency, as to how much "true" material unaccounted for (MUF) is tolerable in a given situation. However, against a backdrop of uncertainties due to measurement, the control problems are greatly multiplied. This is especially true in the control of nuclear materials because the measurement problems are not trivial by any means; the "noise level" is moderately high.

Chapter 3 is concerned with the concept of a statistical "error" associated with a measured value. An error of measurement can be defined as the magnitude and the sign of the difference between a measured value and the corresponding true value. It is important to distinguish between an error and a mistake. A measurement *error* is committed because of limitations of the measurement system. (Although it is standard terminology to speak of an error as being committed, there is no intent to disparage the operator with this expression, i.e., to imply that the resulting error occurs because of poor work or a deliberate act on his part. Rather, an error is committed as a result of an inherent property or limitation of the measurement process.) A *mistake* is made when the operator of the system either does not use the system properly in a given instance or does not record properly the value produced by the system (e.g., he transposes numbers).

It is very difficult to factor the effects of *mistakes* into an analysis because of their unpredictability, with respect to both size and frequency.

This problem was touched on briefly in Sec. 2.9.1 dealing with the detection of outliers that might result from mistakes. Further, in Chap. 9, on inventory verification, an important part of the inspection activities is centered around ensuring that the frequency of mistakes, evaluated against a background of measurement errors, is below a tolerable level. Little else can be done. (This is true from point of view of detection and correction of mistakes. However, management can take positive steps to minimize the number of mistakes. An excessive frequency of human mistakes can render ineffectual an otherwise sound system of control based on a solid measurement and data-handling system.)

It is possible, however, to deal with *errors* of measurement, measurement being used in its broadest meaning to include all sources of error that might affect the quality of a final measured value. Except for a bias an error can be regarded as an observation on a random variable. This is a simple but very important concept to remember. Once understood, the whole discussion on measurement errors should become quite clear. (A looseness in terminology has contributed to some of the confusion that exists. Thus we hear the expression "the measurement error is such and such," which in fact means that the standard deviation of the density function for the error random variable in question is such and such. Thus it is more appropriate to speak of the measurement error standard deviation than simply the measurement error, to emphasize that we do not know the value of the particular error but only the population density function from which the particular error value was drawn.) Thus for each error there is an associated population probability density function, with parameters whose values may or may not be known.

A given observation will, in general, be affected by several individual errors, each drawn from a different population. Some of these error sources are identified; others may not be. The effects of some can be combined and described by one broad error source. In modeling to account for the various error sources that might affect the value of an observation, ideally we endeavor to identify and evaluate the effects of all these sources individually. However, the ideal goal is, for the most part, a physical impossibility. Rather, we group error sources and identify the principal error sources, where an error source is classified as principal either because of the magnitude of the error standard deviation or because of the importance of the operation involved, or for both reasons. Thus the error introduced by the weighing operation, for example, although it may not have a great effect on the size of the total error variance, is generally included in the analysis because of the significance of the weighing operation in nuclear materials control measurements.

This chapter deals specifically with identification of the principal error sources considered in this book and with methods for estimating the appropriate error variances. Subsequent chapters deal with using the results

to make inferences of particular concern and interest in the control of nuclear materials.

Section 3.1 deals with the basic categories, or types, of errors; Sec. 3.2 identifies the error sources treated in subsequent chapters; Sec. 3.3 discusses methods for estimating error variances.

3.1 BASIC ERROR CATEGORIES

Many discussions have taken place in the past, and will quite likely continue to take place in the future, in attempting to reach agreement on the definitions and statistical treatment of different basic types or categories of errors. In particular, opinions differ on the meanings of such terms as *bias*, *random errors*, and *systematic errors*. The definition presented here describes how these terms are used in this book and, by implication, indicates the only reasonable way the error effects can be treated statistically. The definition is very simple but all inclusive in that all terms are included in the same definition. This permits making the distinction among the various terms. Basic to the definition is the idea of a reference set of data, i.e., the definition is meaningful only with regard to this data set.

Definition: An error that affects only a single member of a given data set is called a *random error*. If the error affects some, but not all, members of the data set, it is called a *short-term systematic error*. If it affects all members of the data set, it is a *long-term systematic error* or a *bias*.

In this definition no distinction is made between a long-term systematic error and a bias because these quantities differ with respect to how they may be treated statistically but not with respect to their basic meanings. (In a general sense we can also speak of a short-term bias that affects some but not all the members of the data set. This has the same relationship to a short-term systematic error as bias has to a long-term systematic error.) The statistical treatment depends on the degree of information we have about the error. If the magnitude and direction of the error are known, the error is a *known bias*, and the data presumably are corrected accordingly. If this information is not known, we can describe the effects of the error by regarding it as a random observation from some population of errors. This population should normally have a mean of zero and a standard deviation related to the expected magnitude of the error. This standard deviation is called a long-term systematic-error standard deviation. In a more general sense, the population mean might not be zero. This would be true if a known bias were present but the data were not corrected for some reason, perhaps because of the small size of this bias.

Example 3.A

Assume that the data set in question consists of a number of obser-

vations on percent ^{235}U for UO_2 powder as measured with a mass spectrometer. Each measurement consists of the following:

1. A sample of UO_2 powder (all samples at nominally the same enrichment, designated by μ).
2. A particular mass spectrometer on which to measure the sample.
3. A particular operator to run the sample.

Assume the existence of a population density function to describe the error due to sampling the UO_2, one to describe the differences that exist among mass spectrometers, one to describe the differences that exist among operators, and one to describe the combined effects of all other errors that might affect the reported result. Further, assume that each density function has mean zero and that a known mass-discrimination bias, θ, affects all observations. (The mass-discrimination bias is an inherent feature of many mass spectrometers, and estimation of this bias is a part of the calibration procedure.)

$\epsilon_i = i$th error selected at random from the population of sampling errors

$\eta_j = j$th error selected at random from the population of mass-spectrometer errors (i.e., it describes differences among mass spectrometers)

$\beta_k = k$th error selected at random from the population of operator errors (i.e., it describes differences among operators)

$\omega_l = l$th error selected at random from the population of all other errors

Denote the variances of the population density functions by σ_ϵ^2, σ_η^2, σ_β^2, and σ_ω^2, respectively.

Let the data set in question consist of a single observation, and assume an additive model in the sense that the total error in the observation that occurs as a result of the individual errors is found by algebraically summing these individual errors. This single observation may then be written as

$$y_{1111} = \mu + \theta + \epsilon_1 + \eta_1 + \beta_1 + \omega_1 \tag{3.1}$$

where, by definition, μ is the true percent of ^{235}U, θ is a known bias for the the data set, and the errors ϵ_1, η_1, β_1, and ω_1 can be called either random errors or long-term systematic errors because they each affect only a single member of the set or they also affect all members of the set, whichever viewpoint is taken. There is no distinction for this data set consisting of a single observation.

Now let the data set consist of two observations, consisting of two separate UO_2 samples, both measured on the same mass spectrometer by the same operator. Thus we now have selected two observations at random from the ϵ and ω populations and one from the η and β populations.

These two data points are written as

$$\begin{aligned} y_{1111} &= \mu+\theta+\epsilon_1+\eta_1+\beta_1+\omega_1 \\ y_{2112} &= \mu+\theta+\epsilon_2+\eta_1+\beta_1+\omega_2 \end{aligned} \tag{3.2}$$

where, by definition, θ is a known bias, the errors ϵ_1, ϵ_2, ω_1, and ω_2 are random errors since each affects only a single member of the set, and η_1 and β_1 are both long-term systematic errors since each affects all members of the set.

As the final illustration, suppose now that there are six total observations in the data set. Each pair of observations consists of measurements on the same sample, i.e., there are three UO_2 samples with duplicate measurements on each. All measurements are made on the same mass spectrometer, but two operators make the measurements—operator 1 for observations 1, 2, 4, and 6 and operator 2 for measurements 3 and 5. Then the six observations appear as follows:

	True $\%\ ^{235}U$	Mass-discrimination bias	UO_2 sample	Instrument	Operator	Random errors
y_{1111}	μ	$+\theta$	$+\epsilon_1$	$+\eta_1$	$+\beta_1$	$+\omega_1$
y_{1112}	μ	$+\theta$	$+\epsilon_1$	$+\eta_1$	$+\beta_1$	$+\omega_2$
y_{2123}	μ	$+\theta$	$+\epsilon_2$	$+\eta_1$	$+\beta_2$	$+\omega_3$
y_{2114}	μ	$+\theta$	$+\epsilon_2$	$+\eta_1$	$+\beta_1$	$+\omega_4$
y_{3125}	μ	$+\theta$	$+\epsilon_3$	$+\eta_1$	$+\beta_2$	$+\omega_5$
y_{3116}	μ	$+\theta$	$+\epsilon_3$	$+\eta_1$	$+\beta_1$	$+\omega_6$

(3.3)

In this example, θ is a known bias; ϵ_1, ϵ_2, ϵ_3, β_1, and β_2 are short-term systematic errors; η_1 is a long-term systematic error; ω_1, ω_2, ω_3, ω_4, ω_5, and ω_6 are all random errors. This example shows that some observations from a given error population may be classified as random errors (affecting one data point) and some as short-term systematic errors (affecting two or more data points). To avoid the confusion that would result from this, adopt the convention that if one (or more) observation from a given population is a short-term systematic error, then the corresponding population variance is called a short-term systematic-error variance. Thus with refer-

ence to Eq. 3.2, rather than saying that ϵ_1, ϵ_2, ω_1, and ω_2 are random errors whereas η_1 and β_1 are long-term systematic errors, say that σ_ϵ^2 and σ_ω^2 are random-error variances whereas σ_η^2 and σ_β^2 are long-term systematic-error variances. Similarly, in Eq. 3.3, σ_ω^2 is a random-error variance, σ_ϵ^2 and σ_β^2 are short-term systematic-error variances, and σ_η^2 is a long-term systematic-error variance.

3.2 ERROR SOURCES IN NUCLEAR MATERIALS CONTROL APPLICATIONS

The simple example just concluded suggests that there are many error sources which can conceivably affect an observed value. Clearly, it is a physical impossibility to identify and account for all potential error sources in routine analyses of data. This does not imply that the contributions from some error sources are ignored but rather that they are combined with others to result in principal error sources.

To emphasize this point, let us consider a measurement situation discussed by R. A. Schneider in a teaching outline used at the Argonne School of Safeguards, Argonne National Laboratory (this teaching outline has not been documented, and no specific reference can be cited). The total uranium in a process tank is to be determined by measuring the volume in the tank with a dip-tube manometer system and then measuring the concentration for a sample drawn from the tank. In calculating the total amount of uranium in this fashion, Schneider identifies seven sources of random error and ten sources of systematic error associated with a single observation. These are listed in Table 3.1.

TABLE 3.1 SOURCES OF ERROR IN MEASUREMENT OF TOTAL URANIUM IN A PROCESS TANK

Random-error sources	Systematic-error sources*
Reading the manometer	Uncertainty in volume calibration curve
Measuring the specific gravity	Fixed errors in measuring specific gravity
Distinguishing the titration end point	Normality of titration
Pipetting the sample	Pipet calibration
Reading the buret liquid level	Buret calibration
Sampling the solution (due to imperfect mixing)	Sampling equipment
Sampling the solution (due to presence of solids)	Consistent sampling errors due to presence of solids
	Titratable impurities in sample
	Persistent temperature effects on manometer fluid
	Specific gravity changes in manometer fluid

* In a given context some of these will lead to short-term systematic errors, and some to long-term systematic errors.

With so many sources affecting a single measurement and with so many measurements affecting quantities of interest in the control of nuclear materials, such as MUF, it is evident that we must strike a balance between the amount of detail that can be separately identified and included in an analysis and what is practical.

The amount of detail that should be included in a given data analysis depends upon the motivation for the analysis. If a study of measurement systems is being made to identify and evaluate many error sources, considerable detail will obviously be required. On the other hand, if the problem is one of testing for the significance of a given MUF, the analysis will be less detailed.

The major interest in this book centers on techniques for routine analyses of data, primarily as they affect the interpretation of MUF and shipper–receiver data and the verification of inventories. Therefore there is a limit on the amount of detailed error analysis that can be performed profitably. The amount of detail used in subsequent chapters is described in the following paragraph.

Five basic types of measurement operations are identified: weighing, volume determination, sampling, analysis, and nondestructive assay (NDA). The sampling and analysis operations are defined separately with respect to the element (uranium or plutonium) and the isotope (^{235}U or fissile plutonium). Associated with each measurement operation is a "method". For the weighing operation, the method refers to the scale or balance used; for volume determination, it refers to a given dip-tube manometer system or some other system used to measure volume; for sampling, it indicates the type of material being sampled in combination with the equipment and technique used to draw the sample; for analysis, it is the analytical equipment and technique used; and for an NDA measurement, the method is identified with the equipment and technique used. Finally, for each operation–method combination, three error variances are identified: the random-error variance, the short-term systematic-error variance, and the long-term systematic-error variance.

In effect this procedure combines the effects of all random errors associated with a given operation–method combination into one random-error random variable. The same is true of the short-term and long-term systematic-error variances. This does not limit the scope of the analysis, because it is permissible to combine the effects of the random and long-term systematic errors in this fashion. With respect to the short-term systematic error, we can identify the conditions under which a given measurement operation is performed, and all measurements made under a fixed set of conditions represent the same observation on the short-term-error random variable in question. In this sense, it is often meaningful to relate "conditions" to "time" of the measurement operation, and this is

the sense in which the expressions "short term" and "long term" were coined.

Two other points are made with respect to the short-term systematic error. First, although only one such error variance is assumed for each operation–method combination, there is no reason that more such variances cannot be included if desired, the same being true for random-error variances and long-term systematic-error variances; we are always free to identify and include several separate sources if we wish. This adds nothing to the inherent complexity of the problem except that more computations may be required. Second, for some types of measurement operations, e.g., sampling, it may be difficult to assign a meaning to a short-term systematic error. This poses no difficulties since this source can simply be ignored in the analysis.

3.3 ESTIMATION OF ERROR VARIANCES

As will be evident as the reader progresses through the book, the assumption is frequently made that the various error variances are known quantities. In practice this assumption means that the variances have been estimated on the basis of previous studies, the estimates being continually reviewed as new data are available. Thus, although the error variances may be regarded as known constants or parameters in a given framework, they are actually based on estimated quantities. This brings up the very basic and important problem of which techniques can be used to estimate them.

Measurement parameters are estimated from data. These data may come from special studies designed specifically to provide estimates of the parameters, or they may have been generated in the normal course of doing business. There are a number of statistical techniques that are used to estimate the measurement parameters from a given set of data and from other information that might be available. These techniques are discussed separately in this section. Although the emphasis is on data analysis, indications are given on how experiments can be designed to provide the data needed for analysis. The estimation topics are presented as indicated in Table 3.2.

3.3.1 Paired Data

Paired data occur frequently in nuclear material control. Paired data result from independent measurement of the same item by two

TABLE 3.2 ESTIMATION TOPICS

Topic	Section
Paired data	3.3.1
Use of known standards	3.3.2
Errors in weighing	3.3.3
Analysis of variance studies	3.3.4
Test for homogeneity of variances	3.3.5
Systematic errors in sampling	3.3.6
Synthetic approach to estimating systematic-error variance	3.3.7
Linear calibration—independent data	3.3.8
Linear calibration—cumulative data	3.3.9
Curvilinear calibration—independent data	3.3.10

parties, as in the following nuclear materials control situations:

1. Shipper–receiver measurements, where both the shipper and the receiver make measurements on the same items.
2. Inventory-verification activities, in which the audit team makes measurements on a sample of items previously measured by the operator.
3. Measurements on the same item by two individuals or by two measurement methods, e.g., by sampling and wet chemistry and by NDA.
4. Interlaboratory tests involving two laboratories.

These types of data are very valuable in obtaining realistic estimates of the error variances. Because of the importance of paired data, a complete chapter, Chap. 8, is included on this topic. Further detailed discussion of paired data is deferred until then, but for the present it is worthwhile to indicate what types of information can be derived from analyzing paired data.

With paired data, we can obtain answers to the following questions:

1. What is the estimate of the measurement random-error standard deviation for each party?

   (Depending on how the paired data were generated, the term "measurement" has different meanings. For example, if both parties draw random samples of material from the same item, the effect of sampling error would be included, whereas, if both parties make measurements on the same sample, this sampling effect would not be included. See Chap. 8 for more detailed discussion on this point.)

2. Do both parties have the same true standard deviation?
3. Each party supplies his own value for this standard deviation. Do the data support these values?
4. One party supplies his own value for this standard deviation, whereas the other party does not. Do the data support this value?
5. Is there a significant bias between the two parties?
6. If the measurements are made on a known standard, is party 1 biased? party 2? What is the average for the two parties?
7. What is the best estimate of the true value for each item?

3.3.2 Use of Known Standards

One of the most common ways to estimate random- and systematic-error variances is through the use of known standards. Several nonstatistical difficulties are associated with this practice. Known standards are often not completely representative of the types of samples actually being measured. This means that there may be factors, such as the degree of cleanliness of the standards, which might affect the uncertainty of the result for a production sample but would not affect the result for the standard or would perhaps affect it less. Also, it is difficult to disguise the fact that we are submitting a known standard for analysis. Even the most conscientious analyst has problems being completely objective in determining a value for the sample when he knows what the answer should be. This is especially a problem when the analyst must exercise considerable personal judgment in determining a result.

Nevertheless, the use of known standards does play an important role, especially because it is the only direct means by which we can obtain an estimate of the bias or of the systematic-error variance; these parameters have meaning only with respect to a "true" or known value.

The following steps are taken to estimate the bias and the random- and systematic-error variances with known standards. (Assume in this section that the standards data are collected under fixed conditions, i.e., there is no shifting measurement bias over the range of the data. Thus the idea of a short-term systematic error is not pertinent. The case in which this is not true is considered in Sec. 3.3.3.)

Step 1. Measure the standard n times, designating the measured values $x_1, x_2, \ldots, x_n$.

Step 2. Compute the sample mean, $\bar{x}$, by Eq. 2.56 and the sample variance, s^2, by Eq. 2.60 or Eq. 2.61.

Step 3. With μ_0 as the value assigned the standard, the estimated bias, $\hat{B}$, is $(\bar{x}-\mu_0)$. This estimate has variance s^2/n. The mean of $\hat{B}$ is assumed to be B, the true bias.

Step 4. **a.** If the bias correction is made, the systematic-error variance is

estimated by $s^2/n+s_0^2$, where s_0^2 is the variance that describes the uncertainty in μ_0; s_0^2 is often very small relative to s^2/n.

b. If the bias correction is not made, the systematic-error variance is estimated by $(\bar{x}-\mu_0)^2+s_0^2$. (Some analysts also prefer to use $s^2/n+s_0^2$ as the systematic-error variance when a bias correction is not made. This practice has some merit in the common situation in which a bias correction is not made because its estimate is not significantly different from zero.)

Step 5. The random-error variance is estimated by s^2.

Some further discussion is helpful on step 4. During the calibration, a measured or observed value, x_i, is regarded as the sum of three quantities: the standard value μ_0, the bias B, and the random error, which can be denoted by ϵ_i in this discussion. The bias, B, is estimated by $\hat{B}=(\bar{x}-\mu_0)$, which has variance σ^2/n by Eq. 2.58, where σ^2 is the variance of ϵ_i. Then, in application, a value, y, is observed. If the bias correction is made to this value by subtraction of $\hat{B}$, then, in addition to the random variance, σ^2, the y also has a systematic-error variance due to the uncertainty in $\hat{B}$. This is σ^2/n, which is estimated by s^2/n. On the other hand, if a bias correction is not made, then all future observations not corrected for bias are in error by an amount B, and the total variance of y includes a component, B^2, which can be regarded as the systematic-error variance. The quantity B^2, of course, is not known and can be replaced by its estimate, $\hat{B}^2$, or $(\bar{x}-\mu_0)^2$. Even in this instance, however, when a bias correction is not made, there is a basis for preferring s^2/n over $\hat{B}^2$ as the estimate of the systematic-error variance. This is true because in the usual case the bias correction is not made simply because it is not large relative to its uncertainty, i.e., there is little real evidence that a bias correction is actually needed. This being the case, we might prefer to use s^2/n because it describes the uncertainty associated with a bias correction whether the correction is made or not. To be on the conservative side, we can use as a reasonable alternative the larger of $(\bar{x}-\mu_0)^2$ and s^2/n in the event a bias correction is not made.

Looking ahead to the application of these results in subsequent chapters, we see that a difficulty associated with the problem of systematic-error variance will arise when we consider the combined effects of several random variables. From a purely statistical viewpoint, the preferred approach in the sense of the most defensible one is to make the bias corrections at all times and, hence, to follow step 4a. The propagation of errors is then straightforward and intuitively reasonable. This, however, presents practical problems because no laboratory or operations manager reacts favorably to the idea of making very small bias corrections, especially when they are poorly estimated in a relative sense. In actual fact some bias corrections are generally made, and some are not. Thus the clean statistical approach to describing the error uncertainty for a total result

would consist in first algebraically combining the bias estimates for the variables for which bias corrections were not made and then in appropriately propagating the systematic-error variances for the remaining variables by the methods to be discussed. This approach, however, usually is awkward and not practical in a real application. It is far simpler to regard all the effects as systematic-error variances, whether the bias corrections are made or not. I have treated the latter approach in this book, recognizing that in practice, when bias corrections are not made, the reason is that they are unimportant in their effects.

Example 3.B

Assume that 10 measurements are made on a National Bureau of Standards (NBS) standard by a mass spectrometer to estimate the bias and the random- and systematic-error variances. The standard is assigned a value of 3.046% of ^{235}U. The 10 measurements are given in Table 3.3.

TABLE 3.3 MEASUREMENTS OF PERCENT OF ^{235}U* (Example 3.B)

3.095	3.066	3.082
3.086	3.090	3.045
3.058	3.068	3.084
3.073		

* The standard has an assigned value of 3.046%.

For example 3.B the procedural steps 2 to 5 to estimate the parameters are as follows:

Step 2. $$\bar{x}=\frac{3.095+3.086+\ \ldots\ +3.084}{10}=3.075$$

$$s^2=\frac{(3.095)^2+\ \ldots\ +(3.084)^2-[(3.095+\ \ldots\ +3.084)^2/10]}{9}$$

$$=0.0002442=244.2\times10^{-6}$$

Step 3. $\hat{B}=\bar{x}-\mu_0=3.075-3.046=0.029$

Step 4. Assume that $s_0^2=(0.0006)^2=0.36\times10^{-6}$ is given by a tolerance statement associated with the standard.

a. If the bias correction is made, the estimate of the systematic-error variance is $(244.2/10+0.36)\times10^{-6}=24.78\times10^{-6}$, which gives a standard deviation of $\sqrt{24.78\times10^{-6}}$ or 0.00498% of ^{235}U.

b. If the bias correction is not made, this estimate is $(0.029)^2+0.36\times10^{-6}=841.36\times10^{-6}$, giving a standard deviation of

0.0290% of ^{235}U. (In this instance, however, the bias correction should clearly be made. It is obvious from the data, with 9 of the 10 observations reading high, that a real bias is present.)

Step 5. The random-error variance is estimated by $s^2 = 244.2 \times 10^{-6}$, giving a standard deviation of 0.0156% of ^{235}U.

Example 3.C

(This example was supplied by R. A. Schneider.)

In the second example, two analysts make determinations of percent of plutonium using a known standard with an assigned value of 13.00% of plutonium. The data are given in Table 3.4.

TABLE 3.4 DETERMINATIONS OF PERCENT OF PLUTONIUM*
(Example 3.C)

Analyst 1		Analyst 2	
12.90	13.01	13.01	12.97
12.99	13.03	13.02	13.01
12.98	12.99	12.98	12.95
12.96	13.04	13.04	13.01
12.97	12.94	13.00	13.04

* The standard has an assigned value of 13.00%.

Before estimating the random- and systematic-error variances for the analytical method, we must see if there are differences between the two analysts. The analysts might conceivably differ because one gives higher readings than the other or because the results for one might be more variable than those for the other.

Consider the comparison of the variances first. The variance is computed separately for each analyst. If the variances differ significantly, we cannot speak of the random variance of the analytical method as such but only as it relates to a given analyst. Let s_i^2 $(i = 1,2)$ be the sample variance for analyst i. From Eq. 2.61,

$$s_1^2 = \frac{(12.90)^2 + \ldots + (12.94)^2 - [(12.90 + \ldots + 12.94)^2/10]}{9} = 0.001743$$

$$s_2^2 = \frac{(13.01)^2 + \ldots + (13.04)^2 - [(13.01 + \ldots + 13.04)^2/10]}{9} = 0.000846$$

To test the hypothesis that σ_1^2 equals σ_2^2, where these are the true variances estimated by s_1^2 and s_2^2, respectively, use the F distribution, as

given in Sec. 2.6.4. If the hypothesis is true, $F=s_1^2/s_2^2$ will have the F density function with 9 degrees of freedom in the numerator and 9 in the denominator. Use a significance level of $\alpha=0.05$. This means that, if the analysts truly have the same variances, there is a probability of 0.05 that the opposite conclusion will be reached. Then, from Appendix D, we can reject the hypothesis for a two-sided test of significance if the larger of s_1^2 and s_2^2 exceeds $F_{0.975}$ (9,9) or 4.03. The $F_{0.975}(9,9)$ value is used rather than the $F_{0.95}(9,9)$ value because this is a two-sided test, and the hypothesis can be rejected if s_1^2/s_2^2 is either too large or too small. Since $s_1^2/s_2^2=0.001743/0.000846=2.06$ is less than 4.03, the hypothesis is not rejected. This conclusion permits us to speak of the measurement variance for the analytical method as such, irrespective of who is the analyst. This variance is estimated by the average of the variances for both analysts, or $s^2=0.001295$.

The simple average is used in this case because each analyst made the same number of determinations. In the general case in which one analyst makes m_1 determinations and the other makes m_2, the weighted average is

$$s^2=\frac{(m_1-1)s_1^2+(m_2-1)s_2^2}{(m_1+m_2-2)}$$

Next, does one analyst produce higher readings than the other? Letting μ_i be the mean reading for analyst i ($i=1, 2$), test the hypothesis $\mu_1=\mu_2$, or, equivalently, $\mu_1-\mu_2=0$ as follows:

Step 1. Calculate $\bar{x}_1$ and $\bar{x}_2$, the sample averages.

$$\bar{x}_1=\frac{12.90+\ \ldots\ +12.94}{10}=12.981$$

$$\bar{x}_2=\frac{13.01+\ \ldots\ +13.04}{10}=13.003$$

Step 2. Estimate $(\mu_1-\mu_2)$ by $(\bar{x}_1-\bar{x}_2)$, which is a random variable with zero mean under the hypothesis. The variance of $(\bar{x}_1-\bar{x}_2)$ is found by summing the variances for $\bar{x}_1$ and $\bar{x}_2$ (shown in Chap 4). This is $s^2/10+s^2/10$ or $(2)(0.001295)/10=0.000259$. The standard deviation of $(\bar{x}_1-\bar{x}_2)$ is then $\sqrt{0.000259}=0.016$.

Step 3. Reject the hypothesis if $(\bar{x}_1-\bar{x}_2)$ is either too large or too small, i.e., if $(\bar{x}_1-\bar{x}_2)>c$ or if $(\bar{x}_2-\bar{x}_1)>c$, where c is some constant defining the critical region. If $\alpha=0.05$, select c such that

$$\Pr\,[(\bar{x}_1-\bar{x}_2)>c\,|\,(\mu_1-\mu_2)=0]=0.025$$

Equivalently, choose c such that

$$\Pr\,[(\bar{x}_2-\bar{x}_1)>c\,|\,(\mu_1-\mu_2)=0]=0.025$$

The statistic is standardized by subtracting the mean (zero in this case) and dividing by the standard deviation, 0.016. The resulting statistic has Student's t density function, as given in Sec. 2.6.3.

Thus

$$\Pr\left[\frac{(\bar{x}_1-\bar{x}_2)-0}{0.016}>\frac{c-0}{0.016}\right]=0.025$$

from which $c/0.016=2.101$ or $c=0.034$ from Appendix C. The value 2.101 is the entry under $t_{0.975}$ for 18 degrees of freedom, because 18 degrees of freedom are associated with the estimate of the standard deviation, i.e., 9 degrees of freedom for each analyst.

Now, $(\bar{x}_2-\bar{x}_1)=13.003-12.981=0.022$. Since 0.022 is less than the critical value, 0.034, the hypothesis is not rejected; i.e., we conclude that there is no evidence of a relative bias between the two analysts. Having concluded that the analysts do not differ, we can regard all the 20 observations as having come from the same population, i.e., the one relating to the analytical method regardless of which analyst made the determination. To estimate the bias and the systematic- and random-error variances, find the mean, $\bar{x}$, and the variance, s^2, for the entire set of data.

$$\bar{x}=\frac{(12.90)+\ \ldots\ +(13.04)}{20}=12.992$$

$$s^2=\frac{[(12.90)^2+\ \ldots+(13.04)^2-[(12.90+\ \ldots+13.04)^2/20]}{19}=0.001354$$

Then, for example 3.C, procedural steps 3 to 5 to estimate the measurement parameters are as follows:

Step 3. $\hat{B}=\bar{x}-\mu_0=12.992-13.00=-0.008$

Step 4. **a.** If the bias correction is made, and if we assume $s_0^2=(0.003)^2=0.000009$, the systematic-error variance is

$$\frac{s^2}{n}+s_0^2=\frac{0.001354}{20}+0.000009=0.000077$$

b. If the bias correction is not made, the systematic-error variance is

$$(\bar{x}-\mu_0)^2+s_0^2=(-0.008)^2+(0.003)^2=0.000073$$

(This example represents a borderline case with respect to whether or not future data should be corrected for bias by adding 0.008 to such results. This bias is not statistically significant at some

reasonable value for α, as would be found by a test of the hypothesis $B=0$, but statistical significance is not essential to the decision concerning whether or not to make the bias correction. It is, of course, one factor in making this decision, but other considerations also play a role, e.g., the size of the bias, irrespective of its statistical significance or nonsignificance, and technical judgement as to whether or not the method is inherently biased.)

Step 5. The random-error variance is estimated by $s^2=0.001354$, giving a standard deviation of $\sqrt{0.001354}=0.037\%$ of plutonium.

Example 3.D

(This example was supplied by R. A. Schneider.)

A certain facility applies a bias correction to all uranium analytical results on a monthly basis. A standard is run with each process sample analyzed to arrive at the correction for certain uranyl nitrate hexahydrate transfers. At the end of each month, the recoveries on the standards are calculated, and the need for a bias correction is determined on the basis of these recoveries. From the set of recovery data in Table 3.5, estimate the bias and the appropriate error variances.

TABLE 3.5 DATA ON PERCENT OF RECOVERY
(Example 3.D)

100.36	100.19	100.41	100.47
100.79	100.78	100.84	100.63
100.35	100.86	100.26	100.34
100.57	100.99	100.52	100.07
100.45	100.81	101.01	101.38
100.83	100.51	100.46	100.14
100.87	100.55	100.65	100.56
100.46	100.59	100.81	100.48
99.99	100.76	100.53	101.04

The random variable, X, is defined as the observed percent of recovery minus 100%. With this data transformation, μ_0, the standard value, becomes zero. The variance component, s_0^2, which is the variance of μ_0, is assumed to be negligible. Then in example 3.D the procedural steps 2 to 5 are as follows:

Step 2. $$\bar{x}=\frac{0.36+0.79+\ \ldots\ +1.04}{36}=0.592$$

$$s^2=\frac{(0.36)^2+\ \ldots\ +(1.04)^2-[(0.36+\ \ldots\ +1.04)^2/36]}{35}=0.0870$$

Step 3. $\hat{B} = (\bar{x} - 0) = 0.592$. This has variance $0.0870/36 = 0.002417$, or a standard deviation of $\sqrt{0.002417} = 0.049$. Clearly, comparing 0.049 with $\hat{B} = 0.592$ reveals that there is no question but that the bias is real. Of course, this was evident from the fact that 35 of the 36 numbers exceeded 100%.

Step 4. **a.** The bias correction will be made. Therefore estimate the systematic-error variance by $s^2/n = 0.002417$.

Step 5. Estimate the random-error variance by $s^2 = 0.0870$.

3.3.3 Errors in Weighing

This is treated as a separate topic because two unique aspects are associated with measurement errors in weighing. First, particularly in this application, errors due to rounding may play a dominant role. Also, the role played by tare weights must be factored in.

The measurement performance of scales and balances is controlled by the use of standard weights. The frequency with which such weights are applied depends on the use of the particular scale. In some instances standards may be used once per shift; in other cases standards may be weighed just prior to each use of the scale. Whatever the frequency, it is not uncommon for the scale readings to be in very close agreement with the known weights of the standards. This could lead to an optimistic appraisal of the size of the error variances due to weighing when the methods of Sec. 3.3.2 are applied without modification.

This appraisal may be optimistic for two reasons: (1) in the routine use of the scale, the rounding error may dominate and (2) the use of standards provides information only on the integrity of the gross weight; the uncertainties in the tare-weight determination must also be considered.

First, consider the random-error variance for a net weight. The effect of rounding errors was introduced in Sec. 2.4.4 in a discussion of the uniform density function. The additional point made here is that the effect of rounding must also be included for the tare weight. To illustrate, with reference to the results of Sec. 2.4.4, round the tare weights to the nearest 25 g and round the gross weights to the nearest 50 g (regardless of which scale is used). Then σ_1^2 is the random-error variance due to rounding the tare weight and is equal to $(25)^2/12 = 52.08$; σ_2^2 is the random-error variance due to rounding the gross weight and is equal to $(50)^2/12 = 208.33$; and the random-error variance due to rounding for the net weight is $\sigma_1^2 + \sigma_2^2 = 52.08 + 208.33 = 260.41$ g^2, which gives a standard deviation of 16.1 g.

Some care must be taken in relating the error variance due to rounding to that inherent in the scale in question. Section 3.3.2 was concerned with the use of known standards to estimate error variances. With some modifications this section is applicable to scales also. If in such experiments the

observations on the standards are rounded to the same degree as is done in practice and if the rounding is gross relative to scale capability, it is quite likely that all weighings of the standard will produce the same result, and the data might appear as follows for a 20-kg standard weight rounded to the nearest 25 g.

20.000	20.000
20.000	20.000
	etc.

Or, possibly, an occasional observed value might read 20.025 or 19.975. In any event this is clearly an instance in which the random-error variance for a single weighing is exclusively that due to rounding, and the preceding data do not really provide much information except to verify that rounding error does indeed dominate.

In another situation the standards data can be read with extra care by the use of finer scale divisions and/or visual interpolation by the operator, and readings might be made on the standard to the nearest 5 g and produce data such as the following:

20.005	20.005
20.005	19.995
20.000	20.010
	etc.

These data describe the random-error variance inherent to the scale plus that due to rounding to the nearest 5 g. From the results of Sec. 3.3.2, the variance of the preceding six observations is computed by Eq. 2.60 or Eq. 2.61 to give the random-error variance. For simplicity, the data are expressed in grams, and 20,000 is subtracted from each observation. This gives

$$s^2 = \frac{(5)^2+(5)^2+\ldots+(10)^2-[(5+5+\ldots+10)^2/6]}{5}$$
$$= 26.67 \text{ g}^2$$

This variance includes the effect due to rounding to the nearest 5 g, which is $(5)^2/12 = 2.08$ g^2. Thus the variance due to the inherent performance of the scale is $(26.67-2.08) = 24.59$ g^2. To this value, then, must be added the error due to rounding to the nearest 25 g in practice, namely, $(25)^2/12 = 52.08$ g^2. The total random-error variance for a given gross weight determination thus becomes $(24.59+52.08) = 76.67$ g^2. If, in turn, the tare weight is rounded to the nearest 50 g, its random-error variance is $\{[(50)^2/12]+24.59\} = 232.92$ g^2. Thus the total random-error variance associated with a given net weight is $(76.67+232.92) = 309.59$ g^2, giving a standard deviation of 17.6 g.

To summarize, the steps for determining the random-error variance associated with a given net weight are as follows:

Step 1. Weigh a given standard n times on the scale in question, preferably over a period of time.

Step 2. Compute the variance, s^2, of these observed values, using Eq. 2.60 or Eq. 2.61.

Step 3. When weighing the standard weights, say the values are rounded to the nearest Δ_1 units. Compute $[s^2-(\Delta_1^2/12)]=A_1$.

Step 4. If A_1 is negative, call it zero.

Step 5. Assume that the gross weight is rounded to the nearest Δ_2 units and the tare weight to the nearest Δ_3 units. Then the random-error variance for a net-weight determination is

$$V=2A_1+\frac{\Delta_2^2+\Delta_3^2}{12} \tag{3.4}$$

Step 6. If the tare weight is determined on another scale or if different standards are used for the gross and tare weights, repeat steps 1 to 3 for the other scale or for the tare standard, calling the result A_2. Then

$$V=A_1+A_2+\frac{\Delta_2^2+\Delta_3^2}{12} \tag{3.5}$$

Thus far, only the random-error variance due to weighing has been covered. Now, consider the systematic-error variance. For a given standard weight, the systematic-error variance may be determined by the methods of Sec. 3.3.2 except that the effects of rounding must again be taken into account. For a given standard weight, μ_0, the systematic-error variance was given by step 4 as $(\bar{x}-\mu_0)^2+s_0^2$, where $\bar{x}$ is the average observed weight for the standard. (This was the formula to use if a bias correction is not made, which is the usual practice. When real biases are detected, the scales are normally adjusted, not the data.) Often, because of rounding, $(\bar{x}-\mu_0)$ will be zero. To account for the rounding error, add the quantity $\Delta^2/12$, where the readings on the standard are rounded to the nearest Δ units. As far as the systematic-error variance is concerned, the extent by which the actual observed data for gross and tare weights are rounded has no effect (except in the limiting case in which there is very little true variation in weights from item to item, relative to the rounding error, and this is not considered to be a likely situation in nuclear materials control applications). Thus, for a given standard weight, the systematic-error variance for weighing is

$$s_w^2=(\bar{x}-\mu_0)^2+s_0^2+\frac{\Delta^2}{12} \tag{3.6}$$

where $\bar{x}$ = observed average standard weight
μ_0 = assigned value for the standard weight
Δ = amount of rounding for standard weight
s_0^2 = variance associated with μ_0

This gives the systematic-error variance for either the gross or the tare weight but leaves unanswered the question of what is the systematic-error variance for the net weight. This variance depends on the degree of correlation between a systematic error for the gross weight and a systematic error for a tare weight. If the tare and gross weights are determined on different scales, then this correlation should be near zero, and the systematic-error variance for the net weight is found by summing the variances for the gross and tare weights. However, when the same scale is used for both weight determinations, it is likely that these errors are correlated. A positive correlation means that a high reading for the gross weight tends to produce a high reading for the tare weight, whereas the correlation is negative if a high reading for the gross weight tends to produce a low reading for the tare weight.

Table 3.6 gives the value of the systematic-error variance for the net weight as a function of the degree of correlation between the gross and tare weights. The correlation coefficient (defined explicitly in Eq. 2.55) ranges from -1 (perfect negative correlation) to $+1$ (perfect positive correlation). In Table 3.6, σ_g^2 denotes the systematic-error variance for the gross weight, σ_t^2, for the tare weight, and σ_n^2, for the net weight. If $\sigma_g^2 = \sigma_t^2 = \sigma^2$, then the value for the systematic-error variance for the net weight is denoted by $\sigma_{n'}^2$.

TABLE 3.6 SYSTEMATIC-ERROR VARIANCE FOR NET WEIGHT

Correlation coefficient	σ_n^2	$\sigma_{n'}^2$
-1	$\sigma_g^2+\sigma_t^2+2\sigma_g\sigma_t$	$4\sigma^2$
-0.5	$\sigma_g^2+\sigma_t^2+\sigma_g\sigma_t$	$3\sigma^2$
0	$\sigma_g^2+\sigma_t^2$	$2\sigma^2$
$+0.5$	$\sigma_g^2+\sigma_t^2-\sigma_g\sigma_t$	σ^2
$+1$	$\sigma_g^2+\sigma_t^2-2\sigma_g\sigma_t$	0

Unfortunately the correlation coefficient is difficult to evaluate in this instance. If the terms of the form $(\bar{x}-\mu_0)^2$ in Eq. 3.6 are the dominant contributors to s_w^2, then the systematic-error variance for the net weight can be estimated directly from standards data. Letting x_{gi} represent the ith reading for the gross standard and x_{ti} denote the same quantity for the tare standard, with $i = 1, 2, \ldots, n$, estimate the net-weight systematic-error variance by

$$[(\bar{x}_g-\mu_{g0})-(\bar{x}_t-\mu_{t0})]^2 \qquad (3.7)$$

where $\bar{x}_g$ and $\bar{x}_t$ are the averages of the x_{gi} and x_{ti} values, respectively, and μ_{g0} and μ_{t0} are the assigned values for the standard weights.

In many instances, however, the rounding error, rather than the terms of $(\bar{x}-\mu_0)^2$, will tend to dominate. In this case we must speculate on the size of the systematic-error variance for the net weight. Since the two systematic errors are likely to be positively correlated rather than negatively, a conservative approach is to assume a correlation coefficient of zero and simply sum the systematic-error variances for the gross and tare weights.

To summarize, the steps to find the systematic-error variance associated with a given net weight are as follows:

Step 1. Weigh a given standard n times on the scale in question, preferably over a period of time.

Step 2. Compute the systematic-error variance s_w^2 from Eq. 3.6.

Step 3. If different scales are used for the gross and tare weight determinations, find s_w^2 separately for each scale and sum the results to give the systematic-error variance for the net weight.

Step 4. If the same scale is used for the gross and tare weight determinations and if $(\bar{x}-\mu_0)^2$ is the dominant term in Eq. 3.6, determine the systematic-error variance separately for both the gross and tare weights using the appropriate standards, and use Eq. 3.7 to find the net-weight systematic-error variance.

Step 5. If the same scale is used for the gross and tare weight determinations and if $(\bar{x}-\mu_0)^2$ is not the dominant term in Eq. 3.6, multiply s_w^2 in Eq. 3.6 by 2 to find the net-weight systematic-error variance.

Example 3.E

A given scale is controlled through the use of one standard which nominally weighs 20 kg. Assume that the uncertainty in this standard weight is expressed as a standard deviation of 1 g. When the standard is weighed, the weights are recorded to the nearest 10 g. When used to measure actual containers, the gross weights are rounded to the nearest 50 g and the tares to the nearest 25 g. Both the gross and tare weights are determined on this same scale. The results of 20 weighings on this standard are given in Table 3.7. Use these data to estimate the random- and systematic-error variances for a given net weight.

TABLE 3.7 WEIGHT DATA*
(Example 3.E)

20000	20010	20020	20000
20000	20000	20000	20000
20010	20000	20000	20000
20000	20000	19990	20000
20010	20000	20000	20010

* In grams.

In example 3.E, first consider the six procedural steps to determine the random-error variance:

Step 2. By Eq. 2.61, after coding the data by subtracting 20000 for simplicity,

$$s^2=\frac{(0)^2+\ldots+(10)^2-[(0+\ldots+10)^2/20]}{19}=40.79$$

Step 3. With $\Delta_1=10$,

$$A_1=40.79-\frac{100}{12}=32.46$$

Step 4. With $\Delta_2=50$ and $\Delta_3=25$,

$$V=2(32.46)+\frac{(2500+625)}{12}=325.34 \quad g^2$$

the random-error variance for net-weight determination.

Next, for the systematic-error variance, the appropriate steps to follow are as follows:

Step 2. To use Eq. 3.6, evaluate

$$(\bar{x}-\mu_0)=\frac{0+0+10+\ldots+10}{20}=2.50$$

$$\Delta=10$$

$$s_0^2=1$$

$$s_w^2=(2.50)^2+1+\frac{100}{12}=15.58$$

Step 5. $2s_w^2=31.16 \quad g^2$

the systematic-error variance for net-weight determination.

3.3.4 Analysis of Variance

The analysis of variance is a very large topic and can be covered only very superficially in this book. Four simple but common and useful appli-

cations of the technique are made here. For more complicated situations the user should consult other books on the subject.

Analysis of variance is a statistical technique for dividing a total variance into component parts that can be identified with specific factors. The technique will be illustrated in the following situations:

Situation A. In the case of the known standards of Sec. 3.3.2, the experiment is repeated routinely, and the data are gathered over a period of time.

Situation B. For an estimate of the random-error variances due to sampling and analysis, replicate samples are drawn for a number of items, with replicate analyses made on each sample.

Situation C. Samples are sent to a number of laboratories for analysis (interlaboratory tests).

Situation D. Production data are analyzed to obtain estimates of certain error variances.

Situation A

The standards data are the same as those in Sec. 3.3.2 except that now a time factor has been introduced. The data are given in Table 3.8, where the tabular entries represent measured values on a standard whose assigned value is μ_0.

TABLE 3.8 SCHEMATIC OF MEASUREMENTS ON A STANDARD

	Time 1	Time 2	. . .	Time k
	x_{11}	x_{21}	. . .	x_{k1}
	x_{12}	x_{22}	. . .	x_{k2}
	.	.		.
	.	.		.
	.	.		.
	x_{1n_1}	x_{2n_2}	. . .	x_{kn_k}
Total	T_1	T_2		T_k

The data are structured so that the same number of observations need not necessarily be made during each block of time. The sum of the T_i values over the k columns is denoted by T. The following additional calculations are made:

Step 1. T^2/N, where N is the total number of observations

Step 2. $\bar{x} = T/N$, the overall average

Step 3. $S_1 = \sum_{i=1}^{k} T_i^2$,

Step 4. $S_2 = \sum_{i=1}^{k} \sum_{j=1}^{n_i} x_{ij}^2$

Step 5. $P = \dfrac{N^2 - \sum_{i=1}^{k} n_i^2}{N(k-1)}$

Step 6. $M_1 = \dfrac{S_2 - S_1}{\sum_{i=1}^{k} (n_i - 1)}$

Step 7. $M_2 = \dfrac{\{[S_1 - (T^2/N)]/(k-1)\} - M_1}{P}$

Step 8. $M_3 = \dfrac{M_1 \sum_{i=1}^{k} n_i^2 + M_2 \sum_{i=1}^{k} n_i}{N^2}$

Then the estimates of the error variances of interest are as follows:

M_1 estimates the random-error variance for the analytical method

M_2 estimates the short-term systematic-error variance

$M_3 + s_0^2$ estimates the long-term systematic-error variance if the bias correction is made, where $(\bar{x} - \mu_0)$ is the bias correction and s_0^2 is the variance that describes the uncertainty in μ_0

$(\bar{x} - \mu_0)^2 + s_0^2$ estimates the long-term systematic-error variance if the bias correction is not made*

The preceding analysis is known as a one-way analysis of variance with unequal numbers of observations. This technique is applied to the following data.

Example 3.F

This example represents mass-spectrometer measurements of ^{235}U on a known standard, with $\mu_0 = 3.046$. Given the data in Table 3.9, the calculational steps called for in situation A follow.

* As pointed out earlier in a similar situation, some analysts prefer to use $M_3 + s_0^2$ as the systematic error variance when a bias correction is not made.

TABLE 3.9 MASS SPECTROMETRIC DATA*
(Example 3.F)

Time 1	Time 2	Time 3	Time 4	
3.095	3.044	3.019	3.090	
3.086	3.078	3.045	3.073	
3.058	3.046	3.022	3.053	
3.073	3.060		3.081	
	3.023			
	3.072			
$T_1=12.312$	$T_2=18.323$	$T_3=9.086$	$T_4=12.297$	$T=52.018$
$n_1=4$	$n_2=6$	$n_3=3$	$n_4=4$	$N=17$

* The standard has an assigned value of 3.046%.

Step 1. $\dfrac{T^2}{N}=\dfrac{(52.018)^2}{17}=159.168960$

Step 2. $\bar{x}=\dfrac{T}{N}=\dfrac{52.018}{17}=3.0599$

Step 3. $S_1=\dfrac{(12.312)^2}{4}+\ \ldots\ +\dfrac{(12.297)^2}{4}=159.174242$

Step 4. $S_2=(3.095)^2+(3.086)^2+\ \ldots\ +(3.081)^2=159.178232$

Step 5. $P=\dfrac{(17)^2-[(4)^2+\ \ldots\ +(4)^2]}{(17)(3)}=4.157$

Step 6. $M_1=\dfrac{159.178232-159.174242}{3+5+2+3}=0.0003069$

Step 7. $M_2=\dfrac{[(159.174242-159.168960)/3]-0.0003069}{4.157}=0.0003497$

Step 8. $M_3=\dfrac{(0.0003069)(16+36+9+16)+(0.0003497)(4+6+3+4)}{(17)^2}$

$=0.0001023$

Then,

$M_1=0.0003069$ estimates the random-error variance for the analytical method

$M_2 = 0.0003497$ estimates the short-term systematic-error variance

$(\bar{x} - \mu_0) = 3.0599 - 3.046 = 0.0139$ estimates the bias

$s_0^2 = 0.36 \times 10^{-6}$, input data from the example of Sec. 3.3.2

$M_1 + s_0^2 = 0.0001023 + 0.00000036 = 0.0001027$ estimates the long-term systematic-error variance if the bias correction is made

$(\bar{x} - \mu_0)^2 + s_0^2 = 0.0001936$ estimates the long-term systematic-error variance if the bias correction is not made

Situation B

In this situation, replicate samples are drawn for a number of items, and replicate analyses are made on each sample. This is done to obtain separate estimates of the random-error variance due to sampling and of the random-error variance due to analysis. Because the true value for the item being measured is not known in this instance, we cannot estimate the systematic-error variances in this situation. Such information must come from other sets of data, as in the previous example. The data are shown in Table 3.10.

TABLE 3.10 SCHEMATIC OF MEASUREMENTS
(Situation B)

	Item 1				Item 2 . .				Item k			
Sample	1	2	. . .	m	1	2	. . .	m	1	2	. . .	m
Analysis												
1	x_{111}	x_{121}	. . .	x_{1m1}	x_{211}	. . .		x_{2m1}	x_{k11}	. . .		x_{km1}
2	x_{112}	x_{122}		.	.			.	.			.
.	.	.		.	.			.	.			.
.	.	.		.	.			.	.			.
.	.	.		.	.			.	.			.
n	x_{11n}	x_{12n}	. . .	x_{1mn}	x_{21n}	. . .		x_{2mn}	x_{k1n}	. . .		x_{kmn}

The data are balanced in this design, i.e., there are m samples and n analyses on each sample. This makes for simplicity in analysis, although it is not a necessary condition. The analysis in this situation is called an analysis for a nested (or hierarchical) design with three classifications (items, samples within items, and analyses within samples). For an estimate of the random-error variances due to sampling and analysis, only the two lower classifications are of interest; the only function of the k items in this case is to produce more data and hence better estimates of the error variances.

Before estimating the variances from these data, note the following definitions:

T = sum of all the observations
N = total number of observations
T_i = sum of all observations for item i; $i = 1, 2, \ldots, k$
T_{ij} = sum of all the observations for item i, sample j; $j = 1, 2, \ldots, m$

Then the following calculational steps are made:

Step 1. Find T^2/N

Step 2. Find

$$\sum_{i,j,k} x_{ijk}^2 - \frac{T^2}{N}$$

Call this S_T. The sum indicated is the sum of squared values for all the observations.

Step 3. Find

$$\frac{T_1^2 + T_2^2 + \ldots + T_k^2}{mn} - \frac{T^2}{N}$$

Call this S_I.

Step 4. For item 1, find:

$$\frac{T_{11}^2 + T_{12}^2 + \ldots + T_{1m}^2}{n} - \frac{T_1^2}{mn}$$

Do the same for items 2, 3, . . . , k. Sum these quantities, and call the sum S_S.

Step 5. Find $S_T - S_I - S_S = S_A$

Then the random-error variance due to analysis is estimated by

$$\frac{S_A}{km(n-1)}$$

and the random-error variance due to sampling is estimated by

$$\frac{S_S}{nk(m-1)} - \frac{S_A}{nkm(n-1)}$$

Example 3.G

These results are applied to a set of data (Table 3.11) that represent four samples of ammonium diuranate (ADU) scrap from each of five containers, with two analyses for each sample. An analytical result consists of percent of uranium. Here

$k = 5$ items $\qquad n = 2$ analyses per sample
$m = 4$ samples per item $\qquad \mathcal{N} = kmn = 40$ total observations

TABLE 3.11 PERCENT OF URANIUM IN ADU SCRAP
(Example 3.G)

Container	Analysis	Sample s-1	s-2	s-3	s-4	Total
ADU-1	a-1	44.1	33.8	42.3	40.3	
	a-2	44.0	33.0	42.4	40.1	
		88.1	66.8	84.7	80.4	$T_1 = 320.0$
ADU-2	a-1	24.1	27.3	22.9	25.6	
	a-2	24.2	26.7	22.7	25.9	
		48.3	54.0	45.6	51.5	$T_2 = 199.4$
ADU-3	a-1	76.8	74.3	76.8	74.0	
	a-2	76.5	74.0	76.6	73.8	
		153.3	148.3	153.4	147.8	$T_3 = 602.8$
ADU-4	a-1	79.8	76.5	77.0	77.1	
	a-2	80.2	76.2	77.4	77.3	
		160.0	152.7	154.4	154.4	$T_4 = 621.5$
ADU-5	a-1	26.8	30.0	28.2	31.4	
	a-2	27.0	30.2	28.3	31.9	
		53.8	60.2	56.5	63.3	$T_5 = 233.8$
						$T = 1977.5$

The five steps in the analysis called for in situation B are as follows:

Step 1. $\dfrac{T^2}{\mathcal{N}} = \dfrac{(1977.5)^2}{40} = 97762.66$

Step 2. $S_T = [(44.1)^2 + (44.0)^2 + \ldots + (31.9)^2] - 97762.66 = 20751.67$

Step 3. $S_I = \dfrac{(320.0)^2 + (199.4)^2 + \ldots + (233.8)^2}{8} - 97762.66 = 20543.95$

Step 4. For ADU-1: $\dfrac{(88.1)^2+\ldots+(80.4)^2}{2}-\dfrac{(320.0)^2}{8}=131.05$

For ADU-2: $\dfrac{(48.3)^2+\ldots+(51.5)^2}{2}-\dfrac{(199.4)^2}{8}=20.20$

For ADU-3: $\dfrac{(153.3)^2+\ldots+(147.8)^2}{2}-\dfrac{(602.8)^2}{8}=14.11$

For ADU-4: $\dfrac{(160.0)^2+\ldots+(154.4)^2}{2}-\dfrac{(621.5)^2}{8}=15.22$

For ADU-5: $\dfrac{(53.8)^2+\ldots+(63.3)^2}{2}-\dfrac{(233.8)^2}{8}=26.01$

$S_S=206.59$

Step 5. $S_A=20751.67-20543.95-206.59=1.13$

Then the random-error variance due to analysis is estimated by

$$\frac{S_A}{km(n-1)}=\frac{1.13}{20}=0.0565 \qquad (\%\text{ of U})^2$$

and the random-error variance due to sampling is estimated by

$$\frac{206.59}{30}-\frac{0.0565}{2}=6.86 \qquad (\%\text{ of U})^2$$

Example 3.H

(This example was provided by R. A. Schneider.)

In the previous example, there were $k=5$ items sampled with $m=4$ samples per item and $n=2$ analyses per sample. This second example is a degenerate case of situation B in that $k=n=1$.

A uranium fuel-fabrication plant burns its dry waste in an incinerator. The ash consists of about 10% uranium on a weight basis. The ash is accumulated in drums awaiting chemical leaching and recovery. Since the material is heterogeneous, it presents a sampling problem. To estimate the random-sampling-error variance, obtain ten large samples of the ash from a given drum with a core sampler. Totally dissolve each sample and measure the uranium by an analytical method having a relative standard deviation of 0.2%. From the data for the ten samples (Table 3.12), estimate the random-sampling-error variance.

TABLE 3.12 WEIGHT PERCENT OF URANIUM IN ASH
(Example 3.H)

9.8968	13.5076	11.1304
10.5124	8.5720	11.4592
9.3664	10.2304	12.0460
8.2804		

It should be apparent in this case that the sample variance for the 10 values in the table estimates the combined effects of sampling and analytical random errors. This is, by Eq. 2.61,

$$s^2 = \frac{(9.8968)^2 + \ldots + (12.0460)^2 - [(9.8968 + \ldots + 12.0460)^2/10]}{9}$$
$$= 2.5688$$

To obtain the estimate of the random-error variance due to sampling, subtract that due to analysis. This standard deviation was given as 0.2% relative or $(0.002)(10.50) = 0.021$ wt. %; 10.50% is the average of the 10 numbers in Table 3.12. Therefore the random-error variance due to sampling is estimated by $2.5688 - (0.021)^2 = 2.5684$, giving a standard deviation of $\sqrt{2.5684} = 1.60$ wt. %, or $(1.60)(100)/10.50 = 15.2\%$ relative.

Example 3.H was a very simple example treated as a special case of situation B. We could have applied the formulas of situation B directly and arrived at the same answer.

Situation C

For the simplest interlaboratory testing situation in which two laboratories make measurements on the same samples, the data are paired data, and reference is made to Sec. 3.3.1. In the more general case, k unknown samples are sent to each of m laboratories, with each laboratory making n determinations on each sample. Some reflection will make it apparent that the resulting data will have the same structure as in situation B with "items" replaced by "samples", "samples" by "laboratories", and "analyses" the same in each case. In this instance, $S_A/[km(n-1)]$ remains an estimate of the random-error variance due to analysis, averaged over the laboratories (however, see Sec. 3.3.5 on this point). The quantity $S_S/[k(m-1)]$ becomes a measure of the random-error variance among laboratories. When interest is centered on a particular laboratory, as is often the case, this quantity can be used to describe the systematic-error variance due to analysis for that (or any) laboratory. This is an important technique for obtaining an estimate of the systematic-error variance. This assumes that the average over all the laboratories is an unbiased estimate of the true value.

Many variations of experimental designs are used in interlaboratory testing. We will not discuss these designs other than to mention their existence. Some are very detailed and serve to identify and evaluate the effects of many possible sources of error. Such studies are used primarily to gain a better understanding of the factors that contribute to measurement-error variances. Analysis-of-variance techniques are used, in general, to estimate the various effects. Depending upon the complexities of the experimental design, the calculational details can become quite involved. However, the principle is the same: the total variance is divided into component parts, each part being identified with some factor.

Situation D

The term production data refers to data collected in the course of operating a given facility. They can be collected for such purposes as nuclear materials control, quality control, process improvement, or, more than likely, with several motivations in mind. Although they are normally not collected primarily to obtain estimates of measurement-error variances, these data often provide valuable information about such variances.

Many such sets of data can be analyzed by the techniques of analysis of variance. Quite often a simple one-way analysis of variance, as described in situation A, is applicable.

Example 3.I

Consider measurements made for percent of plutonium on seven UO_2–PuO_2 pellets. Three analyses were made on each pellet. Although these particular data may have been collected to demonstrate product conformance to specifications, they also provide valuable information on random-measurement-error variances. The data, in percent of plutonium, are given in Table 3.13.

TABLE 3.13 PERCENT OF PLUTONIUM IN UO_2–PuO_2 PELLETS
(Example 3.I)

Pellet	Analyses, % of Pu			Total
1	2.51	2.53	2.50	7.54
2	2.46	2.50	2.46	7.42
3	2.47	2.50	2.47	7.44
4	2.49	2.53	2.53	7.55
5	2.51	2.49	2.53	7.53
6	2.45	2.42	2.50	7.37
7	2.47	2.45	2.45	7.37
				52.22

These data fit the pattern of situation A, with "time" replaced by "pellets." Now there is a simplification since the numbers of observations are the same for each pellet. With the steps given under situation A, we get the following:

Step 1. $\dfrac{T^2}{N}=\dfrac{(52.22)^2}{21}=129.8537$

Step 2. $\bar{x}=\dfrac{T}{N}=\dfrac{52.22}{21}=2.487$

Step 3. $S_1=\dfrac{(7.54)^2+(7.42)^2+\ldots+(7.37)^2}{3}=129.8663$

Step 4. $S_2=(2.51)^2+(2.53)^2+\ldots+(2.45)^2=129.8738$

Step 5. $P=\dfrac{(21)^2-(9)(7)}{(21)(6)}=3$

(When the number of items is the same for all categories, as in this example, P is simply this number of items.)

Step 6. $M_1=\dfrac{129.8738-129.8663}{14}=0.000536$

Step 7. $M_2=\dfrac{[(129.8663-129.8537)/6]-0.000536}{3}=0.000521$

Step 8. Not pertinent in this example because there is no true value, μ_0

In this example,

$M_1=0.000536$ estimates the random-error variance due to analysis

$M_2=0.000521$ represents the differences among the pellets and can be regarded as an estimate of the random-error variance due to sampling. In this example the sampling component refers to the pellet-to-pellet variation; in other instances it may refer to the variation within a given container. We should always keep in mind just how the population of interest is defined.

Example 3.J

In Sec. 2.8.2, dealing with control charts, an example was given in which the percent of uranium factor for UO_2 powder was monitored with

a control chart. In that example, the random variable was the average factor per lot of powder, with each average based on five observations. This average was assumed to have a standard deviation of 0.06% in the construction of the control limits. The 0 06% value was based on experience data and estimated by an analysis of variance.

The experience production data used to establish the parameters of the control chart are given in Table 3.14. The data are in percent of uranium minus 87%, e.g., 0.575 corresponds to 87.575% and 0.580 to 87.580%, etc.

TABLE 3.14 PERCENT OF URANIUM FOR UO_2 POWDER *
(Example 3 J)

	Lot 1	Lot 2	Lot 3	Lot 4	Lot 5	Lot 6	
	0.575	0.587	0.535	0.539	0.656	0.590	
	0.580	0.600	0.530	0.538	0.682	0.598	
	0.572	0.604	0.538	0.547	0.650	0.593	
	0.586	0.603	0.552	0.533	0.671	0.572	
	0.577	0.609	0.545	0.508	0.677	0.607	
Total	2.890	3.003	2.700	2.665	3.336	2.960	
	Lot 7	Lot 8	Lot 9	Lot 10	Lot 11	Lot 12	
	0.719	0.613	0.618	0.629	0.442	0.617	
	0.717	0.627	0.610	0.592	0.499	0.614	
	0.667	0.652	0.613	0.628	0.509	0.604	
	0.721	0.659	0.633	0.638	0.509	0.612	
	0.717	0.626	0.610	0.606	0.480	0.612	
Total	3.541	3.177	3.084	3.093	2.439	3.059	$T = 35.947$

* Data are in percent of uranium minus 87%, e g , 0 575 corresponds to 87 575%.

These data fit the pattern of situation A, as did the previous example. Once again, follow the steps given under situation A:

Step 1. $\dfrac{T^2}{N} = \dfrac{(35.947)^2}{60} = 21.536447$

Step 2. $\bar{x} = \dfrac{T}{N} = \dfrac{35.947}{60} = 0.599$ (i.e., 87.599% of uranium)

Step 3. $S_1 = \dfrac{(2.890)^2 + (3.003)^2 + \ldots + (3.059)^2}{5} = 21.733749$

Step 4. $S_2 = (0.575)^2 + (0.580)^2 + \ldots + (0.612)^2 = 21.745445$

Step 5. $P = 5$

Step 6. $M_1 = \dfrac{21.745445 - 21.733749}{48} = 0.000244$

Step 7. $M_2 = \dfrac{[21.733749 - 21.536447/11] - 0.000244}{5} = 0.003539$

Step 8. Not pertinent in this example because there is no true value, μ_0

In this example,

M_1 estimates the random-measurement-error variance for a given sample. This includes the combined effects of sampling and analysis.

M_2 estimates the variance among lots of powder. This includes the effects of real lot-to-lot differences in percent of uranium and the short-term systematic-error variance due to analysis.

The variance of a given lot average is $(M_1/5 + M_2)$, or 0.003588, giving a standard deviation of $\sqrt{0.003588} = 0.06\%$ of uranium. (Since there are five samples per lot, M_1 is divided by 5. The basis for this is developed in Chap. 5.) This is the value used in the control chart construction. It assumes that the data of Table 3.14 represent data collected during a state of control; i.e., they represent the usual variation we would expect to see from lot to lot under well-controlled process conditions.

Before we leave the analysis of variance topic, I should emphasize that we make some rather important assumptions when we apply this method of analyzing data. We assume an additive model, that the various effects are statistically independent, and that the error variances are the same from one experimental unit to another. (This last characteristic is referred to as homogeneity of variance.) The fact that these assumptions have not been stressed in this discussion does not detract from their importance. The last assumption, which is very important, provides a natural introduction to the next topic.

3.3.5 Test for Homogeneity of Variance

By now, it should be apparent that there are many ways in which we can estimate measurement-error variances. Further, within a given

experiment or for a given set of data, there may be several estimates of the same variance. The resulting estimate that is to be used in application is an average (perhaps weighted) of these individual estimates, where it is implicitly assumed that all the quantities are estimating the same parameter.

As an illustration, consider example 3.G in situation B in the previous section, and, in particular, the estimate of the random-error variance due to sampling, 13.77 (% of U)^2. It is evident from calculation step 4 that this variance estimate is an average of five separate estimates, one associated with each container of ADU scrap. Each estimate is based on 3 degrees of freedom, which explains why the overall estimate is based on 15 degrees of freedom. The analysis of variance technique provides the average estimate based on the 15 degrees of freedom because of the important assumption of homogeneous variance implicit in an analysis of variance. We might, however, like to verify the validity of this assumption because, in this instance, for example, it may well be that the sampling-error variance is not the same for the various containers owing to the different kinds of scrap that might be classified as ADU scrap.

A test that can be used to test the hypothesis that k variances are all estimates of the same parameter is known as Bartlett's test. (If $k=2$, then the F test described in Sec. 2.6.4 can be applied.) Bartlett's test, which assumes the underlying population variances have the normal density function, consists of the following steps:

Given the k-sample variances $s_1^2, s_2^2, \ldots, s_k^2$, computed by Eq. 2.61 and based on $\nu_1, \nu_2, \ldots, \nu_k$ degrees of freedom, respectively,

Step 1. Calculate $\nu=\nu_1+\nu_2+\ \ldots\ +\nu_k$

Step 2. Calculate $s^2=\dfrac{\nu_1 s_1^2+\nu_2 s_2^2+\ \ldots\ +\nu_k s_k^2}{\nu}$

Step 3. Find $Q=\nu \ln s^2-\sum_{i=1}^{k} \nu_i \ln s_i^2$

Step 4. Find $B=1+\dfrac{\left(\sum_{i=1}^{k} \dfrac{1}{\nu_i}-\dfrac{1}{\nu}\right)}{3(k-1)}$

Step 5. Compute Q/B.

Step 6. If $Q/B>\chi^2_{1-\alpha}$ as defined by Eq. 2.67 for $(k-1)$ degrees of freedom, reject the hypothesis that $\sigma_1^2=\sigma_2^2=\ \ldots\ =\sigma_k^2$, where s_i^2 is the estimate of σ_i^2. The value of $\chi^2_{1-\alpha}$ can be read from Appendix B.

Example 3.K

In this example the test for homogeneity of variance, with $\alpha = 0.01$, is applied to the data of example 3.G, Sec. 2.3.4. Here, $\nu_i = 3$ for all $i = 1, 2, \ldots, 5$. The s_i^2 values are, from step 4 of situation B:

$$s_1^2 = 131.05/3 = 43.68 \qquad s_4^2 = 15.22/3 = 5.07$$
$$s_2^2 = 20.20/3 = 6.73 \qquad s_5^2 = 26.01/3 = 8.67$$
$$s_3^2 = 14.11/3 = 4.70$$

Step 1. $\nu = 3+3+3+3+3 = 15$

Step 2. $$s^2 = \frac{3(43.68)+3(6.73)+ \ldots +3(8.67)}{15} = \frac{206.55}{15} = 13.770$$

(Compare this with the value for $S_S/[k(m-1)]$ in example 3.G.)

Step 3. $\nu \ln s^2 = 15 \ln 13.770 = 39.337$

$$\sum \nu_i \ln s_i^2 = 3 \sum \ln s_i^2$$

$$\ln s_1^2 = 3.777$$
$$\ln s_2^2 = 1.907$$
$$\ln s_3^2 = 1.548$$
$$\ln s_4^2 = 1.623$$
$$\ln s_5^2 = 2.160$$
$$\overline{11.015}$$

Multiply 11.015 by 3: 33.045

Step 4. $$B = 1 + \frac{(5/3)-(1/15)}{12} = 1.13333$$

Step 5. The $\alpha = 0.01$ critical value is 13.28 from Appendix B.
$Q/B = 13.770/1.1333 = 12.15$

Step 6. Since 12.15 < 13.28, do not reject the hypothesis. Conclude that $\sigma_1^2 = \sigma_2^2 = \ldots = \sigma_5^2$.

In this particular example it might have been preferable to apply a different test for homogeneity of variances. Bartlett's test fits the situation in which the alternative hypothesis is not specified except to say that H_0: $\sigma_1^2 = \sigma_2^2 = \ldots = \sigma_k^2$ is not true. There are other tests that can be applied if the alternative hypothesis is stated more precisely. In particular, if we suspect that *one* of the variances is excessively high or low while the others agree among themselves, we can apply a test known as Cochran's test.

This appears to be the situation with this set of data in which s_1^2 is considerably larger than the other variances. However, the reader is again cautioned on the danger of formulating hypotheses after the data are collected. Unless we have an a priori reason for specifying the alternative hypothesis, it is advisable to apply a generalized test such as Bartlett's.

There are other situations in which we may wish to apply a test of homogeneity of variances. This is often done with interlaboratory testing because in this situation it is important to test for equality of random-error variances for the laboratories involved. As another instance, when historical production data provide information on a given error variance, it is advisable to perform routine tests of the hypothesis that this particular error variance is remaining constant.

3.3.6 Systematic Errors in Sampling

Systematic-error variances due to sampling are perhaps the most difficult of all measurement parameters to estimate. Many sources can contribute to this error, especially in a facility in which sampling of liquids is required. In many instances it is difficult to distinguish between the effects of systematic error due to sampling and the effects due to analytical factors, and we can only estimate their combined effects. Often, this is satisfactory in application, but it provides little insight into the steps that should be taken to reduce error variances when they are too large.

One method of estimating systematic-error variances due to sampling is the synthetic method to be discussed in Sec. 3.3.7. However, this method is often very difficult because of the problems associated with identifying primary error sources on the one hand and of evaluating their variances on the other. In general, the synthetic method cannot be considered a very satisfactory estimation method for sampling error variances.

An alternate approach, and perhaps the only reasonable one, is to conduct special experimental studies whose primary purpose is to evaluate the magnitude of the systematic-sampling-error variance. This is illustrated by example 3.L.

Example 3.L

(This example was supplied by R. A. Schneider.)

A chemical processing facility is to conduct cold start-up tests on the sampling system used for the input-accountability tank. One aim of the test is to determine if the sampling system, which employs an air lift, concentrates or dilutes the sample, i.e., creates a systematic sampling error. The test consists in filling the tank with a solution of uranyl nitrate with a uranium concentration of 300 g/liter. Large-volume samples are then dipped from the tank, and parallel samples are taken by means of the air-

lift system; both samples are sent to the laboratory for analysis of uranium concentration.

It is important to stop at this point and comment on the role of the dip samples. We might argue that since the concentration of the tank is known the air-lift results can be compared directly with this known standard and the techniques of Sec. 3.3.2 can be applied. This approach has some merit and may indeed be the preferred one, but we must recognize that the systematic-error variance thus estimated is the combined effects of such errors due to sampling and analysis. We could, of course, obtain estimates of the systematic-error variance due to analysis by separate experimentation and subtract this error variance from the variance produced by the sampling experiment. On the other hand, if the systematic-error variance for air-lift samples is found by treating the dip-sample results as the known standard, then it should be clear that the effects of systematic errors due to analysis cancel out and the resulting estimate is a direct estimate of the systematic-error variance due to sampling. This particular set of data is treated in this fashion. The data for 16 replications of the test are given in Table 3.15.

TABLE 3.15 ANALYSIS OF URANIUM CONCENTRATION
(Example 3.L)

Replication	Uranium concentration, g/liter	
	Air-lift sample	Dip sample
1	300.5817	299.9514
2	300.1155	299.5146
3	299.6751	300.1134
4	299.9061	299.9829
5	300.1818	300.4068
6	300.2763	299.7246
7	299.5581	300.0036
8	299.7447	299.7267
9	300.0630	300.3711
10	300.3798	299.5848
11	299.8278	300.2877
12	299.8296	300.2193
13	299.9238	300.2151
14	299.7237	299.5101
15	299.6394	300.3342
16	300.0363	300.3453

The steps of Sec. 3.3.2 are applied:

Step 1. $n = 16$ for both the air-lift and dip samples

Step 2. Air lift: $\bar{x}_1 = \dfrac{(300.5817) + \ldots + (300.0363)}{16} = 299.9664$

Dip: $\bar{x}_2 = 300.0182$

Air lift: $s_1^2 = \{(300.5817)^2 + \ldots + (300.0363)^2 - [(300.5817 + \ldots + 300.0363)^2/16]\}/15$
$= 0.082553$

Dip: $s_2^2 = 0.101334$

Step 3. $\mu_0 = 300.0182$ (i.e., $\bar{x}_2$ plays the role of the standard)

Air lift: $\hat{B} = \bar{x}_1 - \bar{x}_2 = -0.0518$

Air lift: Variance $\bar{x}_1 = s_1^2/n = 0.082553/16 = 0.005160$
Standard deviation $\bar{x} = \sqrt{0.005160} = 0.0718$

Dip: Variance $\bar{x}_2 = 0.101334/16 = 0.006333$
Standard deviation $\bar{x}_2 = 0.0796$

Step 4. **a.** If the bias correction is made, i.e., if in application the results will be adjusted by adding 0.0518 g of uranium per liter to the observed concentrations, then the systematic-error variance due to sampling by the air-lift method is estimated by

$$\frac{s_1^2}{n} + s_0^2 = 0.005160 + 0.006333 = 0.011493$$

where s_0^2 is the variance assigned the standard value, i.e., the average for the dip sample, s_2^2/n in this instance.

b. If no bias correction is made, then the systematic-error variance due to sampling by the air-lift method is estimated by

$$(\bar{x}_1 - \bar{x}_2)^2 + s_0^2 = 0.002683 + 0.006333 = 0.009016$$

Step 5. The random-error variance due to sampling plus analysis is estimated by $s_1^2 = 0.082553$. Note that the estimate of the random-error variance includes the effects of both sampling and analysis. The error variance due to analysis must be estimated separately. As an alternative, replicate analytical determinations could have been made to provide an estimate of this variance internal to the experiment.

(We might wish to regard these data as paired in the sense that conditions might change within the tank and/or in the analytical laboratory. In this event the methods of Chap. 8 can be used to provide added insight.)

This is an illustration of how systematic-error variances due to sampling can be estimated. The principle should be very clear in any sampling situation: compare sample results obtained by the usual sampling method with "the truth." The problem comes in determining the truth. In this example the truth was established through the use of a sampling method assumed to produce a sample representative of the true contents of the container. In other instances the truth may be based on intensive sampling of the contents of the container in question.

3.3.7 Synthetic Approach To Estimating Systematic-Error Variance

The synthetic approach to estimating error variances is another approach that can be used to estimate systematic-error variances. This method involves identification of all steps that lead to a reported result. At each step any factor that would, if in error, affect all results in the same way would be a contributor to the systematic-error variance. A technical appraisal must be made of the possible magnitude of each such error. These individual error effects are then combined appropriately by methods to be discussed in the next chapter.

The details of this approach to error estimation are best presented with a simple example. The application to other situations should then be obvious in principle.

Example 3.M

In Sec. 3.2, I mentioned the measurement situation in which total uranium in a process tank is to be determined by measuring the volume in the tank and then measuring the concentration from a tank sample. Consider the systematic-error variance associated with the determination of the uranium concentration. In particular, for illustrative purposes, fix attention on the variance attributable to the uncertainties in two "constants," the normality of the oxidizing solution ($0.2000N$) and the volume of the 2.00-ml pipet in the following equation for uranium concentration:

$$U_{conc} = \frac{(\text{ml})(\text{equiv. wt. of U})(0.2000N)}{2.00 \text{ ml}} \tag{3.8}$$

Since the $0.2000N$ and 2.00-ml values are applied to successive batches, any uncertainty in these values will be described jointly by a systematic-error variance. These two values can be regarded as random variables drawn from density functions with standard deviations of σ_1 and σ_2, respectively. The determination of σ_1 and σ_2 poses another problem. For pipet volume some value can be assigned the standard deviation on the

basis of tolerance statements supplied by the manufacturer or perhaps by the National Bureau of Standards. The normality of the oxidizing solution is determined by repetitive titration of a primary standard, and the value of σ_1 can be determined by methods of Sec. 3.3.2. Whatever technique is used to evaluate σ_1 and σ_2 (including technical judgment) assume that these values are known.

Designate by σ_u the systematic-error standard deviation for the uranium-concentration determination. Looking ahead to the next chapter, and in particular to Eqs. 4.4 and 4.6, we can evaluate σ_u. Write

$$U=\frac{K(0.2000+\Delta_1)}{2.00+\Delta_2} \tag{3.9}$$

where K is the product of (ml) (equivalent wt. of uranium); Δ_1 is a random observation from the population with density function having mean zero and standard deviation σ_1; and Δ_2 is a random observation from the population having mean zero and standard deviation σ_2. Equation 3.9 is in the form of Eq. 4.4 where x is identified with U, x_1 with Δ_1, and x_2 with Δ_2. Then, Eq. 4.6 can be applied. This requires finding the partial derivatives of U with respect to Δ_1 and Δ_2.

$$\frac{\partial U}{\partial \Delta_1}=\frac{K}{(2.00+\Delta_2)} \tag{3.10}$$

$$\frac{\partial U}{\partial \Delta_2}=-\frac{K(0.2000+\Delta_1)}{(2+\Delta_2)^2} \tag{3.11}$$

To apply Eq. 4.6, evaluate these partial derivatives at their means, both of which are assumed to be zero.

$$\frac{\partial U}{\partial \Delta_1}=\frac{\cdot K}{2.00}=0.5K$$

$$\frac{\partial U}{\partial \Delta_2}=-\frac{0.200K}{4}=-0.05K$$

Then from Eq. 4.6,

$$\begin{aligned}\sigma_u^2 &\approx (0.5K)^2\sigma_1^2+(-0.05K)^2\sigma_2^2 \\ &\approx K^2(0.25\sigma_1^2+0.0025\,\sigma_2^2)\end{aligned} \tag{3.12}$$

This gives the systematic-error standard deviation:

$$\sigma_u \approx K(0.25\sigma_1^2+0.0025\sigma_2^2)^{1/2} \tag{3.13}$$

Assume $K=3360$, $\sigma_1=0.0002$, and $\sigma_2=0.006$; then,

$$\sigma_u \approx 3360[(0.25)(4)(10^{-8})+(0.0025)(3600)(10^{-8})]^{1/2}$$
$$\approx 1.0625$$

At this value of K,

$$U=\frac{3360(0.2)}{2}=336.0$$

from Eq. 3.8, and expressing this systematic-error standard deviation on a relative basis gives

$$\frac{\sigma_u}{U}=\frac{1.0625}{336.0}=0.00316=0.316\%$$

This example was simplified for illustrative purposes. There is no intent to imply that the two sources identified are the only ones that contribute to the systematic error in the uranium-concentration determination.

We should note that the synthetic approach is especially valuable as a diagnostic tool, i.e., in evaluating the importance of primary error sources on the total error variance. From this point of view, it is not essential to know precisely the individual standard deviations used in the analysis. In application, it is reasonable to require that standards must ultimately be used to obtain valid estimates of systematic-error variances, or, at least, to confirm that estimates found by other means are reasonably valid.

3.3.8 Linear Calibration, Independent Data

In a sense this section can be regarded as an extension of Sec. 3.3.2. The distinction is that now, rather than calibrating against a known standard, we calibrate against a series of known standards having different assigned standard values.

With this problem a word of caution is in order. Calibration work of the type described here is often performed in connection with calibrating nondestructive assay (NDA) equipment to measure, for example, the amount of ^{235}U in a waste barrel. In this particular instance the standard is known in the sense that the amount of ^{235}U contained in the calibration barrel is known precisely, but the number of counts observed will vary considerably according to how the uranium is dispersed. Thus, in a very real sense, the standard is not really known.

The creation of valid standards for NDA application poses a very real problem. In the example under discussion, one satisfactory approach might be to disperse given amounts of ^{235}U in different ways throughout the barrel during the calibration so that this dispersal will describe how

uranium might actually be reasonably dispersed in the waste barrels to be measured. The resulting scatter in the counts for a given amount of ^{235}U then reflects reality, and the corresponding calibration curve with its uncertainty is reasonably valid. Another possibility is to calibrate against actual waste barrels rather than created standards. This can be done by counting a number of barrels and then selecting some whose contents will be incinerated and leached and the residue carefully assayed for ^{235}U by wet chemistry. The amount of ^{235}U found in a given barrel can then be considered as the standard value. With both methods suggested, the standards can then be considered to be known in the true sense of the word, and the methods discussed in Sec. 3.3.8 can be applied.

The problem now is to estimate the calibration line and to estimate the appropriate random- and systematic-error variances. A very simple mathematical model is assumed. In spite of its simplicity, the model describes a commonly encountered situation which is applicable to many problems likely to occur in the nuclear materials control area. The two basic assumptions are (1) that the calibration relation is linear and (2) that there is statistical independence between any two observations on the random variable.

There is a unique feature of linear-calibration work that sets it apart from the usual problem of fitting a straight line through a set of data. The distinction is noted here. In the traditional problem we fix the values of some independent variable, X, and do so without error. Corresponding to each fixed value of X, a value of a dependent variable, Y, is observed. The variable Y is a random variable and hence is affected by random errors. The usual linear model is of the form

$$y=\alpha+\beta x+\epsilon \tag{3.14}$$

where the parameters α and β are estimated by standard least-squares procedures, i.e., they are chosen such that the sum of the squared distances between the observed values, y_i, and the true values, $(\alpha+\beta x_i)$, is minimized. The ϵ is called the error term and is generally assumed to have mean zero and variance σ_ϵ^2. (If, in addition, ϵ is normally distributed, then the least-squares estimates of α and β are identical with the maximum-likelihood estimates of the parameters. See Sec. 2.7.1 for the definition of maximum-likelihood estimation.)

Thus far this situation is identical with that arising in linear-calibration applications. However, in calibration applications in which the derived model is applied, there is an important difference. Although the calibration line is estimated by fixing x and observing y, in applying the calibration line, we observe y and predict the x value that corresponds to it. Thus the linear relation is used in the reverse form.

$$x = \frac{y-\alpha}{\beta} = \alpha' + \beta' y \tag{3.15}$$

where $\alpha' = -\alpha/\beta$ and $\beta' = 1/\beta$ relates the two sets of parameters. Various investigators have suggested that in this calibration situation the parameters α' and β' be estimated by reversing the roles of x and y, i.e., by treating X as the dependent variable and Y as the independent variable. This approach, called the inverse model, does have some merit, and the statistical properties of the estimates of the resulting parameters are better than those found by the traditional approach under certain defined circumstances. As a general rule, however, it is preferable to follow the direct approach, rather than this inverse approach, and then to use the derived model, Eq. 3.15.

The least-squares estimates of α and β in Eq. 3.14 are given in many texts. If we let the data set be paired values (x_i, y_i) with $i = 1, 2, \ldots, n$, these estimates are

$$\hat{\beta} = \frac{\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i \Big/ n \right)}{\sum_{i=1}^{n} x_i^2 - \left[\left(\sum_{i=1}^{n} x_i \right)^2 \Big/ n \right]} \tag{3.16}$$

and

$$\hat{\alpha} = \bar{y} - \hat{\beta}\bar{x} \tag{3.17}$$

where $\bar{y}$ and $\bar{x}$ are the sample means. The parameters α' and β' are then estimated from

$$\hat{\beta}' = 1/\hat{\beta} \tag{3.18}$$

$$\hat{\alpha}' = -\hat{\alpha}/\hat{\beta} \tag{3.19}$$

From a measurement-error viewpoint, the errors associated with $\hat{\beta}'$ and $\hat{\alpha}'$ are systematic errors as long as the particular estimated calibration line is used.

As a result, the error associated with a predicted value for X for a given known value of Y is also a systematic error. Specifically, because ϵ is a random variable, in a usual linear least-squares situation, the parameter estimates $\hat{\alpha}$ and $\hat{\beta}$ have variances

$$\sigma_{\hat{\alpha}}^2 = \frac{R \sum_{i=1}^{n} x_i^2}{n} \tag{3.20}$$

$$\sigma_{\hat{\beta}}^2 = R \tag{3.21}$$

and their covariance (see Sec. 2.5 for definition) is

$$\sigma_{\hat{\alpha},\hat{\beta}} = -R\bar{x} \tag{3.22}$$

where R is defined by

$$R = \frac{\sigma_\epsilon^2}{\sum_{i=1}^{n} x_i^2 - \left[\left(\sum_{i=1}^{n} x_i\right)^2 \Big/ n\right]} \tag{3.23}$$

and σ_ϵ^2 is estimated by

$$\hat{\sigma}_\epsilon^2 = \sum_{i=1}^{n} \frac{(y_i - \hat{\alpha} - \hat{\beta}x_i)^2}{n-2} \tag{3.24}$$

or, equivalently, by

$$\hat{\sigma}_\epsilon^2 = \frac{\sum_{i=1}^{n} y_i^2 - \hat{\alpha}\sum_{i=1}^{n} y_i - \hat{\beta}\sum_{i=1}^{n} x_i y_i}{n-2} \tag{3.25}$$

Then, looking ahead to the results of Sec. 4.2.2 (see example 4.E), we find the variance of the calibration equation (Eq. 3.15) for a given known value of y, y_0 to be estimated by

$$\hat{\sigma}_s^2 \approx R\frac{\left[\left(\sum_{i=1}^{n} x_i^2\right)\Big/ n\right] + [(y_0 - \hat{\alpha})^2/\hat{\beta}^2] - \{[2(y_0 - \hat{\alpha})\bar{x}]/\hat{\beta}\}}{\hat{\beta}^2} \tag{3.26}$$

This variance is denoted by σ_s^2 to emphasize that it is a systematic-error variance.

If there are two predictions of X, corresponding to two different *known* values of y, say y_1 and y_2, then these two predictions will be correlated. The covariance is designated by σ_{ij} and is equal to

$$\sigma_{ij} \approx R\frac{\left[\left(\sum_{i=1}^{n} x_i^2\right)\Big/ n\right] + \{[(y_1 - \hat{\alpha})(y_2 - \hat{\alpha})]/\hat{\beta}^2\} - \{[(y_1 + y_2 - 2\hat{\alpha})\bar{x}]/\hat{\beta}\}}{\hat{\beta}^2} \tag{3.27}$$

Equation 3.26 gives the systematic-error variance induced by the calibration, assuming that the y value is known. In practice we do not know y but observe a value for y. This observed value of y has a random-error variance, σ_ϵ^2, estimated by $\hat{\sigma}_\epsilon^2$, and it produces a random-error variance in the predicted x of

$$\hat{\sigma}_r^2 = \frac{\hat{\sigma}_\epsilon^2}{\hat{\beta}^2} \tag{3.28}$$

Let us summarize the results of this section. The following steps are performed in a linear-calibration situation:

Step 1. The observed calibration data (x_i, y_i) are used to estimate the calibration parameters with Eqs. 3.16 and 3.17.

Step 2. The parameters for the reverse calibration line (Eq. 3.15) are estimated with Eqs. 3.18 and 3.19.

Step 3. In application a value is observed for Y. Call this value y_0. The corresponding value for X is x_0 and is predicted by using the model of Eq. 3.15 with $y = y_0$.

Step 4. The systematic-error variance associated with x_0 is given by Eq. 3.26.

Step 5. The random-error variance is given by Eq. 3.28.

Step 6. If two values are observed for Y, i.e., y_1 and y_2, and the values of X, i.e., x_1 and x_2, are predicted with Eq. 3.15, then the systematic errors in x_1 and x_2 are correlated. The covariance is given by Eq. 3.27.

Step 7. The systematic-error variance of the sum $(x_1 + x_2)$ can be found by evaluating Eq. 3.26 separately for x_1 and x_2 and adding the results. This sum is then added to twice the covariance of step 6.

Step 8. The random-error variance of the sum can be found by multiplying the result of step 5 by 2.

Step 9. If there are k items in a sum, i.e., if the given data points are $y_1, y_2, \ldots, y_k$, then the total of the corresponding x's, $(x_1 + x_2 + \ldots + x_k)$, denoted by x_T, can be found by using Eq. 3.15 with $k\alpha'$ replacing α' and the sum of the y's replacing y.

Step 10. The systematic-error variance of x_T is given by multiplying Eq. 3.26 by k^2 and replacing y_0 by the average of the k y's.

Step 11. The random-error variance of x_T is given by multiplying Eq. 3.28 by k.

Steps 9 to 11 correspond to a special case of steps 12 to 14 in which all the $c_i = 1$.

Step 12. If the sum of the x's is a general sum of the form $x_s = c_1x_1 + c_2x_2 + \ldots + c_kx_k$, where the c's are arbitrary constants, then x_s can be found by using Eq. 3.15 with $(\alpha' \sum_{i=1}^{k} c_i)$ replacing α' and $(\sum_{i=1}^{k} c_i y_i)$ replacing y.

Step 13. The systematic-error variance of x_s is given by Eq. 3.26 with the first term multiplied by $(\sum_{i=1}^{k} c_i)^2$, y_0 replaced by $(\sum_{i=1}^{k} c_i y_i)$, and $\hat{\alpha}$ replaced by $(\hat{\alpha} \sum_{i=1}^{k} c_i)$.

Step 14. The random-error variance of x_s is found by multiplying Eq. 3.28 by $\sum_{i=1}^{k} c_i^2$.

Example 3.N

Let us now apply these results to a set of calibration data. Let the data consist of measurements for total ^{235}U made by an NDA instrument on 1-gal containers known to contain specified amounts of ^{235}U. The X and Y variables are defined by X = known amount of ^{235}U in a given container and Y = net counts produced by the NDA instrument. If the random-error variance in Y is affected primarily by counting statistics, then σ_ϵ^2 is not constant but increases in proportion to the number of counts observed. It is assumed here, as is often the case, that the counting-statistics source of variation is dominated by other sources of random error and that σ_ϵ^2 can with reasonable validity be assumed to be constant over the range of the data.

The data are given in Table 3.16.

TABLE 3.16 MEASUREMENTS FOR TOTAL ^{235}U
(Example 3.N)

X, g of ^{235}U	Y, net counts
10	890
15	1234
20	1491
25	1815
40	2896
50	3718

Let us apply the summary steps 1 to 6. Certain quantities are calculated, as follows, for use in these steps.

$$\Sigma y = 12{,}044 \qquad \Sigma x^2 = 5450$$
$$\Sigma x = 160 \qquad \Sigma y^2 = 30{,}042{,}502$$
$$\Sigma xy = 404345 \qquad n = 6$$

Step 1. By Eq. 3.16,

$$\hat{\beta} = \frac{404345 - [(160)(12044)/6]}{5450 - [(160)^2/6]} = \frac{83171.6667}{1183.3333} = 70.286$$

By Eq. 3.17,

$$\hat{\alpha}=\frac{12044}{6}-\frac{(70.286)(160)}{6}=133.04$$

Step 2. By Eq. 3.18,

$$\hat{\beta}'=\frac{1}{70.286}=0.01423$$

By Eq. 3.19,

$$\hat{\alpha}'=-\frac{133.04}{70.286}=-1.893$$

Step 3. Assume that a reading is taken on a container whose ^{235}U content is not known and that the observed y value, y_1, is 1000 counts. Then the predicted amount of ^{235}U in the container is, by Eq. 3.15,

$$x_1=-1.893+(0.01423)(1000)=12.34 \text{ g of } ^{235}U$$

Step 4. The systematic-error variance of x_1 is given by Eq. 3.26. First, R must be evaluated. This requires that σ_ϵ^2 be estimated. By Eq. 3.25,

$$\hat{\sigma}_\epsilon^2=\frac{30{,}042{,}502-(133.04)(12044)-(70.286)(404345)}{4}$$

$$=5094$$

By Eq. 3.23,

$$R=\frac{5094}{1183.3333}=4.305$$

By Eq. 3.26,

$$\sigma_\delta^2=4.305\{(5450/6)+[(1000-133.04)^2/(70.286)^2]$$
$$-[2(1000-133.04)(26.667)/70.286]\}/(70.286)^2$$

$$\cong\frac{4.305(908.33+152.15-657.86)}{4940.12}$$

$$=0.3509 \quad g^2 \text{ of } ^{235}U$$

Step 5. The random-error variance is, by Eq. 3.28,

$$\sigma_r^2 \approx \frac{5094}{(70.286)^2} \approx 1.0311 \quad g^2 \text{ of } {}^{235}U$$

Therefore the total variance for the predicted amount of ^{235}U in that container is

$$0.3509 + 1.0311 = 1.382 \quad g^2 \text{ of } {}^{235}U$$

which gives a standard deviation of 1.18 g of ^{235}U, or about 10% of the amount present.

Second Container. Now suppose that another container is counted and produces a count of 2000. By Eq. 3.15, the predicted amount of ^{235}U in that container is

$$x_2 = -1.893 + (0.01423)(2000) = 26.57 \quad g \text{ of } {}^{235}U$$

so that the total for the two cans is

$$T = 12.34 + 26.57 = 38.91 \quad g \text{ of } {}^{235}U$$

Step 6. By the application of Eq. 3.27, the covariance between x_1 and x_2 is estimated by

$$\begin{aligned}\sigma_{12} &\approx 4.305\{(5450/6) + [(1000-133.04)(2000-133.04)/(70.286)^2] \\ &\quad - [(3000-266.08)(26.667)/70.286]\}/(70.286)^2 \\ &\approx \frac{4.305\ (908.33+327.64-1037.27)}{4940.12} \\ &\approx 0.1732 \quad g^2 \text{ of } {}^{235}U\end{aligned}$$

Step 7. For the systematic-error random variance for the total amount in the two containers, the systematic-error variance of x_2 can be found by Eq. 3.26.

$$\begin{aligned}\sigma_{s_2}^2 &\approx 4.305\{(5450/6) + [(2000-133.04)^2/(70.286)^2] \\ &\quad - [2(2000-133.04)(26.667)/70.286]\}/(70.286)^2 \\ &\approx \frac{4.305\ (908.33+705.56-1416.68)}{4940.12} \\ &\approx 0.1719 \quad g^2 \text{ of } {}^{235}U\end{aligned}$$

Then, with this result plus the results of steps 4 and 6, the systematic-error variance of the sum (x_1+x_2) is the variance of each term plus twice the covariance, or

$$0.3509+0.1719+2(0.1732)=0.8692 \quad g^2 \text{ of } {}^{235}U$$

Step 8. The random-error variance for the sum (x_1+x_2) is, from the result of step 5,

$$2(1.0311)=2.0622 \quad g^2 \text{ of } {}^{235}U$$

The total variance of T is

$$0.8692+2.0622=2.9314 \quad g^2 \text{ of } {}^{235}U$$

which gives a standard deviation of 1.712 g of ^{235}U, or about 4.4% of the total amount.

Alternatively, for the total ^{235}U in the two containers, steps 9 to 11 can be applied. Here, $k=2$ and $\sum_{i=1}^{k} y_i = 1000+2000=3000$; so the average y value is 1500.

Step 9. The total amount of ^{235}U in the two containers is

$$x_T=(2)(-1.893)+(0.01423)(3000)=38.91 \quad g \text{ of } {}^{235}U$$

Step 10. The systematic-error variance associated with x_T is

$$\sigma_s^2=\frac{(2)^2(4.305)}{(70.286)^2} \times\left[\frac{5450}{6}+\frac{(1500-133.04)^2}{(70.286)^2}-\frac{2(1500-133.04)(160)}{(6)(70.286)}\right]$$

$$=0.003486(908.3333+378.2457-1037.2554)$$

$$=0.8691 \quad g^2 \text{ of } {}^{235}U$$

in agreement with step 7.

Step 11. The random-error variance associated with x_T is

$$\sigma_r^2=2(1.0311)=2.0622 \quad g^2 \text{ of } {}^{235}U$$

in agreement with step 8.

Example 3.O

Suppose there are five containers whose amounts of ^{235}U are to be

found by using the calibration line estimated in the previous example. Let the counts on these five containers be

$$\left.\begin{aligned} y_1 &= 1000 \\ y_2 &= 2000 \\ y_3 &= 800 \\ y_4 &= 3400 \\ y_5 &= 1300 \end{aligned}\right\} \begin{aligned} &\text{Sum} = 8500 \text{ counts} \\ &\text{Average} = 1700 \text{ counts} \end{aligned}$$

Then we apply steps 9 to 11.

Step 9. The total amount of ^{235}U in the five containers is

$$x_T = 5(-1.893) + (0.01423)(8500) = 111.49 \quad \text{g of } ^{235}U$$

Step 10. The systematic-error variance associated with x_T is

$$\sigma_s^2 = \frac{(5)^2(4.305)}{(70.286)^2} \times \left[\frac{5450}{6} + \frac{(1700-133.04)^2}{(70.286)^2} - \frac{2(1700-133.04)(160)}{(6)(70.286)}\right]$$

$$= 0.02179(908.3333 + 497.0249 - 1189.0163)$$

$$= 4.714 \quad \text{g}^2 \text{ of } ^{235}U$$

Step 11. The random-error variance associated with x_T is

$$\sigma_r^2 = 5(1.0311) = 5.1555 \quad \text{g}^2 \text{ of } ^{235}U$$

For another example see example 6.H.

3.3.9 Linear Calibration, Cumulative Data

In the preceding section, we assumed that any two observations on the random variable were statistically independent. There is a situation in nuclear materials control applications in which this may be a poor assumption.

Consider the calibration of a process vessel. Assume that a linear model is applicable, as is generally the case, or nearly so. The tank is calibrated by adding "known" weights of liquid to the tank and observing the manometer reading. In practice, the tank is not emptied between additions; therefore any errors associated with early additions of liquid affect later total amounts also. Thus the data are cumulative in nature, and the cumulative model is used to describe this calibration situation.

To be consistent with the previous section, since the amount of liquid added at each increment is the controlled variable and the manometer reading is the dependent variable during calibration, we should perhaps identify the X variable with the total amount of liquid added and the Y variable with the manometer reading. However, most writers on this subject make the opposite identification, i.e., Y is identified with the amount of liquid and X with the manometer reading. This is done because it is generally assumed that the manometer reading is not subject to error (i.e., it can be read exactly), whereas the amounts of liquid added at each step have random errors associated with them. By identifying X with the manometer reading and Y with the liquid weight, we thereby estimate the calibration model directly without requiring the inverse relationship since, in application of the calibration line, the manometer is read and the corresponding weight predicted.

It develops that both identifications will give the same result in working with the cumulative model; i.e., we can either call X the manometer reading and Y the weight and use the resulting calibration curve directly, or we can call X the weight and Y the manometer reading and use the inverse of the calibration curve. This freedom of choice does not exist in the previous section, where the actual estimates for the parameters depend on which variable is regarded as the independent variable and which the dependent. Since this is not a consideration for the model under discussion, we choose to be consistent with most workers in the process vessel calibration area and to let X refer to the manometer reading and Y to the cumulative weight.

It should be noted that among workers in the field there is not universal agreement that the cumulative model is the appropriate one to use in process tank calibration work. Some workers argue that the amount of liquid added at each step is known precisely, contrary to the assumptions of this model, while the manometer reading is subject to random error. If this is the case, the model of Sec. 3.3.8 is applicable. Others argue that, although the amounts of liquid added may be known, not all the liquid actually reaches the tank through the piping with each addition, and hence this has the same effect as if the amounts added were not known precisely. In this latter case there is a concern that the random errors associated with the additions of liquid are not independent, which would violate another assumption of the cumulative model. It should be noted that in any modeling situation we attempt to model reality as well as is reasonable, but we recognize that there are often discrepancies between reality and the mathematical models used to describe it. The cumulative model has received sufficient emphasis in process tank calibration work to warrant inclusion in this book. The user is cautioned to exercise his own technical judgment on the validity of the assumptions in any given application.

On the surface the cumulative model appears identical to Eq. 3.14. For the ith point,

$$y_i = \alpha + \beta x_i + \epsilon_i \tag{3.29}$$

For the cumulative model, however, y_i is actually the sum of a number of liquid additions:

$$y_i = \Delta y_1 + \Delta y_2 + \ldots + \Delta y_i \tag{3.30}$$

Assume that

$$\sigma_{\Delta y_i} = \sigma_{\delta_i}^2 = (x_i - x_{i-1})\sigma^2 \tag{3.31}$$

That is, the random-error variance associated with a given addition of liquid is proportional to the amount of liquid added. Because of this error structure, the successive y_i values are not statistically independent, i.e., they have a nonzero covariance. Therefore the assumptions required for a least-squares fit are violated, and α and β cannot be estimated with validity by the methods of the previous section.

There are two ways to proceed with the estimation. One involves application of the so-called "generalized least-squares" approach to estimation, which takes into account the covariance between any two y_i, y_j values. This approach is beyond the scope of this book. The other approach, which yields equivalent results, involves estimating the parameter β by successively differencing the y_i values and thus creating statistical independence. Specifically, it is easy to see that

$$\begin{aligned} y_2 - y_1 &= \beta(x_2 - x_1) + \delta_2 \\ y_3 - y_2 &= \beta(x_3 - x_2) + \delta_3 \\ &\text{etc.} \end{aligned} \tag{3.32}$$

where the δ_i observations on the random error associated with these differences are statistically independent of one another. However, they have different variances unless $(x_i - x_{i-1})$ is the same for all i, i.e., unless equal increments of liquid are added. This does not create a problem since a weighted least-squares approach can be used to give the estimate for β. Upon simplification this is

$$\hat{\beta} = \frac{y_n - y_1}{x_n - x_1} \tag{3.33}$$

Thus for this cumulative model the estimate of the slope is found by

simply fitting the straight line through the first and last points.* The corresponding estimate for α is

$$\hat{\alpha}=y_1-\hat{\beta}x_1 \tag{3.34}$$

These parameter estimates have variances given by

$$\sigma^2_{\hat{\alpha}}=\frac{s^2x_1x_n}{x_n-x_1} \tag{3.35}$$

and

$$\sigma^2_{\hat{\beta}}=\frac{s^2}{x_n-x_1} \tag{3.36}$$

The covariance between $\hat{\alpha}$ and $\hat{\beta}$ is

$$\sigma_{\hat{\alpha},\hat{\beta}}=\frac{-s^2x_1}{x_n-x_1} \tag{3.37}$$

The quantity s^2 is obtained from

$$s^2=\frac{\sum_{i=2}^{n}[(y_i-y_{i-1})^2/(x_i-x_{i-1})]-\hat{\beta}^2(x_n-x_1)}{n-1} \tag{3.38}$$

As in the previous section, the uncertainties in the estimates of α and β create a systematic-error variance for a predicted weight when the calibration curve is used. For this model the predicted weight, y_0, is directly related to an observed manometer reading, x_0, by

$$y_0=\hat{\alpha}+\hat{\beta}x_0 \tag{3.39}$$

Then the systematic-error variance for y_0 is simply, by application of Eq. 4.3,

$$\sigma^2_{y_0}=\sigma^2_{\hat{\alpha}}+x_0^2\sigma^2_{\hat{\beta}}+2x_0\sigma_{\hat{\alpha},\hat{\beta}} \tag{3.40}$$

with $\sigma^2_{\hat{\alpha}}$, $\sigma^2_{\hat{\beta}}$, and $\sigma_{\hat{\alpha},\hat{\beta}}$ given by Eqs. 3.35 to 3.37.

For the assumed model, since the manometer reading is observed

* It may bother some readers that, with the cumulative model, only the first and last points are used to estimate the slope and intercept of the calibration curve. One wonders, perhaps, why the intermediate two points are even required in the calibration exercise. These points serve a two fold purpose (1) to verify that the calibration curve is indeed linear and (2) to provide s^2 in Eq. 3.38, needed to find the variance of the parameters and of estimated amounts of liquid in the vessel.

without error, there is no random-error variance associated with the true weight of liquid in the vessel. A random error is introduced, however, when converting the weight to a volume through a specific-gravity determination.

As with the previous model, there is a covariance between the weights of liquid determined from two manometer readings, x_1 and x_2. This covariance, designated by σ_{12}, is given by

$$\sigma_{12} = \sigma_{\hat{\alpha}}^2 + x_1 x_2 \sigma_{\hat{\beta}}^2 + (x_1 + x_2)\sigma_{\hat{\alpha},\hat{\beta}} \tag{3.41}$$

In application, transfer weights of the form $(y_2 - y_1)$ are of interest. In this instance the systematic-error variance of $(y_2 - y_1)$ is

$$\sigma^2_{(y_2 - y_1)} = \sigma_{\hat{\beta}}^2(x_1^2 + x_2^2 - 2x_1x_2) + 2\sigma_{\hat{\alpha},\hat{\beta}}(x_1 + x_2 - x_1 - x_2) = (x_2 - x_1)^2\sigma_{\hat{\beta}}^2 \tag{3.42}$$

Note that the variance of the transfer weight depends only on the uncertainty in the slope estimate, as is intuitively reasonable.

Let us summarize the results of this section. The following steps are performed in a linear-calibration situation based on the cumulative model.

Step 1. Using the observed calibration data (x_i, y_i), estimate the calibration parameters using Eqs. 3.33 and 3.34.

Step 2. In application, a value is observed for the manometer reading, X. Call this x_0. The corresponding value for the weight of liquid in the tank, designated by y_0, is given by Eq. 3.39.

Step 3. The systematic-error variance associated with y_0 is given by Eq. 3.40. The random-error variance is zero.

Step 4. If two values are observed for X, i.e., x_1 and x_2, and the values of Y, i.e., y_1 and y_2, are predicted by using Eq. 3.39, then the systematic errors in y_1 and y_2 are correlated. The covariance is given by Eq. 3.41.

Step 5. The systematic-error variance for the weight of a transfer amount is given by Eq. 3.42.

Step 6. The systematic-error variance for the total weight of k transfers is found by replacing $(x_2 - x_1)^2$ in Eq. 3.42 by the square of the sum of these differences in x values for the k transfers.

Example 3.P

The vessel-calibration data are given in Table 3.17. Estimate the calibration curve, assuming a cumulative model. The summary steps are applied.

TABLE 3.17 DATA ON VESSEL CALIBRATION
(Example 3.P)

Y (weight, arbitrary units)	X (manometer reading)
1	5.78
2	9.22
3	13.66
4	17.31
5	20.97
6	25.26
7	28.90
8	32.92
9	37.77
10	42.27

Step 1. From Eq. 3.33,

$$\hat{\beta}=\frac{10-1}{42.27-5.78}=0.2466$$

From Eq. 3.34,

$$\hat{\alpha}=1-(0.2466)(5.78)=-0.425$$

Step 2. With a given manometer reading assumed to be 30.00, the estimated weight of the liquid is, by Eq. 3.39,

$$y_0=-0.425+(0.2466)(30)=6.973 \text{ units}$$

Step 3. For the systematic-error variance for this estimate, some preliminary calculations are required. The term s^2 is given by Eq. 3.38. Since (y_i-y_{i-1}) is constant for all i in this example, Eq. 3.38 can be written

$$s^2=\frac{\sum_{i=2}^{n}(x_i-x_{i-1})^{-1}-(0.2466)^2(36.49)}{9}$$

$$=\frac{(2.24810-2.21901)}{9}=0.003232$$

Then, from Eqs. 3.35 to 3.37,

$$\sigma^2_{\hat{\alpha}}=\frac{(0.003232)(5.78)(42.27)}{36.49}=0.02164$$

$$\sigma^2_{\hat{\beta}} = \frac{(0.003232)}{36.49} = 0.00008857$$

$$\sigma_{\hat{\alpha},\hat{\beta}} = \frac{-(0.003232)(5.78)}{36.49} = -0.0005119$$

Then, from Eq. 3.40,

$$\sigma_s^2 = 0.02164 + (30)^2(0.00008857) + (60)(-0.0005119)$$
$$= 0.02164 + 0.07971 - 0.03071 = 0.07064 \quad (\text{units})^2$$

which gives $\sigma_s = 0.266$ units.

Step 4. Not pertinent in this example.

Step 5. Some liquid is now removed; the manometer reading now gives a value of $x = 10.00$. What are the estimated weight of the liquid removed and its systematic-error variance? At $x = 10$, the estimated weight is

$$y_1 = -0.425 + (0.2466)(10) = 2.041 \quad \text{units}$$

Therefore the estimated amount removed is $6.973 - 2.041 = 4.932$ units.
The variance of this quantity is given by Eq. 3.42:

$$\sigma^2_{(y_2 - y_1)} = (30 - 10)^2(0.00008857) = 0.03543 \quad (\text{units})^2$$

which gives a standard deviation of 0.188 units.

Step 6. Not pertinent in this example.

If three transfers are involved with the following pairs of manometer readings:

Before transfer	*After transfer*	*Difference*
30	10	20
33	7	26
41	8	33

then the estimate of the total weight of liquid removed is

$$(0.2466)(20 + 26 + 33) = 19.48 \quad \text{units}$$

The systematic-error variance associated with this total transfer weight is, by step 6,

$$(20+26+33)^2(0.00008857)=0.5528 \quad (\text{units})^2$$

Notice that the percent standard deviation associated with the weight of the liquid removed is constant for a given calibration line. This quantity is $(100)(\sigma_{\hat{\beta}}/\hat{\beta})\%$, which is 3.82% in this example.

3.3.10 Curvilinear Calibration, Independent Data

The same problem as in Sec. 3.3.8 is structured here, except that the relation between y and x is now presumed to be curvilinear rather than linear. This complicates the problem considerably.

There are several alternative approaches that might be used in this situation. One possibility is that within the range of practical interest the relation may be linear, or nearly so, and we can use the method of Sec. 3.3.8, the analysis being restricted to the region where this linear relation is valid. Another possibility is to apply some simple data transformation that will produce a linear relation and to use the methods in Sec. 3.3.8 on the transformed data. For example, the curvilinear relation $y=ax^b$ can be transformed to $\ln y=\ln a+b \ln x$, which is now linear when $\ln y$ is related to $\ln x$. Other relations can also be transformed to achieve a linear model.

On occasion, however, the calibration data may have some curvature that no transformation can adequately remove. In this instance we can fit a polynomial curve of the form

$$y=a_0+a_1x+a_2x^2+ \ldots \tag{3.43}$$

This problem becomes difficult very quickly because the calibration curve must be applied in reverse, i.e., by expressing x as a function of y. It is difficult to handle any case beyond a quadratic, but fortunately a quadratic model is adequate for many calibration curves likely to be encountered. This quadratic model is considered here, with ϵ_i defined as the random-error term and generally assumed to have mean zero and variance σ_ϵ^2.

$$y_i=\alpha'+\beta'x_i+\gamma'x_i^2+\epsilon_i \tag{3.44}$$

First, the estimates of the parameters and their variances and covariances must be found. This problem is still not very simple unless the x_i values are equally spaced. Fortunately, in calibration work the x_i values are chosen by the experimenter, and he is free to select them so

that they are equally spaced. In this case the method of orthogonal polynomials can be applied, and this is done in this section.

The approach is as follows: The x_i values are equally spaced, with x_1 the first point, with x_2 the second, etc., and with $i=1, 2, \ldots, n$. Let the median x be x_m, and transform the x's to u's by the relation

$$u_i=\frac{x_i-x_m}{w} \tag{3.45}$$

where w is the constant difference between any two x values.

Also introduce the variable

$$v_i=u_i^2-\frac{(n^2-1)}{12} \tag{3.46}$$

The quadratic expression in Eq. 3.44 can now be written equivalently as

$$y_i=\alpha+\beta u_i+\gamma v_i+\epsilon_i \tag{3.47}$$

With this transformation the parameters are now easily estimated, and, more important, the estimates are statistically independent of one another, i.e., all covariances between the pairs of estimates are zero. The estimates and their variances are as follows:

$$\hat{\alpha}=\bar{y}=\frac{\sum_{i=1}^{n} y_i}{n} \tag{3.48}$$

$$\hat{\beta}=\frac{\sum_{i=1}^{n} u_i y_i}{\sum_{i=1}^{n} u_i^2} \tag{3.49}$$

$$\hat{\gamma}=\frac{\sum_{i=1}^{n} v_i y_i}{\sum_{i=1}^{n} v_i^2} \tag{3.50}$$

$$\hat{\sigma}_{\hat{\alpha}}^2=\frac{\sigma_\epsilon^2}{n} \tag{3.51}$$

$$\hat{\sigma}_{\hat{\beta}}^2 = \frac{\sigma_\epsilon^2}{\sum_{i=1}^{n} u_i^2} \tag{3.52}$$

$$\hat{\sigma}_{\hat{\gamma}}^2 = \frac{\sigma_\epsilon^2}{\sum_{i=1}^{n} v_i^2} \tag{3.53}$$

where σ_ϵ^2 is estimated by

$$\hat{\sigma}_\epsilon^2 = \left\{ \sum_{i=1}^{n} y_i^2 - \left[\left(\sum_{i=1}^{n} y_i \right)^2 / n \right] - \left[\left(\sum_{i=1}^{n} u_i y_i \right)^2 / \sum_{i=1}^{n} u_i^2 \right] - \left[\left(\sum_{i=1}^{n} v_i y_i \right)^2 / \sum_{i=1}^{n} v_i^2 \right] \right\} / (n-3) \tag{3.54}$$

After the direct relation, Eq. 3.47, is estimated, the calibration curve is used in reverse to estimate x_0 for a given y_0. This can be done in terms of u_0, and then x_0 is calculated by

$$x_0 = x_m + w u_0 \tag{3.55}$$

Equation 3.47 can be written in its equivalent form (by dropping the random error term, ϵ_i, and replacing the parameters by their estimates),

$$y_0 = \hat{\alpha} + \hat{\beta} u_0 + \hat{\gamma} \left(u_0^2 - \frac{n^2-1}{12} \right)$$

or

$$\hat{\gamma} u_0^2 + \hat{\beta} u_0 + (\hat{\alpha} - c\hat{\gamma} - y_0) = 0 \tag{3.56}$$

where c is $(n^2-1)/12$. This is a quadratic equation in u_0 which yields the solution

$$u_0 = \frac{-\hat{\beta} \pm \sqrt{\hat{\beta}^2 - 4\hat{\gamma}(\hat{\alpha} - c\hat{\gamma} - y_0)}}{2\hat{\gamma}} \tag{3.57}$$

It will be obvious in application whether the + or the − sign should be used. The systematic-error variance induced by the estimated calibration curve is then found by noting that the uncertainties in $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ create this variance. The methods of Chap. 4, and in particular Sec. 4.2.2, are used to find the systematic-error variance in u_0, designated by σ_s^2. This is approximated by

$$\hat{\sigma}_s^2 \approx \left(\frac{\partial u_0}{\partial \hat{\alpha}} \right)^2 \sigma_{\hat{\alpha}}^2 + \left(\frac{\partial u_0}{\partial \hat{\beta}} \right)^2 \sigma_{\hat{\beta}}^2 + \left(\frac{\partial u_0}{\partial \hat{\gamma}} \right)^2 \sigma_{\hat{\gamma}}^2 \tag{3.58}$$

where the partial derivatives are evaluated at $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$. These partial derivatives are

$$\frac{\partial u_0}{\partial \hat{\alpha}} = \frac{\pm 1}{\sqrt{\hat{\beta}^2 - 4\hat{\gamma}(\hat{\alpha} - c\hat{\gamma} - y_0)}} \tag{3.59}$$

$$\frac{\partial u_0}{\partial \hat{\beta}} = -\frac{1}{2\hat{\gamma}} \pm \frac{\hat{\beta}}{2\hat{\gamma}\sqrt{\hat{\beta}^2 - 4\hat{\gamma}(\hat{\alpha} - c\hat{\gamma} - y_0)}} \tag{3.60}$$

$$\frac{\partial u_0}{\partial \hat{\gamma}} = \frac{\hat{\gamma}[\pm(-2\hat{\alpha} + 4c\hat{\gamma} + 2y_0)/\sqrt{\hat{\beta}^2 - 4\hat{\gamma}(\hat{\alpha} - c\hat{\gamma} - y_0)}] - [-\hat{\beta} \pm \sqrt{\hat{\beta}^2 - 4\hat{\gamma}(\hat{\alpha} - c\hat{\gamma} - y_0)}]}{2\hat{\gamma}^2} \tag{3.61}$$

The random-error variance in u_0, designated by σ_r^2, is estimated by

$$\hat{\sigma}_r^2 = \frac{\hat{\sigma}_\epsilon^2}{\hat{\beta}^2 - 4\hat{\gamma}(\hat{\alpha} - c\hat{\gamma} - y_0)} \tag{3.62}$$

The systematic- and random-error variances in x_0 are found by multiplying $\hat{\sigma}_s^2$ and $\hat{\sigma}_r^2$ by w^2.

Let us summarize the results of this section. The following steps are performed in a curvilinear calibration situation in which a quadratic calibration curve is used. Steps 10 to 12 cover the case in which the general sum of x values is considered.

Step 1. Choose the x_i values such that they are equally spaced when the calibration is performed. $(i = 1, 2, \ldots, n)$

Step 2. Find the median value of these x_i values. If n is odd, this median value, x_m, is the middle value; if n is even, the median value is the average of the two middle values.

Step 3. Letting $w = (x_i - x_{i-1})$ for any i, calculate u_i corresponding to each x_i by Eq. 3.45.

Step 4. Calculate v_i corresponding to each x_i by Eq. 3.46.

Step 5. Find the estimates for the calibration parameters by using Eqs. 3.48 to 3.50.

Step 6. In application, a value is observed for Y. Call this y_0. Find the corresponding value for x_0 by using Eq. 3.57 to find u_0 and then using Eq. 3.55 to find x_0.

Step 7. The systematic-error variance associated with u_0 is given by Eq. 3.58, where the quantities in the equation are given in Eqs. 3.51 to 3.54 and Eqs. 3.59 to 3.61.

Step 8. The systematic-error variance for x_0 is found by multiplying the result of step 7 by w^2.

Step 9. The random-error variance for u_0 is given by Eq. 3.62, and the corresponding value for x_0 is found by multiplying the result by w^2.

Step 10. If there are k items in a general sum, i.e., if the given data points are $y_1, y_2, \ldots, y_k$, then the general sum of the corresponding x's, $(c_1x_1+c_2x_2+ \ldots +c_kx_k)=x_s$, is found by the formula

$$x_s=x_m \sum_{i=1}^{k} c_i+wu_s \tag{3.63}$$

where

$$u_s=\sum_{i=1}^{k} c_iu_i=\frac{-\hat{\beta}\sum_{i=1}^{k} c_i+\sum_{i=1}^{k} c_i\Gamma_i}{2\gamma} \tag{3.64}$$

and where

$$\Gamma_i=\sqrt{\hat{\beta}^2-4\hat{\gamma}(\hat{\alpha}-c\hat{\gamma}-y_i)} \tag{3.65}$$

Step 11. The systematic-error variance of x_s is w^2 times the systematic variance of u_s. The systematic-error variance of u_s is given by Eq. 3.58 with u_s replacing u_0 and the following partial derivatives defined as

$$\frac{\partial u_s}{\partial \hat{\alpha}}=-\frac{\sum_{i=1}^{k} c_i}{\Gamma_i} \tag{3.66}$$

$$\frac{\partial u_s}{\partial \hat{\beta}}=\frac{-\sum_{i=1}^{k} c_i+\hat{\beta}\sum_{i=1}^{k}[c_i/\Gamma_i]}{2\hat{\gamma}} \tag{3.67}$$

$$\frac{\partial u_s}{\partial \hat{\gamma}}=\frac{\hat{\beta}\sum_{i=1}^{k} c_i-2\hat{\gamma}\sum_{i=1}^{k}[c_i(\hat{\alpha}-2c\hat{\gamma}-y_i)/\Gamma_i]-\sum_{i=1}^{k} c_i\Gamma_i}{2\hat{\gamma}^2} \tag{3.68}$$

Step 12. The random-error variance of x_s is w^2 times the random variance of u_s. The random-error variance of u_s is

$$\hat{\sigma}_r^2 = \hat{\sigma}_\epsilon^2 \sum_{i=1}^{k} \left(\frac{c_i}{\Gamma_i}\right)^2 \tag{3.69}$$

Example 3.Q

Let the calibration data consist of measurements of total ^{235}U made by a nondestructive assay instrument on 5-gal containers known to contain specified amounts of ^{235}U. The X and Y variables are defined by X = known amount of ^{235}U in a given container and Y = net counts produced by the NDA instrument. The data are given in Table 3.18.

TABLE 3.18 MEASUREMENTS OF TOTAL ^{235}U
(Example 3.Q)

x_i, g of ^{235}U	y_i, net counts
20	595
30	867
40	1180
50	1389
60	1627
70	1813
80	2093

Let us apply the summary steps:

Step 2. $x_m = 50$

Step 3. $w = 10$

By Eq. 3.45,

$u_1 = (20-50)/10 = -3$ $\quad u_5 = +1$
$u_2 = (30-50)/10 = -2$ $\quad u_6 = +2$
$u_3 = -1$ $\quad u_7 = +3$
$u_4 = 0$

Step 4. By Eq. 3.46,

$v_1 = (-3)^2 - 4 = 5$ $\quad v_5 = -3$
$v_2 = 4-4 = 0$ $\quad v_6 = 0$
$v_3 = 1-4 = -3$ $\quad v_7 = 5$
$v_4 = 0-4 = -4$

Step 5. The parameters are estimated by Eqs. 3.48 to 3.50:

$$\hat{\alpha} = \frac{595+867+\ldots+2093}{7} = 1366.29$$

$$\hat{\beta} = \frac{(-3)(595)+\ldots+(3)(2093)}{(-3)^2+\ldots+(3)^2}$$

$$= 6833/28 = 244.04$$

$$\hat{\gamma} = \frac{(5)(595)+(0)(867)+\ldots+(5)(2093)}{(5)^2+(0)^2+\ldots+(5)^2}$$

$$= -537/84 = -6.39$$

Step 6. The calibration curve is now used. A net count of 1000 is observed for y_0. What is the estimated amount of ^{235}U in the container? From Eq. 3.57,

$$u_0 = \frac{-244.04 \pm \sqrt{(244.04)^2 - 4(-6.39)[1366.29 - 4(-6.39) - 1000]}}{2(-6.39)}$$

$$= \frac{-244.04 \pm 263.76}{-12.78} = -1.543$$

since the "+" sign need clearly be used. The corresponding value for the amount of ^{235}U, x_0, is given by Eq. 3.55,

$$x = 50 + 10(-1.543) = 34.57 \quad \text{g of } ^{235}U$$

Step 7. For σ_s^2, the systematic-error variance associated with u_0, the variances of the parameter estimates are found from Eqs. 3.51 to 3.54, and the partial derivatives are found in Eqs. 3.59 to 3.61. First, $\hat{\sigma}_\epsilon^2$ is evaluated by Eq. 3.54.

$$\hat{\sigma}_\epsilon^2 = \frac{14742182 - [(9564)^2/7] - [(6833)^2/(28)] - [(-537)^2/84]}{4}$$

$$= 1024.11$$

Then,

$$\hat{\sigma}_{\hat{\alpha}}^2 = 1024.11/7 = 146.30$$

$$\hat{\sigma}_{\hat{\beta}}^2 = 1024.11/28 = 36.58$$

$$\hat{\sigma}_{\hat{\gamma}}^2 = 1024.11/84 = 12.19$$

In the evaluation of the partial derivatives, the "+" sign is used where "±" appears since this was used in finding u_0. Note that

$$\sqrt{\hat{\beta}^2-4\hat{\gamma}(\hat{\alpha}-c\hat{\gamma}-y_0)}=263.76$$

as was determined when u_0 was found. This radical appears in all the partial derivatives. Then,

$$\frac{\partial u_0}{\partial \hat{\alpha}}=\frac{1}{263.76}=0.0037913$$

$$\frac{\partial u_0}{\partial \hat{\beta}}=\frac{1}{2(-6.39)}+\frac{244.04}{2(-6.39)(263.76)}=0.0058502$$

$$\begin{aligned}\frac{\partial u_0}{\partial \hat{\gamma}}&=\{(-6.39)[2(-1366.29-51.12+1000)/233.76]\\&\quad-(-244.04+263.76)\}/2(-6.39)^2\\&=0.0061817\end{aligned}$$

Then, $\hat{\sigma}_s^2$ is, from Eq. 3.58,

$$\begin{aligned}\hat{\sigma}_s^2&\approx 10^{-6}[(3.7913)^2(146.30)+(5.8502)^2(36.58)+(6.1817)^2(12.19)]\\&\approx 0.003821\end{aligned}$$

Step 8. In terms of grams squared of ^{235}U, the systematic-error variance is

$$(10)^2(0.003821)=0.3821 \quad g^2 \text{ of } {}^{235}U$$

Step 9. $\hat{\sigma}_r^2$ is, from Eq. 3.62,

$$\hat{\sigma}_r^2\approx 1024.11/(263.76)^2\approx 0.01472$$

which corresponds to 1.472 g^2 of ^{235}U after it is multiplied by w^2. The total variance associated with the estimated amount of ^{235}U for the container in question is

$$0.3821+1.472=1.854 \quad g^2 \text{ of } {}^{235}U$$

which gives a standard deviation of 1.36 g of ^{235}U or 3.9% of the estimated amount in this example.

Two Additional Containers. Suppose that two additional containers are counted yielding counts of 800 and 1800. Steps 10 to 12 are followed to estimate the total amount of ^{235}U in the three cans and its systematic- and random-error variances.

Step 10. Use $y_1 = 1000$, $y_2 = 800$, and $y_3 = 1800$. Then, by Eq. 3.65,

$$\Gamma_1 = \sqrt{(244.04)^2 - (4)(-6.39)[1366.29 - 4(-6.39) - 1000]}$$
$$= 263.76$$

$$\Gamma_2 = 273.28$$

$$\Gamma_3 = 221.64$$

Thus, by Eq. 3.64, with all the $c_i = 1$,

$$u_s = \frac{-3(244.04) + (263.76 + 273.28 + 221.64)}{2(-6.39)} = -2.08$$

and, by Eq. 3.63,

$$x_s = (3)(50) + (10)(-2.08) = 129.2 \quad \text{g of } {}^{235}\text{U}$$

Step 11. The partial derivatives are evaluated from Eqs. 3.66 to 3.68:

$$\frac{\partial u_s}{\partial \hat{\alpha}} = -\left(\frac{1}{263.76} + \frac{1}{273.28} + \frac{1}{221.64}\right) = -0.01196$$

$$\frac{\partial u_s}{\partial \hat{\beta}} = \frac{-3 + (244.04)(0.01196)}{-12.78} = 0.00636$$

$$\frac{\partial u_s}{\partial \hat{\gamma}} = \frac{3(244.04) + 12.78\left[\dfrac{417.41}{263.76} + \dfrac{617.41}{273.28} - \dfrac{382.59}{221.64}\right] - 758.68}{81.664}$$
$$= 0.00585$$

Then the systematic-error variance of u_s is, by Eq. 3.58,

$$\sigma_s^2 = (0.01196)^2(146.30) + (0.00636)^2(36.58) + (0.00585)^2(12.19)$$
$$= 0.02282$$

The systematic-error variance of x_s is 10^2 times this value, or 2.282 g^2 of ^{235}U, which gives a standard deviation of 1.51 g of ^{235}U.

Step 12. The random-error variance of u_s is, by Eq. 3.69,

$$(1024.11)\left[\frac{1}{(263.76)^2} + \frac{1}{(273.28)^2} + \frac{1}{(221.64)^2}\right] = 0.04928$$

The random-error variance of x_s is then 4.928 g^2 of ^{235}U, which gives a standard deviation of 2.22 g of ^{235}U.

Chapter 4

MEAN AND VARIANCE OF FUNCTIONS OF RANDOM VARIABLES

OVERVIEW

In Chapter 2 the concept of a random variable was introduced, along with its probability density function. It was indicated that the moments provide considerable information about the density function. In particular, if a random variable has a normal probability density function, the first moment about the origin (the mean) and the second moment about the mean (the variance) completely specify this function. Even for a non-normal density function, knowledge of the mean and the variance provide considerable information about the central tendency and spread of the random variable in question, and in many applications higher ordered moments are not required.

In most applications of interest in nuclear materials control, the random variable is a function of other random variables, and its density function is required. As just pointed out, the mean and the variance often provide satisfactory information about this function. Thus it is important to be able to find the mean and the variance for a random variable that is a given function of other random variables.

Commonly the random variable in question is a linear combination of other random variables; this case is treated in Sec. 4.1. Other, more general, functions are considered in Sec. 4.2. In both instances a knowledge of the moments for the original random variable is required. In practice these means and variances may not be known quantities but rather estimates of them. The problem of accounting for this lack of knowledge about the parameters is treated in Sec. 4.3.

4.1 MEAN AND VARIANCE FOR LINEAR COMBINATIONS

4.1.1 Problem and Assumptions

A random variable is a known linear combination, or an algebraic sum, of other random variables. The problem is to find its mean and vari-

ance. Assume that the means and variances of the random variables comprising the linear combination and the covariances between pairs of them are known and finite. Contrary to what is sometimes thought, it is not necessary to assume that the random variables in question are normally distributed.

4.1.2 Solution

Let the random variables $x_1, x_2, \ldots, x_n$ have means $\mu_1, \mu_2, \ldots, \mu_n$ and variances $\sigma_1^2, \sigma_2^2, \ldots, \sigma_n^2$. Let the covariance between x_i and x_j be σ_{ij} and the linear combination of interest be

$$x = a_1x_1 + a_2x_2 + \ldots + a_nx_n \tag{4.1}$$

where the a's are arbitrary constants. Then the mean of x, μ_x, is

$$\mu_x = a_1\mu_1 + a_2\mu_2 + \ldots + a_n\mu_n = \sum_{i=1}^{n} a_i\mu_i \tag{4.2}$$

The variance of x, σ_x^2, is

$$\begin{aligned}\sigma_x^2 = {} & a_1^2\sigma_1^2 + a_2^2\sigma_2^2 + \ldots + a_n^2\sigma_n^2 + 2a_1a_2\sigma_{12} + \ldots + 2a_1a_n\sigma_{1n} \\ & + 2a_2a_3\sigma_{23} + \ldots + 2a_2a_n\sigma_{2n} \\ & \quad \vdots \qquad\qquad \vdots \\ & + \quad \ldots \quad + \\ & \qquad\qquad \vdots \\ & \qquad\qquad + 2a_{n-1}a_n\sigma_{n-1,n} \\ = {} & \sum_{i=1}^{n} a_i^2\sigma_i^2 + 2\sum_{\substack{i=1 \\ i<j}}^{n-1} a_ia_j\sigma_{ij}\end{aligned} \tag{4.3}$$

When all covariances are zero, the second summation in Eq. 4.3 is zero, and the variance of the sum is equal to the sum of the variances. In this situation, the random variables in the linear combination are said to be independently distributed.

Equations 4.2 and 4.3 give the mean and the variance of x but not its density function. If all x_i's in the summation are independently normally distributed, then x will also be normally distributed. Furthermore, as a result of the important central-limit theorem, the density function for the sum of a sufficient number of random variables is approximately normal regardless of the density functions for the variables in the sum. The definition of what constitutes a sufficient number of variables depends on several factors, e.g., the shapes of the density functions of the original variables. Happily, in most nuclear materials control applications in which a

given random variable of interest is the sum of other random variables, the normal density function is an adequate approximation to the density function for the sum in question.

4.1.3 Examples

Example 4.A

The total weight of a fuel rod is the sum of the cladding, end-plug, spring, and fuel weights. If the means and variances of the component weights are as listed in Table 4.1, find the mean and the variance for the total weight of the fuel rod, assuming that all covariances are zero.

TABLE 4.1 WEIGHTS OF COMPONENTS OF FUEL ROD (GRAMS)

Component	Mean weight	Standard deviation	Variance
Cladding	$\mu_1 = 554\ 89$	$\sigma_1 = 4\ 10$	$\sigma_1^2 = 16\ 8100$
Plug	$\mu_2 = 10\ 64$	$\sigma_2 = 0\ 04$	$\sigma_2^2 = 0.0016$
Spring	$\mu_3 = 16\ 07$	$\sigma_3 = 0\ 06$	$\sigma_3^2 = 0\ 0036$
Fuel	$\mu_4 = 1814.85$	$\sigma_4 = 2\ 45$	$\sigma_4^2 = 6\ 0025$

If x in Eq. 4.1 is the weight of the fuel rod and the x_i's are the weights of the component parts, the mean of x, from Eq. 4.2, is

$$\mu_x = 554.89 + 10.64 + 16.07 + 1814.85 = 2396.45 \text{ g}$$

From Eq. 4.3, since all $a_i = 1$, the variance of x is simply the sum of the variances of the x_i's.

$$\sigma_x^2 = 16.8100 + 0.0016 + 0.0036 + 6.0025 = 22.8177 \text{ g}^2$$

The standard deviation is

$$\sigma_x = \sqrt{22.8177} = 4.78 \text{ g}$$

Note that the variances for the plug and spring weights are negligible contributors to the variance of the total rod weight.

Example 4.B

Of a large number of containers in inventory, 30% weigh 10 units, 20% weigh 15 units, 15% weigh 20 units, and 35% weigh 30 units. If five containers are selected at random:

1. What is the expected total weight of the five containers?
2. What is the variance of this total weight?
3. What is the variance of the average weight?

Let the observed weight for the ith container in the sample be x_i, and let x be the sum of the five weights. To find μ_x and σ_x^2, we must first find μ_i and σ_i^2 for any i. (Assume that the random variables in the sum are independently distributed so that σ_{ij} is zero for all i and j.) These values were found in one example in Sec. 2.3 to be $\mu_i = 19.5$ units and $\sigma_i^2 = 69.75$. Then, in answer to question 1, from Eq. 4.2,

$$\mu_x = 19.5 + 19.5 + 19.5 + 19.5 + 19.5 = 97.5 \text{ units}$$

In answer to question 2, from Eq. 4.3,

$$\sigma_x^2 = 69.75 + 69.75 + 69.75 + 69.75 + 69.75 = 348.75 \text{ units}^2$$

$$\sigma_x = \sqrt{348.75} = 18.67 \text{ units}$$

In answer to question 3, since the average weight is $x/5$, the linear combination is

$$\frac{x}{5} = 0.2(x_1 + x_2 + x_3 + x_4 + x_5)$$

i.e., all a_i's in Eq. 4.1 are equal to 0.2. From Eq. 4.3, the variance for the average weight, $\sigma_{\bar{x}}^2$, is

$$\sigma_{\bar{x}}^2 = \underbrace{(0.2)^2(69.75 + \ldots + 69.75)}_{5 \text{ terms}} = 13.95 \text{ units}^2$$

That $\sigma_{\bar{x}}^2$ is one-fifth of σ_i^2 illustrates that the variance of an average for n items, each having the same variance, σ_i^2, is σ_i^2/n, whereas the standard deviation of the average is $\sigma_i/\sqrt{n}$. Also, question 2 illustrates that the variance of the total of the observations for these n items is $n\sigma_i^2$ and the standard deviation is $\sqrt{n}\sigma_i$.

Example 4.C

Successive MUF's (materials unaccounted for) are correlated since the ending inventory for one time period is identically the beginning inventory for the next time period. If the ending inventory is in error on the high side for period i, the MUF for that period tends to be correspondingly low, and the MUF for time period $i+1$ tends to be high. For a given material balance area, let

y_i = ending inventory for period i, or beginning inventory for period $i+1$

x_i = (inputs − outputs) for period i (Inputs are commonly called receipts, and outputs include shipments and measured discards.)

Then, for the first three time periods, the successive MUF's, M_i, can

be written

$$M_1 = y_0 + x_1 - y_1$$
$$M_2 = y_1 + x_2 - y_2$$
$$M_3 = y_2 + x_3 - y_3$$

Assume that all the inventories have the same mean, μ_y, and the same variance, σ_y^2, and that all (inputs − outputs) have the same mean, μ_x, and the same variance, σ_x^2. Further, assume that all covariances between and among the x_i and y_i are zero. Let M be the sum of the M_i's (i.e., the cumulative MUF). Then, from Eq. 4.3,

$$\sigma_M^2 = \sigma_{M1}^2 + \sigma_{M2}^2 + \sigma_{M3}^2 + 2\sigma_{M_1M_2} + 2\sigma_{M_1M_3} + 2\sigma_{M_2M_3}$$

where $\sigma_{M_iM_j}$ denotes the covariance between MUF's for periods i and j.

Apply Eq. 4.3 to find the variance of an individual MUF:

$$\sigma_{M_i}^2 = \sigma_y^2 + \sigma_x^2 + \sigma_y^2 = 2\sigma_y^2 + \sigma_x^2 \qquad \text{for all } i$$

Since the covariance arises in this example because the ending inventory for one period is identically the beginning inventory for the next, $\sigma_{M_iM_j}$ is zero unless $j = i+1$. For $j = i+1$, the covariance is found from Eq. 2.54; note that $E(M_i) = \mu_y + \mu_x - \mu_y$, or simply μ_x, for all i.

$$\begin{aligned}\sigma_{M_iM_{i+1}} &= E(M_iM_{i+1}) - E(M_i)E(M_{i+1}) \\ &= E[(y_{i-1} + x_i - y_i)(y_i + x_{i+1} - y_{i+1})] - \mu_x^2 \\ &= E(y_{i-1}y_i + y_{i-1}x_{i+1} - y_{i-1}y_{i+1} + x_iy_i + x_ix_{i+1} - x_iy_{i+1} \\ &\quad - y_i^2 - y_ix_{i+1} + y_iy_{i+1}) - \mu_x^2\end{aligned}$$

We find the expected value of this algebraic sum by finding the expected value of each term in the sum and adding them. In finding the expected value of each term, we use the fact that, if two random variables are independently distributed, the expected value of their product is equal to the product of their expected values. This follows immediately from the definitive of a covariance in Eq. 2.54, by letting the covariance be zero, as is the case when two variables are independently distributed.

$$\begin{aligned}\sigma_{M_iM_{i+1}} &= \mu_y^2 + \mu_y\mu_x - \mu_y^2 + \mu_x\mu_y + \mu_x^2 - \mu_x\mu_y - E(y^2) - \mu_y\mu_x + \mu_y^2 - \mu_x^2 \\ &= -[E(y^2) - \mu_y^2] \\ &= -\sigma_y^2\end{aligned}$$

by Eq. 2.27.

Thus, for the simple model used in this example, the covariance between successive MUF's is the negative of the variance of the inventory. Therefore the variance of the cumulative MUF ($M = M_1 + M_2 + M_3$) is, by Eq. 4.3, three times the variance of M_i plus twice the covariance be-

tween M_1 and M_2 plus twice the covariance between M_2 and M_3 (the covariance between M_1 and M_3 is zero).

$$\sigma_M^2 = 3(2\sigma_y^2+\sigma_x^2)+2(-\sigma_y^2)+2(-\sigma_y^2) = 2\sigma_y^2+3\sigma_x^2$$

Note in passing that the same result can be found by summing the three M_i's directly before finding the variance; i.e., M can be written

$$M = y_0+x_1+x_2+x_3-y_3$$

and its variance follows immediately from Eq. 4.3, with all the covariances being zero. This approach was not used in this example, because the example is intended to illustrate how covariances enter into the formula for the variance of a linear combination.

Example 4.D

Equations 2.57 to 2.59 are derived by using Eqs. 4.2 and 4.3.

Equation 2.57 indicates that the expected value of the sample mean, $\bar{x}$, is μ. To prove this, write

$$\bar{x} = \frac{x_1+x_2+\ \cdots\ +x_n}{n} = \frac{x_1}{n}+\frac{x_2}{n}+\ \cdots\ +\frac{x_n}{n}$$

Then, applying Eq. 4.2 directly with $a_i = 1/n$ and $\mu_i = \mu$ gives

$$E(\bar{x}) = \sum_{i=1}^{n} a_i\mu_i = \frac{\mu}{n}+\frac{\mu}{n}+\ \cdots\ +\frac{\mu}{n} = \mu$$

which completes the proof.

Equation 2.58 indicates that the variance of $\bar{x}$ is σ^2/n when the sample is from a population of infinite size. As a consequence of the infinite-population-size assumption, the covariance between x_i and x_j, σ_{ij}, is zero for all i and j. Then Eq. 4.3 is applied (again note that $a_i = 1/n$ for all i and $\sigma_i^2 = \sigma^2$ for all i):

$$\sigma_{\bar{x}}^2 = \sum_{i=1}^{n} a_i^2\sigma_i^2 = \frac{\sigma^2}{n^2}+\frac{\sigma^2}{n^2}+\ \cdots\ +\frac{\sigma^2}{n^2} = \frac{\sigma^2}{n}$$

which completes the proof.

When the population is of finite size, Eq. 2.59 indicates that this variance, σ^2/n, must be multiplied by a correction factor, $[(N-n)/(N-1)]$. This occurs because, for a finite population, σ_{ij} is not zero but is rather $-\sigma^2/(N-1)$. Then, applying Eq. 4.3, in which the first summation was already shown to be σ^2/n, yields

$$\sigma_{\bar{x}}^2 = \frac{\sigma^2}{n}+2\sum_{\substack{i=1\\ i<j}}^{n-1}\frac{\sigma_{ij}}{n^2}$$

There are $[n(n-1)]/2$ terms in this second summation. Each term is

$-\sigma^2/[n^2(N-1)]$. Thus, when multiplied by 2, the summation is

$$-\frac{n(n-1)\sigma^2}{n^2(N-1)} = -\frac{(n-1)\sigma^2}{n(N-1)}$$

Therefore

$$\begin{aligned}\sigma_{\bar{x}}^2 &= \frac{\sigma^2}{n} - \frac{(n-1)\sigma^2}{n(N-1)} \\ &= \frac{\sigma^2}{n}\left(1 - \frac{n-1}{N-1}\right) \\ &= \frac{\sigma^2}{n}\,\frac{N-n}{N-1}\end{aligned}$$

which completes the proof.

4.1.4 Basis

Equation 4.2 follows directly from the definition of a mean in Eq. 2.24. Equation 4.3 is derived for the simple case of $n=2$. The generalization to n random variables follows directly from this derivation.

If $x = a_1x_1 + a_2x_2$, then, from Eq. 2.27, the variance of x is

$$\begin{aligned}\sigma_x^2 &= E(x^2) - \mu_x^2 \\ &= E(a_1^2x_1^2 + a_2^2x_2^2 + 2a_1a_2x_1x_2) - (a_1^2\mu_1^2 + a_1^2\mu_2^2 + 2a_1a_2\mu_1\mu_2)\end{aligned}$$

Since the expected value of a sum is the sum of the expected values, the first term can be paired with the fourth, the second with the fifth, and the third with the sixth. Then

$$\begin{aligned}\sigma_x^2 &= a_1^2[E(x_1^2) - \mu_1^2] + a_2^2[E(x_2^2) - \mu_2^2] + 2a_1a_2[E(x_1x_2) - \mu_1\mu_2] \\ &= a_1^2\sigma_1^2 + a_2^2\sigma_2^2 + 2a_1a_2\sigma_{12}\end{aligned}$$

where the last step follows from the definition of a variance in Eq. 2.27 and of a covariance in Eq. 2.54.

4.2 MEAN AND VARIANCE FOR GENERAL FUNCTIONS

4.2.1 Problem and Assumptions

In this section a given random variable of interest is an arbitrary function of the other random variables. The problem is to find its mean and variance. The following assumptions are made:

1. The random variables have finite means and variances.
2. The standard deviations are small relative to the means. (See the discussion following Eq. 4.6 on this point.)

As was true for the linear case in Sec. 4.1, it is not necessary to assume that the random variables are normally distributed, although this is sometimes erroneously stated to be a requirement.

4.2.2 Solution

Let the random variables $x_1, x_2, \ldots, x_n$ have means $\mu_1, \mu_2, \ldots, \mu_n$ and variances $\sigma_1^2, \sigma_2^2, \ldots, \sigma_n^2$. Let the covariance between x_i and x_j be σ_{ij}, and denote the arbitrary function by

$$x = \phi(x_1, x_2, \ldots, x_n) \tag{4.4}$$

where ϕ will be defined specifically in any given application.

Then the mean of x, μ_x, is approximated by

$$\mu_x \approx \phi(\mu_1, \ldots, \mu_n) \tag{4.5}$$

That is, as an approximation the mean of a function of random variables is equal to the function evaluated at the means.

The variance of x, σ_x^2, is approximated by

$$\begin{aligned}
\sigma_x^2 \approx & \left(\frac{\partial \phi}{\partial x_1}\right)^2 \sigma_1^2 + \left(\frac{\partial \phi}{\partial x_2}\right)^2 \sigma_2^2 + \ldots + \left(\frac{\partial \phi}{\partial x_n}\right)^2 \sigma_n^2 \\
& + 2\left(\frac{\partial \phi}{\partial x_1}\right)\left(\frac{\partial \phi}{\partial x_2}\right)\sigma_{12} + \ldots + 2\left(\frac{\partial \phi}{\partial x_1}\right)\left(\frac{\partial \phi}{\partial x_n}\right)\sigma_{1n} \\
& + \ldots + \\
& \quad \vdots \\
& 2\left(\frac{\partial \phi}{\partial x_{n-1}}\right)\left(\frac{\partial \phi}{\partial x_n}\right)\sigma_{n-1,n} \\
\approx & \sum_{i=1}^{n} \left(\frac{\partial \phi}{\partial x_i}\right)^2 \sigma_i^2 + 2 \sum_{\substack{i=1 \\ j>i}}^{n-1} \left(\frac{\partial \phi}{\partial x_i}\right)\left(\frac{\partial \phi}{\partial x_j}\right)\sigma_{ij}
\end{aligned} \tag{4.6}$$

In Eq. 4.6 all the partial derivatives must be evaluated at the mean values of the random variables.

The adequacy of these approximations depends on a number of factors, which interact in their importance. For example, assumption 2 in Sec. 4.2.1 requires that the random variables in the function have small standard deviations relative to their means. How small is "small" depends on the importance of each particular random variable as it affects the random variable of interest. Experience shows that, in most applications of primary interest in the control of nuclear materials, Eqs. 4.5 and 4.6 provide satisfactory approximations. Further, the random variables of

interest may generally be assumed to be normally distributed with reasonable validity. In spite of this assurance, the user is cautioned to be aware that Eqs. 4.5 and 4.6 are only approximations. If there is some concern in a given application that the approximations may not be valid, an indication is given in Sec. 4.2.4 how a judgment can be made as to their validity.

4.2.3 Examples

Example 4.E

Reference is made to Eq. 3.26, the derivation of which requires application of Eq. 4.6. The calibration equation for a given value of y, y_0, was of the form

$$x_0 = \alpha' + \beta' y_0$$

where

$$\alpha' = -\frac{\hat{\alpha}}{\hat{\beta}}$$

and

$$\beta' = \frac{1}{\hat{\beta}}$$

The estimates $\hat{\alpha}$ and $\hat{\beta}$ are derived from the calibration data and have variances and covariances given by

$$\sigma^2_{\hat{\beta}} = R$$

$$\sigma^2_{\hat{\alpha}} = R \sum \frac{x_i^2}{n}$$

$$\sigma_{\hat{\alpha},\hat{\beta}} = -R\bar{x}$$

The problem is to find the variance of x_0 by using this information. We apply Eq. 4.6; this requires taking the partial derivatives of the function x_0 with respect to $\hat{\alpha}$ and $\hat{\beta}$. [These partial derivatives are to be evaluated at the means of $\hat{\alpha}$ and $\hat{\beta}$. Since these means, being the true values of the α and β parameters, are not known, their best estimates are used (i.e., α and β).] First, x_0 is written as a function of $\hat{\alpha}$ and $\hat{\beta}$ rather than of α' and β'.

$$x_0 = \frac{-\hat{\alpha}}{\hat{\beta}} + \frac{y_0}{\hat{\beta}} = -\frac{\hat{\alpha} + y_0}{\hat{\beta}} = \frac{y_0 - \hat{\alpha}}{\hat{\beta}}$$

The partial derivatives are

$$\frac{\partial x_0}{\partial \hat{\alpha}} = -\frac{1}{\hat{\beta}}$$

$$\frac{\partial x_0}{\partial \hat{\beta}} = -\frac{y_0 - \hat{\alpha}}{\hat{\beta}^2}$$

Equation 4.6 can now be applied to give the variance of x_0, denoted by σ_s^2 in Eq. 3.26:

$$\sigma_s^2 \approx \left(\frac{\partial x_0}{\partial \hat{\alpha}}\right)^2 \sigma_{\hat{\alpha}}^2 + \left(\frac{\partial x_0}{\partial \hat{\beta}}\right)^2 \sigma_{\hat{\beta}}^2 + 2\left(\frac{\partial x_0}{\partial \hat{\alpha}}\right)\left(\frac{\partial x_0}{\partial \hat{\beta}}\right)\sigma_{\hat{\alpha},\hat{\beta}}$$

$$\approx \frac{R \sum x_i^2}{n\hat{\beta}^2} + \frac{R(y_0 - \hat{\alpha})^2}{\hat{\beta}^4} - \frac{2(y_0 - \hat{\alpha})\bar{x}}{\hat{\beta}^3}$$

$$\approx \frac{R\{(\sum x_i^2/n) + [(y_0 - \hat{\alpha})^2/\hat{\beta}^2] - [2(y_0 - \hat{\alpha})\bar{x}/\hat{\beta}]\}}{\hat{\beta}^2}$$

which is Eq. 3.26 and completes the exercise.

Example 4.F

The amount of ^{235}U in a container of UO_2 powder is measured by determining the net weight of the powder and drawing a sample of powder for analysis of percent uranium and percent ^{235}U. The random variables are:

w = net weight of UO_2 powder, with mean μ_w and measurement variance σ_w^2

u = ratio of uranium to UO_2 (proportion of uranium), with mean μ_u and measurement variance σ_u^2

v = ratio of ^{235}U to uranium, with mean μ_v and measurement variance σ_v^2

x = estimated amount of ^{235}U in the container, with mean μ_x and variance due to measurement of σ_x^2

The function ϕ of Eq. 4.4 is

$$x = \phi(w, u, v) = wuv$$

Assume the following parameter values:

$$\mu_w = 20.0 \text{ kg} \qquad \sigma_w = 0.05$$

$$\mu_u = 0.876 \qquad \sigma_u = 0.001$$

$$\mu_v = 0.0425 \qquad \sigma_v = 0.0002$$

and further assume that all covariances are zero. Then the mean of x is approximated by Eq. 4.5:

$$u_x \approx (20.0)(0.876)(0.0425) \approx 0.7446 \text{ kg } ^{235}U$$

or

$$\frac{\sigma_x^2}{\mu_x^2} \approx \frac{\sigma_w^2}{\mu_w^2} + \frac{\sigma_u^2}{\mu_u^2} + \frac{\sigma_i^2}{\mu_i^2}$$

When writing the variance in this form, we see that the variance of a product of random variables on a relative basis is equal to the sum of the variances of the random variables, where these are also expressed on relative bases. If we replace μ_x^2 with its approximate equivalent, $\mu_u^2\mu_u^2\mu_i^2$, we see that σ_x^2 reduces to exactly the same result as in example 4.F.

4.2.4 Basis

Formulas 4.5 and 4.6 are derived by approximating the function ϕ by the linear terms of a Taylor's series expansion around the mean values of the random variables. (The Taylor's series expansion is given in most calculus textbooks.) Using the same notation as in Sec. 4.2.2, we can approximate ϕ by

$$\phi(x_1, x_2, \ldots, x_n) \approx \phi(\mu_1, \mu_2, \ldots, \mu_n) + \sum_{i=1}^{n} \frac{\partial \phi}{\partial x_i} (x_i - \mu_i) \qquad (4.7)$$

Since $E(x_i)$ is μ_i, by definition, when the expected value of ϕ is found by using Eq. 4.7, all terms in the summation become zero, and only $\phi(\mu_1, \mu_2, \ldots, \mu_n)$ is left. This is the basis for Eq. 4.5. The variance of ϕ is also found quite easily by noting that the Taylor's series approximation in Eq 4.7 is linear in the random variables. This permits direct application of Eq. 4.3 to give Eq. 4.6.

The adequacy of approximations 4.5 and 4.6 depends on how closely the summed linear terms of the Taylor's series expansion approximates the exact function, ϕ, over the range of the variables in question. As indicated in Sec. 4.2.2, this depends on a number of factors, but, when the standard deviations of the random variables are small relative to the means, the approximation is quite satisfactory.

In most applications to problems in nuclear materials control, there is little need to be concerned about the adequacy of these approximations. Quite often only estimated values of the parameters are available anyway, and the errors introduced by using these estimates normally overshadow the errors that might be introduced by an inadequate approximation of the function ϕ. Even if this were not the case, approximate results are often in very close agreement with exact results.

Nevertheless, in some instance the user may be concerned about the validity of applying Eqs. 4.5 and 4.6. In this case we can obtain at least a qualitative check on the adequacy of the approximation by comparing values of the exact function evaluated at selected points with those given by the Taylor's series expansion.

To find σ_x^2, we evaluate the partial derivatives at the mean values of the random variables.

$$\frac{\partial \phi}{\partial w} = uv = (0.876)(0.0425) = 0.03723$$

$$\frac{\partial \phi}{\partial u} = wv = (20.0)(0.0425) = 0.850$$

$$\frac{\partial \phi}{\partial v} = wu = (20.0)(0.876) = 17.52$$

Then, from Eq. 4.6,

$$\sigma_x^2 \approx (0.03723)^2(0.05)^2 + (0.850)^2(0.001)^2 + (17.52)^2(0.0002)^2$$

$$\approx 10^{-6}(3.465 + 0.723 + 12.278) \approx 16.466 \times 10^{-6} \quad \text{kg}^2\ {}^{235}\text{U}$$

$$\sigma_x \approx \sqrt{16.466 \times 10^{-6}} \approx 0.0041 \quad \text{kg } {}^{235}\text{U}$$

Example 4.G

An alternative approach can be used for the situation in example 4.F: Write the relation in its equivalent form, $\ln x = \ln w + \ln u + \ln v$, which then becomes a linear combination. This permits us to apply the methods of Sec. 4.1. The function is linear in the logarithms, however. The means and variances of the logarithmically transformed random variables must be found first by the methods of Eqs. 4.5 and 4.6.

For any arbitrary random variable y, with mean μ_y and variance σ_y^2, we can apply Eqs. 4.5 and 4.6 to give the approximations

$$E(\ln y) \approx \ln \mu_y$$

$$\sigma_{\ln y}^2 \approx \left(\frac{\partial \ln y}{\partial y}\right)^2 \sigma_y^2 \approx \left(\frac{1}{y}\right)^2 \sigma_y^2$$

which, when we evaluate at the mean of y, gives

$$\sigma_{\ln y}^2 \approx \frac{\sigma_y^2}{\mu_y^2}$$

This result is used in finding the mean and variance of $\ln x$. The mean is found by applying Eq. 4.2:

$$E(\ln x) = E(\ln w) + E(\ln u) + E(\ln v)$$

or

$$\ln \mu_x \approx \ln \mu_w + \ln \mu_u + \ln \mu_v$$

According to the definition of a logarithm, this is equivalent to $\mu_x \approx \mu_w \mu_u \mu_v$ as in example 4.F. The variance of $\ln x$ is found by applying Eq. 4.3:

$$\sigma_{\ln x}^2 = \sigma_{\ln w}^2 + \sigma_{\ln u}^2 + \sigma_{\ln v}^2$$

To illustrate, in example 4.F a set of values for the parameters that could reasonably occur is

$$w = 20.1 \qquad u = 0.878 \qquad v = 0.0429$$

(These values of w, u, and v are all two standard deviations away from their respective means. To choose values much further removed from their means is not reasonable, because such a set of values would be unlikely to occur.) The *exact* value for x for this set of values is

$$x = (20.1)(0.878)(0.0429) = 0.75709$$

The corresponding value is found by the Taylor's series approximation by using the values for the partial derivatives found for example 4.F.

$$\begin{aligned} x &\approx \mu_w \mu_u \mu_v + \frac{\partial x}{\partial w}(w - \mu_w) + \frac{\partial x}{\partial u}(u - \mu_u) + \frac{\partial x}{\partial v}(v - \mu_v) \\ &\approx (20.0)(0.0876)(0.0425) + (0.03723)(20.1 - 20.0) \\ &\quad + (0.850)(0.878 - 0.876) + (17.52)(0.0429 - 0.0425) \\ &= 0.744600 + 0.003723 + 0.001700 + 0.007008 = 0.75703 \end{aligned}$$

Since this value agrees quite well with the exact value of 0.75709, reassurance is provided that the approximation is adequate in this instance.

4.3 USE OF ESTIMATED MEANS AND VARIANCES

4.3.1 Problem and Assumptions

Thus far in this chapter the means and variances of random variables that are functions of other random variables have been expressed as functions of known parameter values. In practical application the means, variances, and covariances involved are often estimated values rather than known values. In this section we consider the effect on the analysis of using estimated values rather than known values. It is assumed that all the variances are finite, that estimates of these quantities are given, along with their associated degrees of freedom, and that the covariances are all zero. Further, the random variables are now required to be normally distributed; this was not a required assumption in previous discussions.

The techniques for finding the mean and the variance for the random variable in question are identical to those given in the previous sections. The only difference is that now the known means and variances are replaced by estimates.

If the analysis were not carried on beyond this point (i.e., if only estimates of the means and variances are required), there would be no need to carry this discussion any further. However, the resulting parameter esti-

mates are often used to construct probability intervals. As discussed in Sec 2 7 2(a), knowledge of the degrees of freedom associated with the estimate of the variance is required * The determination of these degrees of freedom is the specific problem considered here. †

4.3.2 Solution

The solution is given in general terms. Let an estimated variance, s_0^2, be expressed as an algebraic sum of k independently distributed sample variances, $s_1^2, s_2^2, \ldots, s_k^2$, where s_i^2 is based on n_i degrees of freedom. Express this sum as

$$s_0^2 = a_1 s_1^2 + a_2 s_2^2 + \ldots + a_k s_k^2 \tag{4.8}$$

Then the approximate degrees of freedom for s_0^2, n_0, is calculated by

$$n_0 = \frac{s_0^4}{(a_1^2 s_1^4/n_1) + (a_2^2 s_2^4/n_2) + \ldots + (a_k^2 s_k^4/n_k)} \tag{4.9}$$

4.3.3 Examples

Example 4.H

In example 4.A assume that the standard deviations given, σ_i, are replaced by estimated values, s_i, based on n_i degrees of freedom. Given the data in Table 4.2, how many degrees of freedom are associated with σ_x^2?

TABLE 4.2 ESTIMATED STANDARD DEVIATIONS AND DEGREES OF FREEDOM

$s_1 = 5\ 08$	$n_1 = 6$
$s_2 = 0\ 032$	$n_2 = 50$
$s_3 = 0.083$	$n_3 = 30$
$s_4 = 3\ 11$	$n_4 = 100$*

* Before you continue with the example, what is your guess as to the answer?

The solution for n_0 is given by Eqs 4.8 and 4.9 (each $a_i = 1$) since in this problem the variance of x, the total weight of the fuel rod, is simply the sum of the variances of the component parts.

$$s_0^2 = (5.08)^2 + (0.032)^2 + (0.083)^2 + (3.11)^2 = 35.4864$$

* In particular, the problem discussed here reduces to case 2 of Sec 2 7 2(a), whereas previously case 1 of Sec 2 7 2(a) was implied.

† The Overview to Chap 5 emphasizes the practical necessity of taking into account the fact that parameters may be estimated rather than known in a given situation

Then

$$n_0 = \frac{(35.4864)^2}{[(5.08)^4/6]+[(0.032)^4/50]+[(0.083)^4/30]+[(3.11)^4/100]}$$

$$= \frac{1259.28}{111.00+0.00+0.00+0.94} = 11.2 \quad \text{degrees of freedom}$$

Note that the number of degrees of freedom is heavily dominated by the small number of degrees of freedom associated with s_1^2 and that s_1^2 is the dominant term in the calculation of s_0^2, accounting for about 73% of the total variance.

Example 4.I

In example 4.F assume that the standard deviations are replaced by the estimated values given in Table 4.3. How many degrees of freedom are associated with σ_x^2? (Again, what is your guess?)

TABLE 4.3 SAMPLE MEANS, STANDARD DEVATIONS, AND DEGREES OF FREEDOM

$\bar{w} = 20.02$	$s_w = 0.048$	$n_w = 15$
$\bar{u} = 0.8758$	$s_u = 0.0017$	$n_u = 24$
$\bar{v} = 0.0428$	$s_v = 0.00014$	$n_v = 4$

To find s_x^2, we use Eq. 4.6 in the form of Eq. 4.8. It is necessary to use the sample means because the population means are not known. Replacing the population means by sample means does not affect the calculation of the degrees of freedom for the variance, except to the extent that it affects the values of the a_i. The a_i values are calculated from the partial derivatives evaluated at the observed sample means rather than the population means as follows:

$$\frac{\partial \phi}{\partial w} = \bar{u}\bar{v} = (0.8758)(0.0428) = 0.03748$$

$$\frac{\partial \phi}{\partial u} = \bar{w}\bar{v} = (20.02)(0.0428) = 0.8569$$

$$\frac{\partial \phi}{\partial v} = \bar{w}\bar{u} = (20.02)(0.8758) = 17.534$$

Then, from Eq. 4.6, when we replace parameters by their estimates (in the notation of Eq. 4.8, a_1 is 0.001405, s_1 is 0.048, a_2 is 0.7343, etc.),

$$s_x^2 \approx (0.03748)^2(0.048)^2 + (0.8569)^2(0.0017)^2 + (17.534)^2(0.00014)^2$$

$$\approx 0.001405(0.048)^2 + 0.7343(0.0017)^2 + 307.44(0.00014)^2$$

$$\approx (3.24+2.12+6.03)\times 10^{-6} \approx 11.39\times 10^{-6}$$

The corresponding value was 16.47×10^{-6} in example 4.F.

The number of degrees of freedom for s_x^2 is calculated from Eq. 4.9:

$$n_x \approx \frac{(11.39)^2 \times 10^{-12}}{10^{-12}\{[(0.001405)^2(48)^4/15]+[(0.7343)^2(1.7)^4/24]+[(307.44)^2(0.14)^4/4]\}}$$

$$\approx \frac{129.73}{0.6986+0.1876+9.0776} \approx 13.0 \quad \text{degrees of freedom}$$

Example 4.J

One common situation in which we may be required to calculate the degrees of freedom using Eq. 4.9 is that in which variances are estimated from an analysis-of-variance table. Consider the following data.

Six lots of UO_2 powder are characterized for percent uranium by sampling from five containers for each lot, a total of 30 observations. The resulting one-way analysis-of-variance table (see Sec. 3.3.4) provides estimates of the "within" (σ_w^2) and "between" (σ_b^2) lot variance components as follows:

1. s_1^2 estimates ($\sigma_w^2+5\sigma_b^2$) based on 5 degrees of freedom (its value is 0.009231).
2. s_2^2 estimates (σ_w^2) based on 24 degrees of freedom (its value is 0.000885).

Assume that the variance of interest is that associated with the percent uranium of a sample of powder drawn from a container selected at random from a randomly selected lot. This variance is ($\sigma_w^2+\sigma_b^2$), which is estimated by ($\hat{\sigma}_w^2+\hat{\sigma}_b^2$). From these data,

$$\hat{\sigma}_w^2 = 0.000885$$

$$\hat{\sigma}_b^2 = \frac{0.009231-0.000885}{5} = 0.001669$$

$$\hat{\sigma}_w^2+\hat{\sigma}_b^2 = 0.002554$$

Note that ($\hat{\sigma}_w^2+\hat{\sigma}_b^2$) can be written in the form of Eq. 4.8:

$$\hat{\sigma}_w^2+\hat{\sigma}_b^2 = s_2^2+\frac{s_1^2-s_2^2}{5} = 0.2s_1^2+0.8s_2^2$$

Then Eq. 4.9 can be applied directly to find n_0, the degrees of freedom associated with ($\hat{\sigma}_w^2+\hat{\sigma}_b^2$). Here a_1 is 0.2 and a_2 is 0.8.

$$n_0 = \frac{(0.002554)^2}{[(0.2)^2(0.009231)^2/5]+[(0.8)^2(0.000885)^2/24]}$$

$$= \frac{6.5229\times10^{-6}}{10^{-6}(0.0209+0.6817)} = 9.3 \quad \text{degrees of freedom}$$

4.3.4 Basis

Formula 4.9 is commonly referred to as Satterthwaite's formula for degrees of freedom. With the notation of Eq. 4.8, it is derived by noting that, when sampling is from a normal distribution, the variance of a sample variance, s_i^2, is $2\sigma_i^4/n_i$, where σ_i^2 is the corresponding population variance (from Eq. 2.64.). When the variances of both sides of Eq. 4.8 are equated, the result is

$$\frac{2\sigma_0^4}{n_0} = \frac{2a_1^2\sigma_1^4}{n_1} + \frac{2a_2^2\sigma_2^4}{n_2} + \ldots + \frac{2a_k^2\sigma_k^4}{n_k}$$

Solving this for n_0 gives the solution of Eq. 4.9 when the σ_i's are replaced by the s_i's:

$$n_0 = \frac{2\sigma_0^4}{(a_1^2\sigma_1^4/n_1) + (a_2^2\sigma_2^4/n_2) + \ldots + (a_k^2\sigma_k^4/n_k)}$$

Chapter 5

LIMITS OF ERROR ON INDIVIDUAL ITEMS

OVERVIEW

In this chapter the results of Chaps. 3 and 4 are applied to determine the limits of error for the special nuclear material (SNM) content of an individual item of SNM-bearing material. The term "item" applies to a given container (e.g., a cylinder of UF_6, a can of PuO_2 powder, a fuel rod, a process vessel, or a barrel of solid waste) or to a discrete, uncontained quantity, such as a transfer volume in a reprocessing plant. The SNM in question may be total uranium, total plutonium, total ^{235}U, etc. In Chap. 6 the results are extended to include the total SNM content for several items and, more generally, the algebraic sum of these SNM values.

In the vernacular of nuclear materials control practitioners, the term "limits of error" (LE) is defined to mean the end points of a 95% confidence interval on a population mean. Here the population mean in question is the true amount of SNM for the item. As discussed in Sec. 2.7.2, the method of construction of the confidence interval depends on the degrees of freedom associated with the estimate of the variance used in the construction. Since the variance in question is often comprised of several variances, all of which may be based on different numbers of degrees of freedom, an exact calculation of the limits of error based on the appropriately determined number of degrees of freedom (see Sec. 4.3) can be laborious. In many situations it is questionable whether such exactness is required.

In routine applications the variances used in the calculation are commonly treated like known constants rather than estimated parameters to permit calculation of limits of error without an undue amount of effort. In this case, assuming that the measured SNM content is a normally distributed random variable, the limits of error can be found by adding to or subtracting from the estimated amount 1.96 times the standard deviation. (The 1.96 factor comes from Appendix A. It is the z_p value that is exceeded by the standardized normal random variable with a probability of 0.025. For a two-sided 95% confidence interval, there is 0.025 probability in each tail.) The calculation is often simplified further by use of the factor 2 rather than 1.96. It is also common practice to define the limit of error as being twice the standard deviation, thereby denoting half the length of

the interval rather than the end points. This causes no confusion in communication.

The use of the factor 1.96 (or 2) to transform a standard deviation to LE is defensible on two important grounds. First, it greatly simplifies the calculations; of course, this in itself is scarcely a defensible argument. A second, more compelling motivation is the argument that input variances are often based, at least in part, on data from years of experience, and, even though data are continually revised and updated to reflect current experience, they may be regarded more as known constants than as estimated quantities.

Nevertheless, a situation may arise in which a given variance should be regarded as an estimate rather than a known quantity. This occurs when we have limited knowledge about the sizes of one or more important measurement error variance. By applying the results of Sec. 4.3, we can calculate the appropriate number of degrees of freedom required in such an instance and can construct the confidence interval by the methods of Sec. 2.7.2.

With these thoughts in mind and without loss of generality, we can focus our attention in this chapter on finding the variance and standard deviation, rather than the limits of error, for the SNM in question. In this approach the input parameters can be regarded as known quantities and can be replaced by their estimates as necessary in application. The method of conversion from standard deviation to limits of error is then left open. Technical bases were provided in Sec. 2.7.2 to accomplish this conversion, depending on whether the standard deviations in question are regarded as estimates or as known parameters.

The specific aim of this chapter is to provide methods for combining the effects of errors resulting from bulk determination, sampling, and analysis to produce the variance of the reported amount of SNM in a given container. Thus this discussion is restricted to the wet-chemistry approach to determining the amount of SNM in a container. The alternate use of nondestructive assay methods is not overlooked, however, and the methods of Secs. 3.3.8 and 3.3.10 are applicable in this instance.

Bulk determination refers to determining the net weight or volume of the SNM-bearing material in a given container. In most applications net weight is measured directly on a scale, with the net weight of the contents being the difference between the observed gross weight and the tare weight of the container. The volume of contents in a process vessel can be measured by alternate approaches, e.g., by the use of a weigh tank together with a specific gravity determination or by the board manometer–specific gravity approach. Alternately, specific gravity determination can be avoided by performing the analysis on the basis of percent element by weight rather than percent element by volume.

The preceding paragraph illustrates that a reported bulk determination result is affected by several error sources, depending on the measurement methods and procedures in use. The same is true of an analytical determination, in which case even more primary-error sources can be identified. Identifying and evaluating all of them in routine practical applications is an impossible task and is not really considered necessary. Here we will characterize each measurement by a single random-error component made up of all sources, identified or not, which contribute to the total random error, by a single short-term systematic-error component, and by a single long-term systematic-error component, where the systematic errors may also include contributions from several error sources. (The distinction between the short-term systematic-error component and the long-term component is described in detail in Sec. 3.1.)

We are in no way limited by defining the error sources this way. Thus, if we wish, when treating the random-error component for a net volume determination of the contents of a process vessel, for example, we can separately identify the component resulting from the manometer reading and that from the specific gravity determination rather than evaluating their combined effects. This introduces no additional complication conceptually but does, of course, require an additional step in application.

Regardless of how detailed the identification and evaluation of primary error sources is, it is emphasized that evaluation of each given error component must include the effects of all potential sources that contribute to it. For example, if several analysts routinely perform a given analysis, the possible differences among analysts must be included because they may affect the values assigned the short-term systematic- and/or the random-error variances. Contrariwise, if only one analyst performs the analysis, the differences among analysts would affect the size of the long-term systematic-error variance. There is always the danger of understating the size of error variances because they may have been estimated under ideal laboratory conditions when attempts were made to hold conditions constant rather than to vary them purposely to include all error sources that will normally affect a given analysis.

Keeping these remarks in mind, in the next two sections we discuss the determination of the measurement variance associated with the SNM content of a given item. Section 5.1 deals with the additive model in which the various errors are expressed on an absolute basis, and Sec. 5.2 deals with the treatment of relative errors. In application the result will be the same, and it is largely a matter of preference as to which model is used.

Finally, Sec. 5.3 contains a brief discussion of the interpretation of assigned limits of error as they are associated with the SNM content of a container.

5.1 ADDITIVE MODEL (ABSOLUTE ERRORS)

5.1.1 Problem and Assumptions

The amount of element (uranium or plutonium) in a given container is determined by the wet-chemistry approach; i.e., a bulk determination is made which gives a net weight (or volume) of the container contents. This is then multiplied by an element factor to give the total amount of element calculated for the container. The product, in turn, is multiplied by an isotope factor to give the total amount of isotope (e.g., ^{235}U or fissile plutonium) calculated for the container. The element factor is the ratio of the amount of element to the total contents, and the isotope factor is the ratio of the amount of isotope to the amount of element.

The following assumptions are made:

1. A single bulk determination is made.

2. The element factor is an average factor based on m samples and d total analyses made either on the composite or with d/m analyses per sample. This factor may be unique to the container in question, or it may represent an average factor that applies to several containers. The m samples, therefore, may all be drawn from one container or may be drawn from several nominally similar containers, all of which will be assigned this element factor. The interpretation of the variance due to sampling changes accordingly.

3. With respect to the short-term systematic error due to sampling for the element factor, s_i samples are drawn under short-term sampling conditions i; $i = 1, 2, \ldots, S$, with

$$\sum_{i=1}^{S} s_i = m$$

4. With respect to the short-term systematic error due to the element factor analysis, a_i analyses are performed under short-term analytical conditions i; $i = 1, 2, \ldots, A$, with

$$\sum_{i=1}^{A} a_i = d$$

5. The isotope factor is an average factor based on p samples and k total isotopic analyses.

6. With respect to the short-term systematic error due to sampling for the isotope factor, r_i samples are drawn under short-term sampling conditions i; $i = 1, 2, \ldots, R$, with

$$\sum_{i=1}^{R} r_i = p$$

7. With respect to the short-term systematic error due to the isotope

factor analysis, b_i analyses are performed under short-term analytical conditions i; $i = 1, 2, \ldots, B$, with

$$\sum_{i=1}^{B} b_i = k$$

8. All error-component random variables are unbiased; i.e., they are distributed with zero means. This means that, if any known measurement biases exist, the data are appropriately corrected.

9. All error components are uncorrelated; i.e., all covariances between the error-component random variables are zero.

The standard deviations are defined in Table 5.1. Each is expressed in absolute units, i.e., in the same units as the related measurement.

TABLE 5.1 DEFINITION OF STANDARD DEVIATIONS

Operation	Type of error component		
	Long-term systematic	Short-term systematic	Random
Bulk measurement	σ_β	σ_ϕ	σ_ϵ
Sampling, element	σ_Δ	σ_ψ	σ_η
Analytical, element	σ_θ	σ_β	σ_ω
Sampling, isotope	σ_λ	σ_π	σ_μ
Analytical, isotope	σ_γ	σ_α	σ_ν

The problem is to find the variances associated with the calculated amount of element and isotope in the container in question.

5.1.2 Solution

The standard deviations, given in Table 5.1, are in absolute units. In addition:

w = observed net weight (or volume) of container contents
$\bar{p}$ = element factor applied to the contents
$\bar{t}$ = isotope factor applied to the contents
m = number of samples on which $\bar{p}$ is based
d = number of analytical determinations on which $\bar{p}$ is based
s_i = number of samples drawn under condition i for element analysis, with $\sum_{i=1}^{S} s_i = m$
a_i = number of element analyses made under condition i, with $\sum_{i=1}^{A} a_i = d$
p = number of samples on which $\bar{t}$ is based
k = number of analytical determinations on which $\bar{t}$ is based

r_i = number of samples drawn under condition i for isotope analysis, with $\sum_{i=1}^{R} r_i = p$

b_i = number of isotope analyses made under conditions i, with $\sum_{i=1}^{B} b_i = k$

Then the variance of the calculated element weight for the container in question, V_E, is

$$V_E = w^2\left(\sigma_\Delta^2+\sigma_\theta^2+c_0\sigma_\psi^2+c_1\sigma_\beta^2+\frac{\sigma_\eta^2}{m}+\frac{\sigma_\omega^2}{d}\right)+\bar{p}^2(\sigma_\delta^2+\sigma_\phi^2+\sigma_\epsilon^2) \tag{5.1}$$

where

$$c_0 = \sum_{i=1}^{S}\frac{s_i^2}{m^2} \tag{5.2}$$

and

$$c_1 = \sum_{i=1}^{A}\frac{a_i^2}{d^2} \tag{5.3}$$

The result of Eq. 5.1 is no doubt familiar to many readers, except for the inclusion of the short-term systematic-error variances σ_ψ^2 and σ_β^2. The equation indicates that the long-term systematic-error variances are independent of the number of determinations made, whereas the random-error variances decrease in direct proportion to the number of determinations.

The variance of the calculated isotope weight for the container in question, V_I, is

$$V_I = (w\bar{p})^2\left(\sigma_\lambda^2+\sigma_\gamma^2+g_0\sigma_\pi^2+g_1\sigma_\alpha^2+\frac{\sigma_\mu^2}{p}+\frac{\sigma_\nu^2}{k}\right)$$
$$+(w\bar{l})^2\left(\sigma_\Delta^2+\sigma_\theta^2+c_0\sigma_\psi^2+c_1\sigma_\beta^2+\frac{\sigma_\eta^2}{m}+\frac{\sigma_\omega^2}{d}\right)+(p\bar{l})^2(\sigma_\delta^2+\sigma_\phi^2+\sigma_\epsilon^2) \tag{5.4}$$

where c_0 and c_1 are as defined in Eqs. 5.2 and 5.3 and where

$$g_0 = \sum_{i=1}^{R}\frac{r_i^2}{p^2} \tag{5.5}$$

and

$$g_1 = \sum_{i=1}^{B}\frac{b_i^2}{k^2} \tag{5.6}$$

5.1.3 Examples

Example 5.A

Find the standard deviation on the total amount of plutonium calculated for a dissolver batch in a chemical reprocessing facility. The volume is based on a single determination, and the percent plutonium is determined from a duplicate sample with a single analysis per sample. After the first

sample is drawn, the vessel contents are thoroughly mixed before the second sample is taken. The two samples are therefore regarded as having been drawn under two sets of conditions. Both analyses are performed under the same set of conditions. Thus

$$m=2 \qquad d=2 \qquad a_1=2$$
$$s_1=1 \qquad s_2=1$$

In this application the bulk determination consists of a volume rather than a weight. Assume the following values for the observed data and for the various standard deviations:

$$w=4542 \text{ liters} \qquad \bar{p}=3.09 \text{ g/liter}$$

$$\sigma_\delta=15 \qquad \sigma_\phi=8 \qquad \sigma_\epsilon=20$$
$$\sigma_\Delta=0.005 \qquad \sigma_\psi=0.003 \qquad \sigma_\eta=0.010$$
$$\sigma_\theta=0.005 \qquad \sigma_\beta=0.005 \qquad \sigma_\omega=0.024$$

From Eqs. 5.2 and 5.3,

$$c_0=\frac{1}{4}+\frac{1}{4}=0.50 \qquad c_1=\frac{4}{4}=1$$

Then V_E is calculated from Eq. 5.1:

$$V_E=(4542)^2(10^{-6})(25+25+4.5+25+50+288)$$
$$+(3.09)^2(225+64+400)=8613+6579=15192 \quad \text{g}^2 \text{ of Pu}$$

The standard deviation is $\sqrt{V_E}=123$ g of plutonium. This is 0.88% of the calculated amount [(4542)(3.09) = 14.035 kg of Pu.]

Example 5.B

Find the standard deviation on the total amount of uranium and on the total amount of ^{235}U in a can of UO_2 powder. The net contents are based on a single weighing. The uranium factor is the average of five samples with one analytical determination per sample. The samples are all drawn by using the same sampling technique and are assumed to have been drawn under the same set of conditions. The analyses are performed under two sets of conditions (this may refer to two operators, two sets of equipment, two periods of time, etc.), with two analyses under condition 1 and three under condition 2. The isotopic factor is based on two samples, with one mass spectrometric determination per sample. Both samples are drawn and both determinations are made under the same sets of conditions.* This gives rise to the following parameter values:

$$m=5 \qquad k=2 \qquad a_1=2$$
$$p=2 \qquad s_1=5 \qquad a_2=3$$
$$d=5 \qquad r_1=2 \qquad b_1=2$$

* Samples might be considered drawn under different sets of conditions if an average isotope factor is based on sampling different forms of the material (UF_6, powder, pellets).

Assume the following values for the observed data and for the various standard deviations:

$w = 20.02$ kg	$\bar{p} = 0.8758$	$\bar{t} = 0.0428$
$\sigma_\delta = 0.005$	$\sigma_\phi = 0$	$\sigma_\epsilon = 0.015$
$\sigma_\Delta = 0.00015$	$\sigma_\psi = 0.00005$	$\sigma_\eta = 0.0002$
$\sigma_\theta = 0.0001$	$\sigma_\beta = 0.00025$	$\sigma_\omega = 0.0003$
$\sigma_\lambda = 0.000008$	$\sigma_\pi = 0.00001$	$\sigma_\mu = 0.00001$
$\sigma_\gamma = 0.00003$	$\sigma_\alpha = 0.00005$	$\sigma_\nu = 0.0002$

To find V_E, we first calculate c_0 and c_1 from Eqs. 5.2 and 5.3:

$$c_0 = \frac{25}{25} = 1 \qquad c_1 = \frac{4+9}{25} = \frac{13}{25}$$

Then, from Eq. 5.1,

$$V_E = (20.02)^2(10^{-10})(225+100+25+325+80+180) + (0.8758)^2(10^{-6})(25+0+225)$$

$$V_E = 0.00003747 + 0.00019176 = 0.00022923 \quad \text{kg}^2 \text{ of U}$$

Therefore the standard deviation is $\sqrt{V_E} = 0.0151$ kg of uranium. This is 0.086% of the calculated amount [(20.02)(0.8758) = 17.53 kg of U].

To find V_I, we first note that g_0 from Eq. 5.5 and g_1 from Eq. 5.6 are both 1. Then, from Eq. 5.4,

$$V_I = [(20.02)(0.8758)]^2(10^{-10})(0.64+9+1+25+0.5+200) + [(20.02)(0.0428)]^2(10^{-10})(225+100+25+325+80+180) + [(0.8758)(0.0428)]^2(10^{-6})(25+0+225)$$

$$V_I = 10^{-6}(7.2595+0.0686+0.3513) = 7.6794 \times 10^{-6} \quad \text{kg}^2\ ^{235}\text{U}$$

Therefore the standard deviation is $\sqrt{V_I} = 0.00277$ kg of ^{235}U. This is 0.37% of the calculated amount [(20.02)(0.8758)(0.0428) = 0.7504 kg of ^{235}U].

5.1.4 Basis

When each error standard deviation is expressed on an absolute basis, the descriptive model can be developed as follows: Let w be the average net weight (or net volume) determined by a single determination, which is common practice. (The model will be developed in terms of weights, but volumes can be substituted for weights with no essential changes in the development.) Write

$$w = W + \delta + \phi + \epsilon \tag{5.7}$$

where W = true net weight of the container contents in some arbitrary unit (lb, g, kg, etc.)

δ = long-term systematic error due to weighing

ϕ = short-term systematic error due to weighing
ϵ = random error due to weighing

In this model the δ, ϕ, and ϵ errors are expressed in the same units as the net weight. Each error was selected at random from its corresponding population density function. All population density functions have a mean of zero, and their standard deviations are σ_δ, σ_ϕ, and σ_ϵ. No subscripts are used on these errors because only a single weight determination was made. Clearly in this instance we could combine the δ and ϕ components to achieve an overall systematic error. However, they are kept separate to permit the transition to the results of Chap. 6.

To continue, let $\bar{p}$ represent the average element factor expressed as the ratio of the amount of element (uranium or plutonium) to the total amount of material in the container. Depending on the material, this factor may apply to several items in a given category, in which case it will probably be based on several determinations. (Even if it applies only to a given container, it could also, of course, be based on several determinations.) Specifically, let the factor be based on drawing m samples with d total analyses. It is assumed that these d analyses either are made on the composite of the m samples or are the result of d/m analyses per sample. Further, to account for the short-term systematic sampling and analytical errors, we assume that s_i samples are drawn under sampling conditions i, with $i = 1, 2, \ldots, S$ and $\sum_{i=1}^{S} s_i = m$, and that a_i analyses are performed under short-term analytical conditions i, with $i = 1, 2, \ldots, A$, and $\sum_{i=1}^{A} a_i = d$. Then the model can be written

$$\bar{p} = P + \Delta + \bar{\psi}(S) + \bar{\eta}(m) + \theta + \bar{\beta}(A) + \bar{\omega}(d) \tag{5.8}$$

where P = true element factor
Δ = systematic error due to sampling for element
$\bar{\psi}(S)$ = average short-term systematic error due to sampling for element, determined over S sets of sampling conditions
$\bar{\eta}(m)$ = average random error due to sampling for element, based on m samples
θ = long-term systematic error due to element analysis
$\bar{\beta}(A)$ = average short-term systematic error due to element analysis, determined over A sets of analytical conditions
$\omega(d)$ = average random error due to element analysis, based on d analyses

Note that $\bar{\eta}(m)$, the random error due to sampling, includes the error due to sampling from within a container plus that due to sampling from different containers, as applicable. The latter source exists only when an average element factor is used to apply to a number of items of a given type.

The errors in Eq. 5.8 are assumed to have been sampled from popula-

tions with zero means. Also, the standard deviations of these population density functions are σ_Δ, σ_ψ, σ_η, σ_θ, σ_β, and σ_ω.

The amount of element determined for the item in question is now calculated from Eqs. 5.7 and 5.8 as the product $w\bar{p}$:

$$w\bar{p} = (W+\delta+\phi+\epsilon)[P+\Delta+\bar{\psi}(S)+\bar{\eta}(m)+\theta+\bar{\beta}(A)+\bar{\omega}(d)] \qquad (5.9)$$

This is multiplied out, and the variance of the sum is found by applying Eqs. 4.3 and 4.6. It is assumed that all the random variables denoting the error components have zero covariances. Further, in finding the variance of the sum, we ignore second-order terms, e.g., the product of σ_δ^2 and σ_Δ^2. These are normally very small relative to the terms that are retained.

The variance of $w\bar{p}$ is then found to be

$$\sigma_{w\bar{p}}^2 = W^2(\sigma_\Delta^2+\sigma_{\bar{\psi}}^2+\sigma_{\bar{\eta}}^2+\sigma_\theta^2+\sigma_{\bar{\beta}}^2+\sigma_{\bar{\omega}}^2)+P^2(\sigma_\delta^2+\sigma_\theta^2+\sigma_\epsilon^2) \qquad (5.10)$$

where

$$\sigma_{\bar{\psi}}^2 = c_0\sigma_\psi^2 \qquad \sigma_{\bar{\eta}}^2 = \frac{\sigma_\eta^2}{m}$$
$$\sigma_{\bar{\omega}}^2 = \frac{\sigma_\omega^2}{d} \qquad \sigma_{\bar{\beta}}^2 = c_1\sigma_\beta^2 \qquad (5.11)$$

with

$$c_0 = \sum_{i=1}^{S} \frac{s_i^2}{m^2} \qquad c_1 = \sum_{i=1}^{A} \frac{a_i^2}{d^2}$$

It is helpful to see how $\sigma_{\bar{\psi}}^2$ is derived. From Eq. 5.8, considering only the $\bar{\psi}(S)$ contribution to $\bar{p}$, we can write

$$\bar{p} = [\underbrace{(\psi_1+\psi_1+\ldots+\psi_1)}_{s_1 \text{ terms}} + \underbrace{(\psi_2+\psi_2+\ldots+\psi_2)}_{s_2 \text{ terms}} + \ldots$$
$$+ \underbrace{(\psi_s+\psi_s+\ldots+\psi_s)}_{s_s \text{ terms}}]/m$$
$$= \frac{s_1\psi_1+s_2\psi_2+\ldots+s_s\psi_s}{m}$$

Then, by Eq. 4.3,

$$\sigma_{\bar{p}}^2 = \sigma_\psi^2 \frac{s_1^2+s_2^2+\ldots+s_s^2}{m^2} = \sigma_\psi^2 \sum_{i=1}^{S} \frac{s_i^2}{m^2}$$

Similar derivations apply to $\sigma_{\bar{\eta}}^2$, $\sigma_{\bar{\beta}}^2$, $\sigma_{\bar{\omega}}^2$, etc.

Equation 5.10 and its defining relations (Eq. 5.11) give the variance of element weight expressed in squared units; these units are the same as those used to express the net weight of the contents for the container in question. Since W and P are not known, they are replaced by w and $\bar{p}$ in the evaluation.

The extension to calculate the variance of the isotope weight is straightforward. If $w\bar{p}$ is the calculated element weight, then $w\bar{p}\bar{t}$ is the

calculated weight of the isotope, where $\bar{t}$ is the average isotope factor expressed as the ratio of the amount of isotope to the amount of element. Let $\bar{t}$ be based on drawing p samples with k total isotope determinations. In practice, k will often equal p since one determination is usually made per sample; this is not a necessary requirement, however. To account for the short-term systematic errors associated with the isotope determination, we assume that r_i samples are drawn under sampling condition i, with $i=1, 2, \ldots, R$ and $\sum_{i=1}^{R} r_i = p$, and that b_i analyses are made under short-term condition i, with $i=1, 2, \ldots, B$ and $\sum_{i=1}^{B} b_i = k$. Then t is expressed as

$$\bar{t} = T+\lambda+\bar{\pi}(R)+\bar{\mu}(p)+\gamma+\bar{\alpha}(B)+\bar{\nu}(k) \tag{5.12}$$

where T = true isotopic factor
λ = long-term systematic error due to sampling for isotope
$\bar{\pi}(R)$ = average short-term systematic error due to sampling for isotope, determined over R sets of sampling conditions
$\bar{\mu}(p)$ = average random error due to sampling for isotope, based on p samples
γ = long-term systematic error due to isotope analysis
$\bar{\alpha}(B)$ = average short-term systematic error due to isotope analysis, determined over B sets of analytical conditions
$\bar{\nu}(k)$ = average random error due to isotope analysis, based on k analyses

Again assuming zero means, standard deviations of σ_η, σ_π, σ_μ, σ_γ, σ_α, and σ_ν, and uncorrelated random variables and again ignoring second-order and higher terms, we find the variance of the calculated amount of isotope, $\overline{wpt}$, by applying Eqs. 4.3 and 4.6 to the product:

$$\begin{aligned}\overline{wpt} = {} & (W+\delta+\phi+\epsilon)[P+\Delta+\bar{\psi}(S)+\bar{\eta}(m)+\theta+\bar{\beta}(A)+\bar{\omega}(d)] \\ & \times[T+\lambda+\bar{\pi}(R)+\bar{\mu}(p)+\gamma+\bar{\alpha}(B)+\bar{\nu}(k)]\end{aligned} \tag{5.13}$$

The resulting variance is

$$\begin{aligned}\sigma^2_{\overline{wpt}} = {} & (WP)^2(\sigma^2_\lambda+\sigma^2_{\bar{\pi}}+\sigma^2_{\bar{\mu}}+\sigma^2_\gamma+\sigma^2_{\bar{\alpha}}+\sigma^2_{\bar{\nu}}) \\ & +(WT)^2(\sigma^2_\Delta+\sigma^2_{\bar{\psi}}+\sigma^2_{\bar{\eta}}+\sigma^2_\theta+\sigma^2_{\bar{\beta}}+\sigma^2_{\bar{\omega}})+(PT)^2(\sigma^2_\delta+\sigma^2_\phi+\sigma^2_\epsilon)\end{aligned} \tag{5.14}$$

where $\sigma^2_{\bar{\psi}}$, $\sigma^2_{\bar{\eta}}$, $\sigma^2_{\bar{\beta}}$, and $\sigma^2_{\bar{\omega}}$ are as defined in Eq. 5.11 and where

$$\begin{aligned} \sigma^2_{\bar{\pi}} &= g_0\sigma^2_\pi & \sigma^2_{\bar{\mu}} &= \frac{\sigma^2_\mu}{p} \\ \sigma^2_{\bar{\nu}} &= \frac{\sigma^2_\nu}{k} & \sigma^2_{\bar{\alpha}} &= g_1\sigma^2_\alpha \end{aligned} \tag{5.15}$$

with

$$g_0 = \sum_{i=1}^{R} \frac{r_i^2}{p^2} \qquad g_1 = \sum_{i=1}^{B} \frac{b_i^2}{k^2}$$

Equation 5.14 and its defining relations (Eqs. 5.11 and 5.15) give the variance of isotope weight expressed in squared units; these units are the same as those used to express the net weight of the contents for the container in question. Again, W, P, and T are replaced by w, $\bar{p}$, and $\bar{t}$, respectively, in application.

5.2 MULTIPLICATIVE MODEL (RELATIVE ERRORS)

5.2.1 Problem and Assumptions

The presentation in Sec. 5.1.1 for the additive model is also generally applicable for the multiplicative model. The only difference is in the interpretation of the σ's in Table 5.1. In this section the σ's are all expressed on a relative basis. For example, a standard deviation of 0.3% would be written 0.003; this means that the standard deviation is 0.3% of the true value for the measurement in question. No confusion should result from the use of the same notation for both the relative and absolute-error models. Asterisks or some other distinguishing mark could be used, however, to designate relative errors as opposed to absolute errors, but this introduces complexity in the notation which is not really needed.

5.2.2 Solution

The quantities w, $\bar{p}$, $\bar{t}$, m, d, s_i, a_i, p, k, r_i, and b_i are as defined in Sec. 5.1.2.

The variance of the calculated element weight for the container in question, V_E, is found by application of the following steps (formula 5.1 for the absolute error model could have been presented as a set of steps similar to these but somewhat more complicated):

Step 1. Sum the variances for the long-term systematic-error components and for the short-term systematic-error component associated with the bulk determination. (The short-term systematic-error variance for the bulk determination is included because only a single bulk determination is assumed to have been made. In this circumstance the short-term error has the same effect as a long-term error.)

Step 2. Multiply the variance for the short-term systematic sampling component by $c_0 = \sum_{i=1}^{S} (s_i^2/m^2)$.

Step 3. Multiply the variance for the short-term systematic analytical component by $c_1 = \sum_{i=1}^{A} (a_i^2/d^2)$.

Step 4. Divide each variance for the random-error components by the

appropriate number of determinations (samples or analyses), and sum the results.

Step 5. To obtain the variance, V_E, sum the quantities in steps 1 to 4 and multiply by the square of the observed element weight. [If the variance of element (or isotope) weights is to be expressed on a relative basis also, this variance is simply the sum of the quantities in steps 1 to 4. The relative standard deviation is then the square root of this sum.]

The error components identified in these steps include only those associated with the bulk measurement and the sampling and analytical components for the element determination. To find the variance of the observed isotope weight, we include in steps 1 to 4 the sampling and analytical components for the isotope determination, and we replace element weight in step 5 by isotope weight.

If formulas are preferred to words, these are

$$V_E = (w\bar{p})^2\left(\sigma_\delta^2+\sigma_\Delta^2+\sigma_\theta^2+\sigma_\phi^2+c_0\sigma_\psi^2+c_1\sigma_\beta^2+\sigma_\epsilon^2+\frac{\sigma_\eta^2}{m}+\frac{\sigma_\omega^2}{d}\right) \tag{5.16}$$

where

$$c_0 = \sum_{i=1}^{S}\frac{s_i^2}{m^2} \tag{5.17}$$

and

$$c_1 = \sum_{i=1}^{A}\frac{a_i^2}{d^2} \tag{5.18}$$

$$V_I = (w\bar{p}\bar{t})^2\left(\sigma_\delta^2+\sigma_\Delta^2+\sigma_\theta^2+\sigma_\lambda^2+\sigma_\gamma^2+\sigma_\phi^2+c_0\sigma_\psi^2+c_1\sigma_\beta^2+g_0\sigma_\pi^2+g_1\sigma_\alpha^2 + \sigma_\epsilon^2+\frac{\sigma_\eta^2}{m}+\frac{\sigma_\omega^2}{d}+\frac{\sigma_\mu^2}{p}+\frac{\sigma_\nu^2}{k}\right) \tag{5.19}$$

where c_0 and c_1 are as defined in Eqs. 5.17 and 5.18 and where

$$g_0 = \sum_{i=1}^{R}\frac{r_i^2}{p^2} \tag{5.20}$$

and

$$g_1 = \sum_{i=1}^{B}\frac{b_i^2}{k^2} \tag{5.21}$$

5.2.3 Examples

The first two examples in this section parallel those in Sec. 5.1.3 except that error standard deviations are now expressed on a relative basis.

Example 5.C

See example 5.A. The values for the parameters are:

$m=2$ $\quad d=2$ $\quad a_1=2$

$s_1=1$ $\quad s_2=1$

The observed data are:

$$w = 4542 \text{ liters} \qquad \bar{p} = 3.09 \text{ g/liter}$$

On the relative basis, the standard deviations corresponding to those given in example 5.A are:

$$\sigma_\delta = 15/4542 = 0.00330 \qquad \sigma_\eta = 0.010/3.09 = 0.00324$$
$$\sigma_\phi = 8/4542 = 0.00176 \qquad \sigma_\theta = 0.005/3.09 = 0.00162$$
$$\sigma_\epsilon = 20/4542 = 0.00440 \qquad \sigma_\beta = 0.005/3.09 = 0.00162$$
$$\sigma_\Delta = 0.005/3.09 = 0.00162 \qquad \sigma_\omega = 0.024/3.09 = 0.00777$$
$$\sigma_\psi = 0.003/3.09 = 0.00097$$

Compute V_E from the steps of Sec. 5.2.2:

Step 1. $(0.00330)^2 + (0.00162)^2 + (0.00162)^2 + (0.00176)^2 = 19.2364 \times 10^{-6}$

Step 2. $c_0 = 1/4 + 1/4 = 0.50$
$(0.50)(0.00097)^2 = 0.4705 \times 10^{-6}$

Step 3. $c_1 = (2)^2/(2)^2 = 1$
$(1)(0.00162)^2 = 2.6244 \times 10^{-6}$

Step 4. $$\frac{(0.00440)^2}{1} + \frac{(0.00324)^2}{2} + \frac{(0.00777)^2}{2} = 54.7953 \times 10^{-6}$$

Step 5. $(\text{element weight})^2 = [(4542)(3.09)]^2 = 196.975 \times 10^6$

$V_E = (196.975)(19.2364 + 0.4705 + 2.6244 + 54.7953) = 15192$ g² of Pu

This agrees with the value found in example 5.A.

Example 5.D

See example 5.B. The values for the parameters are:

$$m = 5 \qquad a_1 = 2 \qquad k = 2$$
$$d = 5 \qquad a_2 = 3 \qquad r_1 = 2$$
$$s_1 = 5 \qquad p = 2 \qquad b_1 = 2$$

The observed data are:

$$w = 20.02 \qquad \bar{p} = 0.8758 \qquad \bar{t} = 0.0428$$

On a relative basis the standard deviations corresponding to those given in example 5.B are:

$$\sigma_\delta = \frac{0.005}{20.02} = 0.00025 \qquad \sigma_\phi = 0 \qquad \sigma_\epsilon = 0.00075$$

$$\sigma_\Delta = \frac{0.00015}{0.8758} = 0.00017 \qquad \sigma_\psi = 0.000057 \qquad \sigma_\eta = 0.00023$$

$$\sigma_\theta = \frac{0.0001}{0.8758} = 0.00011 \qquad \sigma_\beta = 0.00029 \qquad \sigma_\omega = 0.00034$$

$$\sigma_\lambda = \frac{0.000008}{0.0428} = 0.00019 \qquad \sigma_\pi = 0.00023 \qquad \sigma_\mu = 0.00023$$

$$\sigma_\gamma = \frac{0.00003}{0.0428} = 0.00070 \qquad \sigma_\alpha = 0.00117 \qquad \sigma_\nu = 0.00467$$

Compute V_E from the steps in Sec. 5.2.2:

Step 1. $10^{-10}[(25)^2+(17)^2+(11)^2+(0)^2] = 1035\times10^{-10}$

Step 2. $c_0 = (5)^2/(5)^2 = 1$
$(1)(5.7)^2\times10^{-10} = 32\times10^{-10}$

Step 3. $c_1 = \dfrac{(2)^2+(3)^2}{(5)^2} = \dfrac{13}{25}$
$(13/25)(29)^2\times10^{-10} = 437\times10^{-10}$

Step 4. $10^{-10}\left(\dfrac{(75)^2}{1}+\dfrac{(23)^2}{5}+\dfrac{(34)^2}{5}\right) = 5962\times10^{-10}$

Step 5. (Uranium weight)$^2 = [(20.02)(0.8758)]^2 = 307.42$ kg^2 of U

$V_E = (307.42)(1035+32+437+5962)(10^{-10}) = 0.000229$ kg^2 of U

This agrees with the value found in example 5.B.

Next, compute V_I from the steps of Sec. 5.2.2. In step 5, isotope weight replaces element weight.

Step 1. $10^{-10}[1035+(19)^2+(70)^2] = 6296\times10^{-10}$

Step 2. $g_0 = (2)^2/(2)^2 = 1$
$10^{-10}[32+(1)(23)^2] = 561\times10^{-10}$

Step 3. $g_1 = (2)^2/(2)^2 = 1$
$10^{-10}[437+(1)(117)^2] = 14126\times10^{-10}$

Step 4. $10^{-10}[5962+(23)^2/2+(467)^2/2] = 115271\times10^{-10}$

Step 5. (^{235}U weight)$^2 = [(20.02)(0.8758)(0.0428)]^2$
$= 0.5632$ kg^2 of ^{235}U

$V_I = (0.5632)(6296+561+14126+115271)(10^{-10})$
$= 7.67\times10^{-6}$ kg^2 of ^{235}U

This agrees with the value found in example 5.B.

The values of the first terms in the sums in steps 1 to 4 were calculated when V_E was found. Additional terms are now included to account for the uncertainties in the isotope factor.

Example 5.E

A fuel rod contains PuO_2–UO_2 pellets. Given the following information, find the relative standard deviation associated with the amount of fissile plutonium in the rod. The relative standard deviations are:

$\sigma_\delta = 0.0001$	$\sigma_\phi = 0$	$\sigma_\epsilon = 0.0002$
$\sigma_\Delta = 0.0032$	$\sigma_\psi = 0.0014$	$\sigma_\eta = 0.0090$
$\sigma_\theta = 0.0010$	$\sigma_\beta = 0.0008$	$\sigma_\omega = 0.0075$
$\sigma_\lambda = 0.0001$	$\sigma_\pi = 0.0001$	$\sigma_\mu = 0.00005$
$\sigma_\gamma = 0.0003$	$\sigma_\alpha = 0.0002$	$\sigma_\nu = 0.00012$

A single weighing is made of the net weight of the pellets in the rod. The plutonium factor is based on 12 samples with three analyses per sample. The 12 samples consist of two pellets from each of six batches, and each batch can be considered as corresponding to a given sampling condition. The 36 analyses are performed under analytical conditions 1, 2, and 3, with 9, 6, and 21 analyses, respectively, made under each condition. The fissile plutonium factor is based on seven samples, with one analysis per sample. Three samples are drawn from the PuO_2 powder (sampling condition 1), two from the PuO_2–UO_2 powder (condition 2), and two from the PuO_2–UO_2 pellets (condition 3). All seven analyses are performed under the same set of analytical conditions.

This information can be summarized by the following parameter values:

$$s_1 = s_2 = s_3 = s_4 = s_5 = s_6 = 2$$

$m = 12$	$a_2 = 6$	$r_1 = 3$	$k = 7$
$d = 36$	$a_3 = 21$	$r_2 = 2$	$b_1 = 7$
$a_1 = 9$	$p = 7$	$r_3 = 2$	

The steps in Sec. 5.2.2 are applied:

Step 1. $(0.0001)^2 + (0.0032)^2 + (0.0010)^2 + (0.0001)^2 + (0.0003)^2 = 1135 \times 10^{-8}$

Step 2. $c_0 = 6(2)^2/144 = 0.1667$

$(0.1667)(0.0014)^2 = 33 \times 10^{-8}$

$$g_0 = \frac{(3)^2 + (2)^2 + (2)^2}{49} = 0.3469$$

$(0.3469)(0.0001)^2 = 0 \times 10^{-8}$

Step 3. $c_1 = \dfrac{(9)^2+(6)^2+(21)^2}{1296} = 0.4306$

$(0.4306)(0.0008)^2 = 28\times10^{-8}$

$g_1 = (7)^2/49 = 1$

$(1)(0.0002)^2 = 4\times10^{-8}$

Step 4. $\dfrac{(0.0002)^2}{1}+\dfrac{(0.0090)^2}{12}+\dfrac{(0.0075)^2}{36}+\dfrac{(0.0005)^2}{7}+\dfrac{(0.00012)^2}{7}$
$= 835\times10^{-8}$

Therefore, on a relative basis,

$$\frac{V_I}{I} = 10^{-8}(1135+33+0+28+4+835) = 2035\times10^{-8}$$

The relative standard deviation is $\sqrt{V_I/I} = 0.0045$, or 0.45%.

5.2.4 Basis

When the error standard deviations are expressed on a relative basis, the model can be developed as follows: Let the notation be the same as that used in Sec. 5.1.4 in the sense that δ refers to the long-term systematic error due to bulk determination, ϕ to the corresponding short-term systematic error, etc. However, the density functions for these random variables will differ from those in the previous development.

For the additive model in Sec. 5.1.4, which applies when errors are expressed on an absolute basis, each error random variable has a mean of zero and a standard deviation expressed in the same units as the corresponding measured value. For the multiplicative model, used when errors are expressed on a relative basis, each error random variable has either a mean of zero or a mean of one, depending on how the model is written, and a standard deviation expressed in relative units. For example, a 0.3% relative standard deviation is written as $\sigma = 0.003$.

Using notation analogous to that in Sec. 5.1.4, we can model the observed bulk measurement with relative errors as

$$w = W+\delta W+\phi W+\epsilon W = W(1+\delta+\phi+\epsilon) \tag{5.22}$$

where δ, ϕ, and ϵ have zero means. Alternately, we could write

$$w = W\delta\phi\epsilon \tag{5.23}$$

where δ, ϕ, and ϵ have means of one.

Although these models are not equivalent, they will yield equivalent results when used to find the variance of w by application of Eq. 4.6.

Application of Eq. 4.6 assumes that the relative variances are small,* and this is a situation in which Eqs. 5.22 and 5.23 yield essentially equivalent results.

To illustrate, consider the following equivalent values for the three random variables under the two models.

TABLE 5.2 ERRORS FOR TWO MULTIPLICATIVE MODELS

Model of Eq. 5.22	Model of Eq. 5.23
$\delta = 0.04$	$\delta = 1.04$
$\phi = -0.01$	$\phi = 0.99$
$\epsilon = 0.03$	$\epsilon = 1.03$

The resulting value for w, from Eq. 5.22, is

$$w = W(1+0.04-0.01+0.03) = 1.06W$$

From Eq. 5.23, it is

$$w = W(1.04)(0.99)(1.03) = 1.060488W$$

These values are essentially the same for all practical purposes.

Further, equivalence is demonstrated by application of Eq. 4.6 to find the variance of w in each case. For the model of Eq. 5.22,

$$\sigma_w^2 = W^2(\sigma_\delta^2+\sigma_\phi^2+\sigma_\epsilon^2)$$

This follows since

$$\frac{\partial w}{\partial \delta} = \frac{\partial w}{\partial \phi} = \frac{\partial w}{\partial \epsilon} = W$$

For the model of Eq. 5.23,

$$\sigma_w^2 = W^2(\sigma_\delta^2+\sigma_\phi^2+\sigma_\epsilon^2)$$

an identical result. This follows since

$$\frac{\partial w}{\partial \delta} = W\phi\epsilon$$

which, when evaluated at the mean values $\phi = \epsilon = 1$, is simply W. Similar results hold for $\partial w/\partial \phi$ and $\partial w/\partial \epsilon$.

Equivalence also holds for the product $w\bar{p}$. The first model gives

$$w\bar{p} = WP(1+\delta+\phi+\epsilon)(1+\Delta+\bar{\psi}+\bar{\eta}+\theta+\bar{\beta}+\bar{\omega}) \tag{5.24}$$

The second model is written

$$w\bar{p} = WP\delta\phi\epsilon\Delta\bar{\psi}\bar{\eta}\theta\bar{\beta}\bar{\omega} \tag{5.25}$$

* See the discussion following Eq. 4.6.

Again, applying Eq. 4.6 to find the variance of $\bar{wp}$ yields equivalent results for both models:

$$\sigma^2_{\bar{wp}} = (WP)^2(\sigma^2_{\delta}+\sigma^2_{\phi}+\sigma^2_{\epsilon}+\sigma^2_{\Delta}+\sigma^2_{\bar{\psi}}+\sigma^2_{\bar{\eta}}+\sigma^2_{\theta}+\sigma^2_{\bar{\beta}}+\sigma^2_{\bar{\omega}}) \tag{5.26}$$

where $\sigma^2_{\bar{\psi}}$, $\sigma^2_{\bar{\eta}}$, $\sigma^2_{\bar{\beta}}$, and $\sigma^2_{\bar{\omega}}$ are defined as in Eq. 5.11.

This follows from the model of Eq. 5.22 since $\partial\bar{wp}/\partial\delta = WP(1+\Delta+\bar{\psi}+\bar{\eta}+\theta+\bar{\beta}+\bar{\omega})$, which, when evaluated at the mean values ($\Delta=\bar{\psi}=\bar{\eta}=\theta=\bar{\beta}=\bar{\omega}=0$), is simply WP. Similar results hold for $\partial\bar{wp}/\partial\Delta$, $\partial\bar{wp}/\partial\bar{\psi}$, etc. This also follows with the model of Eq. 5.23 since $\partial\bar{wp}/\partial\delta = WP\phi\epsilon\Delta \ldots \bar{\omega}$, which, when evaluated at the mean values ($\Delta=\phi=\ldots=\bar{\omega}=1$), is simply WP. Similar results hold for $\partial\bar{wp}/\partial\Delta$, $\partial\bar{wp}/\partial\psi$, etc.

Finally, applying Eq. 4.6 to find the variance of $\bar{wpt}$ yields

$$\begin{aligned}\sigma^2_{\bar{wpt}} = (WPT)^2(&\sigma^2_{\delta}+\sigma^2_{\phi}+\sigma^2_{\epsilon}+\sigma^2_{\Delta}+\sigma^2_{\bar{\psi}}+\sigma^2_{\bar{\eta}}+\sigma^2_{\theta}+\sigma^2_{\bar{\beta}}+\sigma^2_{\bar{\omega}}+\sigma^2_{\lambda}\\ &+\sigma^2_{\bar{\pi}}+\sigma^2_{\bar{\mu}}+\sigma^2_{\bar{\gamma}}+\sigma^2_{\bar{\alpha}}+\sigma^2_{\bar{\nu}})\end{aligned} \tag{5.27}$$

where $\sigma^2_{\bar{\mu}}$, $\sigma^2_{\bar{\nu}}$, and $\sigma^2_{\bar{\nu}}$ are defined as in Eq. 5.15.

As a final note, a logarithmic model could also be used when error standard deviations are expressed on a relative basis. This was demonstrated in example 4.G. Although this approach is suitable for a single item, it is awkward to handle in the common nuclear materials control application in which algebraic sums of SNM contents are of interest. Thus, although Eq. 5.25 could be written as an additive model,

$$\ln(\bar{wp}) = \ln W + \ln P + \ln\delta + \ldots + \ln\bar{\omega} \tag{5.28}$$

this is not helpful in summing $\bar{wp}$ values over several items; the model would have to be retransformed to that of Eq. 5.25 to accomplish this.

5.3 INTERPRETATION OF ASSIGNED LIMITS OF ERROR

The limits of error assigned the SNM content of a given container should be carefully interpreted. They are meaningful only as applied to the container in question, and we must take care when we combine limits of error for several containers.

For example, the variance of the sum of SNM in two containers, or of the difference, generally cannot be found by simply summing the variances for the contents of both containers. The measured SNM values may be correlated for one or more reasons, thereby invalidating this procedure. For example, both containers may have identically the same element factor applied. If this factor is in error on the high side, the resulting sum of element weights will be high by that amount (excluding the combined effects of other errors). This error would cancel when the difference in weights was the quantity of interest. Even if the factors in

question are different, they may be related by virtue of having been determined by use of the same analytical technique, or, if the same scale was used for both containers, its systematic error would affect both net weight determinations. There are other ways in which correlations can be introduced.

With these points in mind, we must consider the calculation of variances or of limits of error for groups of items, taking into account the various ways in which the calculated SNM values can be correlated. This is the subject of Chap. 6.

One additional point should be made. We should emphasize that the practice of taking multiple samples from a container or group of containers and basing the limits of error on the scatter observed in the results is not valid in general. The reason for this is that observed variation often reflects only the effects of the random-error components. In nuclear materials control applications, it is often the effects of the systematic errors which tend to be of dominating importance. Although these error variances are sometimes difficult to evaluate, their effects cannot be ignored.

Chapter 6

LIMITS OF ERROR FOR GENERAL ALGEBRAIC SUMS

OVERVIEW

In Chap. 5, limits of error were found for the special nuclear material (SNM) content of an individual item. This is of limited practical interest in nuclear materials control applications, where attention is focused more on such quantities as shipper–receiver differences, total amounts of SNM in inventory, and material unaccounted for (MUF) than on the SNM content of a single item. The primary interest in Chap. 5 is that it provides a basis on which the more useful results of this chapter can be developed.

The quantities just mentioned are all related in the sense that all are algebraic sums, or linear combinations, of SNM contents for individual items. Thus it is not necessary to develop separate methods for determining limits of error for total amounts in inventory, for example, and for material unaccounted for. Rather, a general method is developed which applies to both these quantities, as well as to others of interest.

In this chapter, we assume that the SNM contents of individual items are determined by the wet-chemistry approach involving a bulk determination, a percent element measurement, and a percent isotopic measurement. If nondestructive assay measurements are made on some or all of the items comprising the algebraic sum, they can be included in the analysis by methods given in Secs. 3.3.8 and 3.3.10. Example 6.H illustrates this.

To establish the motivation for the approach to calculating limits of error used in this chapter, consider this calculation for MUF. The fact that MUF is an algebraic sum of SNM contents for individual items has generally been used in finding the MUF variance. First, the variances of the MUF components (beginning and ending inventories, inputs, and outputs) are found; these are then combined to give the variance of MUF by application of Eq. 4.3. However, the covariance terms in Eq. 4.3 are generally either ignored completely or are only partially accounted for. This is understandable because it is difficult to identify and account for all the covariances since they are caused by one or more of several factors. For example, covariances occur because of such factors as the commonality of percent element factors, the existence of identical items in inputs and ending inventories, and biases in measurements that affect several items.

Proper accounting for all such covariances is obviously a formidable task. However, we can circumvent this problem by calculating the vari-

ances attributed to all the individual, uncorrelated primary error sources instead of finding and combining the variances for individual groups of items in the algebraic sum. (These primary error sources were identified in Chap. 5.) Equation 4.3 can then be used to calculate the variance of the algebraic sum directly without being concerned about the covariance terms; these are all zero if the model is properly constructed. Of course, if there is a separate interest in the components of MUF, such as the inventories, inputs, and outputs, the associated variances can also be found by applying the methods of this chapter. However, these variances will not generally sum to give the variance of MUF.

In addition to circumventing the problem of accounting for covariances, the approach given in this chapter to finding the variance of the algebraic sum also pinpoints those areas in which corrective action may be required to reduce the uncertainty associated with the quantity in question. It does this by evaluating the contribution to the total uncertainty for each primary source of error.

In this chapter we again assume that the various standard deviations are known quantities that can be replaced by their estimates in application. Further, we restrict our attention to finding variances or standard deviations rather than limits of error to avoid the problem of making the transition from one to the other. For further discussion on this point, see the overview in Chap. 5.

The multiplicative model based on a structure of relative-error standard deviations is assumed to apply. This model was chosen because the applicable-measurement standard deviations are generally expressed on a relative basis. This is not always true, however. With scales and balances, for example, absolute-error standard deviations are usually quoted, but, since in application a given scale is generally used to weigh items within a relatively restricted range of values, the absolute-error standard deviations are readily expressible on a relative basis. The multiplicative model can therefore be used. This approach is considered preferable to the use of a mixed model in which some errors are expressed on an absolute and some on a relative basis.

Because of the important practical significance of the results of this chapter, the application of the results to specific examples is heavily emphasized. The intent is to cover most types of applications likely to be encountered in practice.

6.1 VARIANCE OF AN ALGEBRAIC SUM OF SNM

6.1.1 Problem and Assumptions

Each container included in a given algebraic sum has associated with it a calculated amount of SNM determined on the bases of a bulk measurement and the application of a percent element and a percent isotopic

factor, as appropriate. If the SNM in question is an element (uranium or plutonium), the isotopic factor does not apply, of course. "Container" refers in general to any discrete quantity that has associated with it a calculated amount of SNM. Examples include a batch of liquid waste, a transfer batch in a chemical reprocessing facility, a tray of sintered UO_2 pellets, a UF_6 cylinder, etc.

All error standard deviations are expressed on a relative basis. For example, a 0.3% relative error is expressed as $\sigma = 0.003$. The notation used to define each primary-error standard deviation is given in Table 5.1. Note that there may be several error components of each type. For example, there is a long-term systematic error, a short-term systematic error, and a random error associated with each weigh scale. Similarly, sampling errors depend on the type of material being sampled, and analytical errors depend on the analytical method used. Thus, from Table 5.1, although there are only 15 types of error components, there are generally many more separately identified components in a given application. All primary-error random variables are assumed to be independently distributed; i.e., the covariances are zero.

The problem is to find the variance of the SNM which represents the algebraic sum of SNM contents for the individual containers. All reasonably conceivable error sources are included in this formulation. In practice, experience will indicate in a given situation which sources, if any, are of negligible importance and can reasonably be ignored in a given application.

6.1.2 Solution

As indicated in Table 5.1, there are five basic types of measurement operations: bulk determination, sampling for element, analysis for element, sampling for isotope, and analysis for isotope. With each type of measurement, a number of specific operations are identified as set forth in Table 6.1.

TABLE 6.1 SPECIFIC MEASUREMENT OPERATIONS

Type of operation	Specific operation
Bulk determination (weighing or volume)	Weighing performed on scale i, or volume of vessel i; $i = 1, 2, \ldots, n_i$
Sampling for element	Sampling from material type j or by method j; $j = 1, 2, \ldots, n_j$
Analysis for element	Analytical method k; $k = 1, 2, \ldots, n_k$
Sampling for isotopic factor	Sampling from material type l or by method l; $l = 1, 2, \ldots, n_l$
Analysis for isotopic factor	Analytical method m; $m = 1, 2, \ldots, n_m$

In the model each specific operation has associated with it a long-term systematic, a short-term systematic, and a random error. (This is for generality. In some applications corresponding standard deviations may be assigned the value zero.) Each combination of a specific operation and a type of error contributes a term to the overall variance of the SNM in the algebraic sum. This term consists of a coefficient times an appropriate variance. From the notation of Tables 5.1 and 6.1, the terms are of the following form:

$$C_{\delta_i}\sigma^2_{\delta_i};\ C_{\phi_i}\sigma^2_{\phi_i};\ \ldots;\ C_{\nu_m}\sigma^2_{\nu_m}$$

with the ranges for i, j, k, l, and m given in Table 6.1.

The procedure for finding the variance of the SNM in question is then reduced to finding these C coefficients. Simple rules for doing this are given. The resulting terms, of the form $C\sigma^2$, are then summed to give the desired result.

First, rules are given for the case in which element weight is of interest. Then additional rules are given for the case where isotope weights are involved. All sums referred to in the rules in Table 6.2 are algebraic sums. Let me emphasize that the sign of each term in the sum is taken into account; this point is of crucial importance.

TABLE 6.2 RULES FOR FINDING THE COEFFICIENTS NEEDED IN CALCULATING THE VARIANCE OF THE ALGEBRAIC SUM OF ELEMENT WEIGHTS

Rules 1, 2, and 3 relate to bulk measurements. The operation may refer to weighing on scale i or to finding the volume for vessel i, whichever is appropriate. The rules are given in terms of the weighing operation to avoid excessive repetition, but they may also be expressed in terms of volume.

Rule 1. Long-term systematic error.

Step a. Sum the element weights for all items weighed on scale i.
Step b. Square this sum. This is C_{δ_i}.

Rule 2. Short-term systematic error.

Step a. Sum the element weights for all items weighed on scale i under a given set of conditions. (A "set of conditions" may refer to a given calibration period, a given operator, etc. If the result is independent of such factors, the corresponding systematic-error variance is zero.)
Step b. Square each sum in step a.
Step c. Sum these squares over all sets of conditions. This is C_{ϕ_i}.

Rule 3. Random error.

Step a. Square each element weight for items weighed on scale i.
Step b. Divide each square by the number of weighings made to determine the element weight. (This is normally one, in which case step b is eliminated.)
Step c. Sum the terms in step b over all items. This is C_{ϵ_i}.

TABLE 6.2 (Continued)

Rules 4, 5, and 6 relate to sampling for the element factor.

Rule 4. Long-term systematic error.

Step a. Sum the element weights for all items with element factors based on sampling from material type j.

Step b. Square this sum. This is $C_{\Delta j}$.

Rule 5. Short-term systematic error.

Step a. Sum the element weights over all items for each element factor based on sampling from material type j.

Step b. For each factor, find the fraction of total samples drawn under a given set of conditions. (A "set of conditions" may refer to samples drawn by the same sampling technique or perhaps may relate to replicate samples drawn from a container with no remixing of contents.) These fractions must sum to 1 over all conditions for each factor.

Step c. Multiply the sums in step a by the fractions in step b, and sum the products over all factors for each set of sampling conditions.

Step d. Square each sum in step c.

Step e. Sum the squares in step d over all sets of sampling conditions. This is $C_{\psi j}$.

Rule 6. Random error.

Step a. Sum the element weights for all items that have a common element factor based on sampling from material type j. There may be more than one sum.

Step b. Square each sum in step a.

Step c. Divide each result in step b by the number of samples on which the corresponding element factor is based.

Step d. Sum the terms in step c over all groups of items which have element factors based on sampling from material type j. This is C_{η_j}.

Rules 7, 8, and 9 relate to analysis for the element factor.

Rule 7. Long-term systematic error.

Step a. Sum the element weights for all items with element factors determined using analytical method k.

Step b. Square this sum. This is $C_{\theta k}$.

Rule 8. Short-term systematic error.

Step a. Sum the element weights over all items for each element factor determined using analytical method k.

Step b. For each factor, find the fraction of total analyses performed under a given set of analytical conditions. These fractions must sum to 1 over all conditions for each factor. (Rule 8 can be applied more than once to account for different kinds of analytical conditions. For example, analytical conditions might relate to the use of different operators, different pieces of analytical equipment, etc. In this case the various effects can, if one wishes, be accounted for separately by repeated application of Rule 8. See example 6.D in this regard. Similar remarks apply to other short-term systematic-error rules.)

Step c. Multiply the sums in step a by the fractions in step b, and sum the products over all factors for each set of analytical conditions.

TABLE 6.2 (Continued)

Step d.	Square each sum in step c.
Step e.	Sum the squares in step d over all sets of analytical conditions. This is C_{β_k}.
Rule 9. Random error.	
Step a.	Sum the element weights for all items that have a common element factor determined using analytical method k.
Step b.	Square each such sum in step a.
Step c.	Divide each result in step b by the number of analyses on which the corresponding element factor is based.
Step d.	Sum the terms in step c over all groups of items which have element factors determined using analytical method k. This is $C_{\omega k}$.

The rules of Table 6.2 apply for element weights. If isotope weights are involved, rules 1 to 9 still apply except that isotope weights are used in place of element weights throughout. Also, there are other rules that must be applied as well. These are given in Table 6.3 as rules 10 to 15.

Unlike common element factors, common isotopic factors may logically be based on sampling from different material types. For example, in a fuel fabrication plant, samples may be drawn from UO_2 powder and from UO_2 pellets with the average isotopic factor then applied to both types of material. This possibility is most conveniently handled by defining only one "material type" for the isotopic factor. (Rules 10 and 11, however, include the possibility of there being more than one material type for generality.) Then the different materials sampled to establish a given factor may be regarded as different sampling conditions, with their effect reflected in the short-term systematic error (see footnote to example 5.B, Sec. 5.1.3). This approach is considered valid because sampling errors for isotopic factors are often of minor importance.

6.1.3 Examples

Example 6.A

A shipper ships five containers of PuO_2. Before placing the PuO_2 in containers, he draws three samples and performs one analytical determination per sample for percent plutonium. He determines the net weight for each of the five containers by a single weighing of each container and applies the same percent plutonium factor to all containers. This average factor is 0.8718. Table 6.4 gives the net weights of PuO_2 and the calculated amounts of plutonium.

TABLE 6 3 ADDITIONAL RULES FOR FINDING THE COEFFICIENTS NEEDED IN CALCULATING THE VARIANCE OF THE ALGEBRAIC SUM OF ISOTOPE WEIGHTS

Rules 10, 11, and 12 relate to sampling for the isotopic factor

Rule 10. Long-term systematic error.

Step a Sum the isotope weights for all items with isotope factors based on sampling from the given material type

Step b Square this sum This is C_{λ_l}

Rule 11. Short-term systematic error.

Step a Sum the isotope weights over all items for each isotope factor based on sampling from material type l

Step b For each factor, find the fraction of total samples drawn under a given set of conditions These fractions must sum to 1 over all conditions for each factor

Step c Multiply the sums in step a by the fractions in step b, and sum the products over all factors for each set of sampling conditions

Step d Square each sum in step c

Step e Sum the squares in step d over all sets of sampling conditions This is C_{π_l}

Rule 12. Random error.

Step a Sum the isotope weights for all items that have a common isotope factor based on sampling from material type l

Step b Square each sum in step a

Step c Divide each result in step b by the number of samples on which the corresponding isotope factor is based

Step d Sum the terms in step c over all groups of items which have isotope factors based on sampling from material type l This is C_{μ_l}

Rules 13, 14, and 15 relate to analysis for the isotopic factor.

Rule 13. Long-term systematic error.

Step a Sum the isotope weights for all items with isotope factors determined using analytical method m

Step b Square this sum This is C_{γ_m}

Rule 14. Short-term systematic error.

Step a Sum the isotope weights over all items for each isotope factor determined using analytical method m

Step b For each factor, find the fractions of total analyses performed for each factor under a given set of analytical conditions These fractions must sum to 1

Step c Multiply the sums in step a by the fractions in step b, and sum the products over all factors for each set of analytical conditions

Step d Square each sum in step c

Step e Sum the squares in step d over all sets of analytical conditions This is C_{α_m}

Rule 15. Random error.

Step a Sum the isotope weights for all items that have a common isotope factor determined using analytical method m

Step b Square each sum in step a

Step c Divide each result in step b by the number of analyses on which the corresponding isotope factor is based

Step d Sum the terms in step c over all groups of items which have isotope factors determined using analytical method m This is C_{ν_m}

TABLE 6.4 SHIPPER DATA
(Example 6.A)

Container	Net weight of PuO_2, kg	Weight of plutonium, kg
1	1.3632	1.1884
2	1.4197	1.2377
3	1.3861	1.2084
4	1.3914	1.2130
5	1.4022	1.2224
Total	6.9626	6.0699
Average	1.3925	

The shipper quotes a systematic-error and a random-error standard deviation due to weighing of 0.5 and 1.0 g, respectively. He does not quote sampling errors. His analytical-error standard deviations are 0.05 and 0.25% relative for the systematic and random errors, respectively. For both the weighing and the analytical determinations, no distinction is made between the long-term and the short-term systematic errors.

The receiver also determines the net weight of each container, using a scale with systematic- and random-error standard deviations of 0.3 and 0.5 g, respectively. He opens one can at random, draws a single sample, and performs duplicate analyses on that sample, performing both analyses under nominally the same conditions. He assumes sampling-error standard deviations of 0.02 and 0.03% relative for the systematic and random components. His analytical method is different from that used by the shipper, and his quoted relative standard deviations are 0.03, 0.02, and 0.15% for the long-term systematic, short-term systematic, and random errors, respectively.

The receiver's average factor is 0.8731, and his weights are listed in Table 6.5.

TABLE 6.5 RECEIVER DATA
(Example 6.A)

Container	Net weight of PuO_2, kg	Weight of plutonium, kg
1	1.3625	1.1896
2	1.4192	1.2391
3	1.3850	1.2092
4	1.3915	1.2149
5	1.4016	1.2237
Total	6.9598	6.0765
Average	1.3920	

The shipper–receiver difference is $(6.0699-6.0765)=-0.0066$ kg of plutonium. What is the standard deviation of this difference? (Chapter 8 gives a thorough discussion of shipper–receiver differences, with attention centered on making inferences about stated uncertainties by using the actual shipper and receiver data. In the example here, however, accept the stated values in finding the standard deviation of the shipper–receiver difference.)

The shipper–receiver difference is an algebraic sum that can be written as $(1.1884+1.2377+\ldots-1.2149-1.2237)$. The variance of the algebraic sum is found by applying the rules of Sec. 6.1.2.

The preceding input data can be summarized as follows:

Bulk Determination

Shipper's scale:

$$\sigma_{\delta_1}=\frac{0.0005}{1.3925}=0.00036$$

$$\sigma_{\epsilon_1}=\frac{0.001}{1.3925}=0.00072$$

Receiver's scale:

$$\sigma_{\delta_2}=\frac{0.0003}{1.3920}=0.00022$$

$$\sigma_{\epsilon_2}=\frac{0.0005}{1.3920}=0.00036$$

Sampling for Plutonium

Both parties sample from the same material and will have the same sampling-error standard deviations as quoted by the receiver.

$$\sigma_{\Delta_1}=0.0002 \qquad \sigma_{\eta_1}=0.0003$$

Analysis

Shipper's method:

$$\sigma_{\theta_1}=0.0005$$

$$\sigma_{\beta_1}=0$$

$$\sigma_{\omega_1}=0.0025$$

Receiver's method:

$$\sigma_{\theta_2}=0.0003$$

$$\sigma_{\beta_2}=0.0002$$

$$\sigma_{\omega_2}=0.0015$$

Let us apply the rules. Only the rules of Table 6.2 are applicable, since the plutonium (element) weight, rather than fissile plutonium (isotope), is the quantity of interest.

Rule 1: $C_{\delta_1}=(6.0699)^2=36.8437$

$C_{\delta_2}=(-6.0765)^2=36.9239$

Rule 2: (Not applicable)

Rule 3: $C_{\epsilon_1}=(1.1884)^2+\ldots+(1.2224)^2=7.3701$

$C_{\epsilon_2}=(-1.1896)^2+\ldots+(-1.2237)^2=7.3861$

Rule 4: $C_{\Delta_1} = (6.0699 - 6.0765)^2 = (-0.0066)^2$

$= 0.000044$

Rule 5: (Not applicable)

Rule 6: Step a. Sum $1 = 6.0699$

Sum $2 = -6.0765$

Step b. $(6.0699)^2 = 36.8437$

$(-6.0765)^2 = 36.9239$

Step c. $36.8437/3 = 12.2812$

$36.9239/1 = 36.9239$

Step d. $C_{\eta_1} = 12.2812 + 36.9239 = 49.2051$

Rule 7:* $C_{\theta_1} = (6.0699)^2 = 36.8437$

$C_{\theta_2} = (-6.0765)^2 = 36.9239$

Rule 8: (Do not calculate $C_{\beta 1}$ since $\sigma_{\beta 1}$ is zero)

For C_{β_2}, steps a to f of rule 8 will be applied, although the exercise is trivial in this instance.

Step a. Sum $= -6.0765$
Step b. Fraction $= 1$
Step c. $(-6.0765)(1) = -6.0765$
Step d. Only one factor$\rightarrow$sum $= -6.0765$
Step e. $(-6.0765)^2 = 36.9239$
Step f. One set of conditions$\rightarrow$sum $= 36.9239 = C_{\beta_2}$

Rule 9: $C_{\omega 1} = (6.0699)^2/3 = 12.2812$

$C_{\omega 2} = (-6.0765)^2/2 = 18.4619$

These coefficients are then applied to the given variances.

Bulk Determination

$C_{\delta 1}\sigma_{\delta 1}{}^2 = (36.8437)(0.00036)^2 = 4.77 \times 10^{-6}$

$C_{\delta_2}\sigma_{\delta_2}{}^2 = (36.9239)(0.00022)^2 = 1.79 \times 10^{-6}$

$C_{\epsilon 1}\sigma_{\epsilon 1}{}^2 = (7.3701)(0.00072)^2 = 3.82 \times 10^{-6}$

$C_{\epsilon_2}\sigma_{\epsilon_2}{}^2 = (7.3861)(0.00036)^2 = 0.96 \times 10^{-6}$

* Note the distinction between application of rules 4 and 7. Both parties use the same sampling method, but different analytical methods are used.

Sampling

$$C_{\Delta_1}\sigma_{\Delta_1}^2 = (0.000044)(0.0002)^2 = 0.00 \times 10^{-6}$$

$$C_{\eta_1}\sigma_{\eta_1}^2 = (49.2051)(0.0003)^2 = 4.43 \times 10^{-6}$$

Analysis

$$C_{\theta_1}\sigma_{\theta_1}^2 = (36.8437)(0.005)^2 = 9.21 \times 10^{-6}$$

$$C_{\theta_2}\sigma_{\theta_2}^2 = (36.9239)(0.0003)^2 = 3.32 \times 10^{-6}$$

$$C_{\beta_2}\sigma_{\beta_2}^2 = (36.9239)(0.0002)^2 = 1.48 \times 10^{-6}$$

$$C_{\omega_1}\sigma_{\omega_1}^2 = (12.2812)(0.0025)^2 = 76.76 \times 10^{-6}$$

$$C_{\omega_2}\sigma_{\omega_2}^2 = (18.4619)(0.0015)^2 = 41.54 \times 10^{-6}$$

Total variance 148.08 g^2 of Pu

Standard deviation 12.2 g of Pu

Example 6.B

(The data for this example were provided by R. D. Smith.)

At the conclusion of a campaign, a facility has on inventory seven batches of material which contain uranium. To measure the uranium content, two scales were used, two types of material were sampled, and three analytical methods were employed. The short- and long-term systematic errors are combined and labeled long-term errors since all analyses of a given type were performed under one set of conditions. Each of the seven batches has its own percent uranium factor, each factor being based on a single sample and a single analysis. Assume a single bulk determination for each batch. Tables 6.6 to 6.8 give all the data and measurement parameters.

TABLE 6.6 MATERIAL IN INVENTORY
(Example 6.B)

Batch	Net weight, g	Uranium factor	Uranium, g
1	90,347	0.0814	7354
2	94,122	0.0639	6014
3	35,091	0.0777	2727
4	4,332	0.2795	1211
5	4,106	0.2801	1150
6	3,893	0.2866	1116
7	257,071	0.0086	2211
		Total	21,783

TABLE 6.7 METHODS USED*
(Example 6.B)

Batch	Weighing	Sampling	Analysis
1	1	1	1
2	1	1	1
3	1	1	2
4	2	2	2
5	2	2	2
6	2	2	2
7	1	2	3

* Scale, material type, analytical method.

TABLE 6.8 ERROR STANDARD DEVIATIONS
(Example 6.B)

Operation	Method	Systematic error	Random error
Weighing	1	$\sigma_{\delta 1}=0.00025$	$\sigma_{\epsilon 1}=0.00025$
	2	$\sigma_{\delta 2}=0.000025$	$\sigma_{\epsilon 2}=0.000025$
Sampling	1	$\sigma_{\Delta 1}=0.0011$	$\sigma_{\eta 1}=0.0060$
	2	$\sigma_{\Delta 2}=0.00005$	$\sigma_{\eta 2}=0.0001$
Analysis	1	$\sigma_{\theta 1}=0.0015$	$\sigma_{\omega 1}=0.0095$
	2	$\sigma_{\theta 2}=0.0005$	$\sigma_{\omega 2}=0.0015$
	3	$\sigma_{\theta 3}=0.0075$	$\sigma_{\omega 3}=0.016$

To find the standard deviation associated with the total amount of uranium in inventory, let us apply the rules of Table 6.1. In this application, an item corresponds to a batch.

Rule 1 — **Product:** $C\sigma^2$, g^2

$C_{\delta 1}=(7354+6014+2727+2211)^2$
$=335,109,636 \times (0.00025)^2 = 20.94$

$C_{\delta 2}=(1211+1150+1116)^2$
$=12,089,529 \times (0.000025)^2 = 0.01$

Rule 3

$C_{\epsilon 1}=(7354)^2+(6014)^2+(2727)^2+(2211)^2$
$=102,574,562 \times (0.00025)^2 = 6.41$

$C_{\epsilon 2}=(1211)^2+(1150)^2+(1116)^2$
$=4,034,477 \times (0.000025)^2 = 0.00$

				Product: $C\sigma^2$, g^2
Rule 4				
$C_{\Delta_1}=(7354+6014+2727)^2$				
$=259{,}049{,}025$	$\times$	$(0.0011)^2$	$=$	313.45
$C_{\Delta_2}=(1211+1150+1116+2211)^2$				
$=32{,}353{,}344$	$\times$	$(0.00005)^2$	$=$	0.08
Rule 6				
$C_{\eta_1}=(7354)^2+(6014)^2+(2727)^2$				
$=97{,}686{,}041$	$\times$	$(0.0060)^2$	$=$	3516.70
$C_{\eta_2}=(1211)^2+(1150)^2+(1116)^2+(2211)^2$				
$=8{,}922{,}998$	$\times$	$(0.0001)^2$	$=$	0.09
Rule 7				
$C_{\theta_1}=(7354+6014)^2$				
$=178{,}703{,}424$	$\times$	$(0.0015)^2$	$=$	402.08
$C_{\theta_2}=(2727+1211+1150+1116)^2$				
$=38{,}489{,}616$	$\times$	$(0.0005)^2$	$=$	9.62
$C_{\theta_3}=(2211)^2$				
$=4{,}888{,}521$	$\times$	$(0.0075)^2$	$=$	274.98
Rule 9				
$C_{\omega_1}=(7354)^2+(6014)^2$				
$=90{,}249{,}512$	$\times$	$(0.0095)^2$	$=$	8145.02
$C_{\omega_2}=(2727)^2+(1211)^2+(1150)^2+(1116)^2$				
$=11{,}471{,}006$	$\times$	$(0.0015)^2$	$=$	25.81
$C_{\omega_3}=(2211)^2$				
$=4{,}888{,}521$	$\times$	$(0.016)^2$	$=$	1251.46
			Total variance	13966.65 g^2 of U
			Total standard deviation	118 g of U

It is immediately apparent that σ_{ω_1} is the dominant source of variation. Its effect can be reduced by replicate analyses of the first two batches.

Example 6.C

This somewhat artificially contrived example is included to illustrate application of rules 1 to 9 in their more complex forms. Consider an algebraic sum of 10 items whose element weights are depicted by S_1, S_2, . . . , S_{10}. The algebraic sum S is

$$S=S_1+S_2-S_3-S_4+S_5-S_6+S_7+S_8+S_9+S_{10}$$

Assumptions. Make the following assumptions about how the S_i's were determined:

1. Each item is weighed once, with three scales in use.
   - Scale 1 for items 1, 2, and 8.
   - Scale 2 for items 3 and 10.
   - Scale 3 for items 4, 5, 6, 7, and 9.

2. Scale 3 was recalibrated after items 4, 5, and 6 were weighed.

3. Three element factors are used.
   - Factor 1 for items 1, 2, 5, and 6.
   - Factor 2 for items 3 and 9.
   - Factor 3 for items 4, 7, 8, and 10.

4. The numbers of samples and analyses used to calculate each factor are as follows:
   - Factor 1 is based on four samples with two analyses per sample.
   - Factor 2 is based on 20 samples with each group of four samples composited and two analyses performed on each composite.
   - Factor 3 is based on 20 samples with one analysis per sample.

5. The factors are based on sampling from three types of material.
   - Factor 1 from material type 1.
   - Factors 2 and 3 from material type 2.

6. The first 12 samples drawn to establish factor 2 utilize one sampling technique; a different technique is used for the last eight samples. The latter technique is used for all samples drawn to establish factor 3.

7. Two analytical methods are used.
   - Factors 1 and 2 use method 1.
   - Factor 3 uses method 2.

8. For each analytical method, analyses are performed under different sets of conditions.
   - Analytical method 1
     Factor 1 based on three analyses under condition 1 and five under condition 2.
     Factor 2 based on two analyses under condition 2 and eight under condition 3.
   - Analytical method 2
     Factor 3 based on eight analyses under condition 1, two under condition 2, and 10 under condition 3. (Conditions 1, 2, and 3 for analytical method 2 are, of course, not the same as conditions 1, 2, and 3 for method 1.)

Let us now apply the rules of Table 6.2 to give the following components of variance. Again it is emphasized that the signs in the algebraic sum must be preserved.

Rule 1

Scale 1: $(S_1+S_2+S_8)^2\sigma_{\delta_1}{}^2$

Scale 2: $(-S_3+S_{10})^2\sigma_{\delta_2}{}^2$

Scale 3: $(-S_4+S_5-S_6+S_7+S_9)^2\sigma_{\delta_3}{}^2$

Rule 2

Scale 1: $(S_1+S_2+S_8)^2\sigma_{\phi_1}{}^2$

Scale 2: $(-S_3+S_{10})^2\sigma_{\phi_2}{}^2$

Scale 3: $[(-S_4+S_5-S_6)^2+(S_7+S_9)^2]\sigma_{\phi_3}{}^2$

Rule 3

Scale 1: $(S_1{}^2+S_2{}^2+S_8{}^2)\sigma_{\epsilon_1}{}^2$

Scale 2: $(S_3{}^2+S_{10}{}^2)\sigma_{\epsilon_2}{}^2$

Scale 3: $(S_4{}^2+S_5{}^2+S_6{}^2+S_7{}^2+S_9{}^2)\sigma_{\epsilon_3}{}^2$

Rule 4

Material type 1: $(S_1+S_2+S_5-S_6)^2\sigma_{\Delta_1}{}^2$

Material type 2: $(-S_3+S_9-S_4+S_7+S_8+S_{10})^2\sigma_{\Delta_2}{}^2$

Rule 5

Step a. Material type 1:

Factor 1 sum $=(S_1+S_2+S_5-S_6)$

Material type 2:

Factor 2 sum $=(-S_3+S_9)$

Factor 3 sum $=(-S_4+S_7+S_8+S_{10})$

Step b. Material type 1:

Factor 1 fraction $=1$

Material type 2:

Factor 2 fractions $=12/20$ (for condition 1)

$=8/20$ (for condition 2)

Factor 3 fraction $=0$ (for condition 1)

$=1$ (for condition 2)

Step c. Material type 1:

$$[(S_1+S_2+S_5-S_6)(1)]$$

Material type 2:

Condition 1: $(-S_3+S_9)(12/20)+(-S_4+S_7+S_8+S_{10})(0)$

Condition 2: $(-S_3+S_9)(8/20)+(-S_4+S_7+S_8+S_{10})(1)$

Step d. Material type 1:

$$(S_1+S_2+S_5-S_6)^2$$

Material type 2:

Condition 1: $[(-S_3+S_9)(12/20)]^2$

Condition 2: $[(-S_3+S_9)(8/20)+(-S_4+S_7+S_8+S_{12})]^2$

Step e. Material type 1:

$$(S_1+S_2+S_5-S_6)^2\sigma_{\psi_1}{}^2$$

Material type 2:

$$\{[(-S_3+S_9)(12/20)]^2+[(-S_3+S_9)(8/20)+(-S_4+S_7+S_8+S_{10})]^2\}\sigma_{\psi_1}{}^2$$

Rule 6

Material type 1: $\dfrac{(S_1+S_2+S_5-S_6)^2}{4}\sigma_{\eta_1}{}^2$

Material type 2: $\left[\dfrac{(-S_3+S_9)^2}{20}+\dfrac{(-S_4+S_7+S_8+S_{10})^2}{20}\right]\sigma_{\eta_2}{}^2$

Rule 7

Method 1: $(S_1+S_2+S_5-S_6-S_3+S_9)^2\sigma_{\theta_1}{}^2$

Method 2: $(-S_4+S_7+S_8+S_{10})^2\sigma_{\theta_2}{}^2$

Rule 8

Method 1:
$$\{[(S_1+S_2+S_5-S_6)(3/8)+(-S_3+S_9)(0)]^2+[(S_1+S_2+S_5-S_6)(5/8)+(-S_3+S_9)(2/10)]^2+[(S_1+S_2+S_5-S_6)(0)+(-S_3+S_9)(8/10)]^2\}\sigma_{\beta_1}{}^2$$

Method 2:
$$\{[(-S_4+S_7+S_8+S_{10})(8/20)]^2+[(-S_4+S_7+S_8+S_{10})(2/20)]^2+[(-S_4+S_7+S_8+S_{10})(10/20)]^2\}\sigma_{\beta_2}{}^2$$
$$=\frac{(-S_4+S_7+S_8+S_{10})^2}{400}(64+4+100)\sigma_{\beta_2}{}^2$$

Rule 9

$$\text{Method 1:} \quad \left[\frac{(S_1+S_2+S_5-S_6)^2}{8}+\frac{(-S_3+S_9)^2}{10}\right]\sigma_{\omega_1}{}^2$$

$$\text{Method 2:} \quad \frac{(-S_4+S_7+S_8+S_{10})^2}{20}\sigma_{\omega_2}{}^2$$

These various quantities are then summed to give the variance of the algebraic sum S.

Example 6.D

In example 6.C, for analytical method 1 three different analytical conditions were specified; these affect the coefficient for the short-term systematic-analytical-error component, $\sigma_{\beta_1}{}^2$. The conditions were not specified further, but they could refer to some time-associated variable, with the analyses being performed in three different blocks of time, such as shifts or half-shifts.

Situations may arise in which a further specification can be made of such conditions. It is then possible to apply rule 8 more than once to account for whatever specification is made. This is illustrated in this example.

For the data of example 6.C and for analytical method 1, assume that condition 1 refers to operator 1 on instrument 1, condition 2 to operator 2 on instrument 1, and condition 3 to operator 2 on instrument 2. Further, replace $\sigma_{\beta_1}{}^2$ by two components, one describing the variance between operators ($\sigma_O{}^2$) and the other describing the variance between instruments ($\sigma_I{}^2$). Rule 8 is then applied twice, once to account for the short-term systematic error due to operators and once to take into account this error source for instruments. The long-term systematic-error variance remains unchanged.

From rule 8 and the data of example 6.C, the coefficient for $\sigma_O{}^2$ is found by replacing "analytical condition" by "operator"; this gives

$$[(S_1+S_2+S_5-S_6)(3/8)+(-S_3+S_9)(0)]^2 + [(S_1+S_2+S_5-S_6)(5/8)+(-S_3+S_9)(10/10)]^2$$

Similarly, the coefficient for $\sigma_I{}^2$, which describes the between-instrument variance, is

$$[(S_1+S_2+S_5-S_6)(8/8)+(-S_3+S_9)(2/10)]^2 + [(S_1+S_2+S_5-S_6)(0)+(-S_3+S_9)(8/10)]^2$$

Clearly, this can be extended to include any number of short-term systematic-error components.

TABLE 6.9 MATERIAL BALANCE DATA
(Example 6.E)

	Type of material	MUF component	3.3% ^{235}U	4.2% ^{235}U
1	UF_6 cylinders	BI	9.942 (3)*	8.384 (2)*
		R	6.576 (2)	21.055 (5)
	(U-factor = 0.6760)	EI	3.310 (1)	4.203 (1)
2	Cans of UO_2 powder	BI	2.035 (5)	4.108 (8)
		EI	5.478 (14)	10.396 (21)
	(U-factor = 0.8760)			
3	Boats of sintered pellets	BI	0	0
		EI	7.443 (37)	15.020 (60)
	(U-factor = 0.8807)			
4	Cans of hard scrap	BI	0	0
		EI	0.161 (1)	0.434 (1)
	(U-factor = 0.8807)			
5	Cans of green scrap	BI	0.418 (2)	0.732 (3)
		EI	0.622 (3)	1.166 (4)
	(U-factor = 0.8760)			
6	Cans of dirty powder	BI	DP-1: 0.121 (0.8727)	DP-4: 0.156 (0.8702)
			DP-2: 0.148 (0.8738)	DP-5: 0.129 (0.8688)
		EI	DP-1: 0.121 (0.8727)	DP-4: 0.156 (0.8702)
			DP-2: 0.148 (0.8738)	DP-5: 0.129 (0.8688)
			DP-3: 0.096 (0.8694)	DP-6: 0.187 (0.8724)

7	Cans of grinder sludge		BI	0		0
			EI	SL-1: 0.023 (0.685)	SL-2:	0.041 (0.560)
8	Cans of ADU† scrap		BI	A-1: 0.231 (0.501)	A-14:	0.287 (0.477)
				A-2: 0.417 (0.770)	A-15:	0.315 (0.722)
				A-3: 0.186 (0.242)	A-16:	0.192 (0.249)
				A-4: 0.401 (0.798)		
				A-5: 0.387 (0.610)		
			EI‡			
				A-6: 0.315 (0.743)	A-17:	0.184 (0.220)
				A-7: 0.155 (0.286)	A-18:	0.277 (0.419)
				A-8: 0.287 (0.318)	A-19:	0.190 (0.342)
				A-9: 0.130 (0.240)	A-20:	0.315 (0.693)
				A-10: 0.118 (0.226)	A-21:	0.362 (0.741)
				A-11: 0.224 (0.383)	A-22:	0.299 (0.512)
				A-12: 0.216 (0.511)	A-23:	0.301 (0.322)
				A-13: 0.333 (0.763)	A-24:	0.114 (0.214)
					A-25:	0.380 (0.532)
					A-26:	0.284 (0.286)
		Total	BI	14.286		14.303
		Total	R	6.576		21.055
		Total	EI	20.802		35.232

* Numbers in parentheses are the number of discrete items for material types 1 to 5, and uranium factors for material types 6 to 8.
† ADU is ammonium diuranate.
‡ The EI for 3.3% ^{235}U includes A-1 to A-5 and A-6 to A-13; EI for 4.2% ^{235}U includes A-14 to A-16 and A-17 to A-26.

Example 6.E

Consider the ^{235}U MUF across a small-scale fuel fabrication facility for a 1-month time period. The material is at two nominal enrichments, as indicated. The data are classified by material type. The abbreviations BI and EI are beginning and ending inventories, respectively, and R is receipts. Assume no shipments and no measured discards, so MUF = BI + R − EI.

The material balance data are given in Table 6.9. For the mainstream items (UF_6 cylinders, UO_2 powder cans, and boats of sintered pellets) and for hard and green scrap, the numbers in parentheses in the table are the numbers of discrete items involved. It is assumed that the discrete items in each class have equal amounts of ^{235}U. This is a reasonable assumption for this type of analysis since a moderate amount of item-to-item variation in isotope weight has little effect on the result. The factors used to convert net weight to total uranium are given in the table for each of these categories.

For the scrap items, assume that a separate factor is established for each discrete item. These items are listed individually in the table, and the parenthetical values are the uranium factors established for each item.

The ^{235}U isotopic factor is 0.03311 for all items at the nominal enrichment of 3.3% and 0.04189 for all items at 4.2%. Tabular entries are given in kilograms of ^{235}U.

The two UF_6 cylinders in ending inventory are both identical to those in receipts. For the UO_2 powder, the beginning and ending inventory items are all physically different. One new container of green scrap was created for each enrichment, with the five containers in beginning inventory still being in ending inventory. In such an instance the common items will drop out of the algebraic sum before the variance of the sum is found. This is an important point to keep in mind. If a new determination were made for a given item in ending inventory, however, and the value changed accordingly, then the item would be carried in the algebraic sum as both a plus and a minus and the rules would be applied as if they were different items.

Assume the values given in Table 6.10 for the error parameters, with $\sigma_{\phi_i} = 0$ for all i and $\sigma_{\psi_j} = 0$ for all j.

The uranium factors are based on the following data:

UF_6: three samples with one analysis per sample (all under same conditions).

UO_2 powder: 20 samples with one analysis per sample under four sets of conditions (five analyses per set).

UO_2 pellets: 16 samples with one analysis per sample under two sets of conditions (eight analyses per set).

TABLE 6.10 MEASUREMENT ERROR STANDARD DEVIATIONS
(Example 6.E)

Scale	Type of material	σ_{δ_i}	σ_{ϵ_i}
1	UF_6 cylinders	0.0005	0.0001
2	UO_2 powder+scrap items	0.00034	0.00047
3	Sintered pellets	0.0001	0.0001
Uranium sampling, material types		σ_{Δ_j}	σ_{η_j}
UF_6		0.00025	0.0006
UO_2 powder		0.00018	0.00016
UO_2 pellets		0.00018	0.00006
Dirty powder		0.003	0.023
Sludge		0.049	0.170
ADU scrap		0.022	0.076
Uranium analysis, methods	σ_{θ_k}	σ_{β_k}	σ_{ω_k}
(UF_6)	0.00029	0.00032	0.0006
(UO_2 powder)	0.00028	0.00032	0.00032
(UO_2 pellets)	0.00028	0.00028	0.00011
(Scrap items)	0.00038	0.00045	0.0020
^{235}U sampling, material type	σ_{λ_l}	σ_{π_l}	σ_{μ_l}
UF_6; UO_2 powder; UO_2 pellets	0.00019	0.0002	0.0003
^{235}U Analysis	σ_{γ_m}	σ_{α_m}	σ_{ν_m}
	0.0007	0.0011	0.0050

Scrap items: one analysis per sample with one, two, or four samples per item as indicated below:

	Analytical condition		
Material	**1**	**2**	**3**
DP-1, 2, 4, 5		1	
DP-3, 6			1
SL-1, 2			1
A-1, 2, 14, 16	1		
A-3, 4, 5, 15	1	1	
A-6, 8, 9, 11, 13, 18		1	
A-7, 10, 17, 19, 22	1	1	2
A-12, 20, 21, 23, 26			1
A-24, 25		1	1

The ^{235}U factors are each based on five samples with one analysis per sample. For each factor one sample is drawn from the UF_6 and two each from the UO_2 powder and the UO_2 pellets. All analyses are performed under the same set of analytical conditions.

The data are now complete, and rules 1 to 15 can be applied. All variances are multiplied by 10^6 to convert kilograms squared to grams squared.

			Product: $C\sigma^2$, g^2
Rule 1			
$C_{\delta_1} = (9.942+6.576-3.310+8.384+21.055-4.203)^2$			
$= (38.444)^2 = 1477.94$	$\times\ (0.5)^2$	=	369.49
$C_{\delta_2} = (2.035-5.478+4.108-10.396-0.161$			
$-0.434+0.418-0.622+0.732-1.166$			
$-0.096-0.187-0.023- \ldots -0.284)^2$			
$= (-15.795)^2 = 249.48$	$\times (0.34)^2$	=	28.84
$C_{\delta_3} = (-7.443-15.020)^2$			
$= 504.59$	$\times (0.10)^2$	=	5.05
	Total		**403.38**
Rule 3			
$C_{\epsilon_1} = (9.942/3)^2(3)+(3.266)^2$			
$+(8.384/2)^2(2)+(16.852/4)^2(4)$			
$= 149.76$	$\times (0.10)^2$	=	1.50*
$C_{\epsilon_2} = (2.035/5)^2(5)+(-5.478/14)^2(14)+ \ldots$			
$+(-0.161)^2+ \ldots +(-0.204)^2+ \ldots$			
$= 11.96$	$\times (0.47)^2$	=	2.64
$C_{\epsilon_3} = (-7.443/37)^2(37)+(-15.020/60)^2(60)$			
$= 5.26$	$\times (0.10)^2$	=	0.05
	Total		**4.19**
Rule 4			
$C_{\Delta_1} = 1477.94$ (Same as C_{δ_1})	$\times (0.25)^2$	=	92.37

* The second term in the sum, $(3.266)^2$, relates to the cylinder that is included as a receipt but is not in ending inventory. A similar statement applies to the four cylinders whose total ^{235}U weight is 16.852 kg.

$C_{\Delta_2} = (2.035-5.478+4.108-10.396-0.204-0.434)^2$			
$= 107.52$	$\times (0.18)^2$	$=$	3.48*
$C_{\Delta_3} = (-7.443-15.020-0.161-0.434)^2$			
$= 531.67$	$\times (0.18)^2$	$=$	17.23
$C_{\Delta_4} = (-0.096-0.187)^2$			
$= 0.08$	$\times (3.0)^2$	$=$	0.72
$C_{\Delta_5} = (-0.023-0.041)^2$			
$= 0.004096$	$\times \quad (49)^2$	$=$	9.83
$C_{\Delta_6} = (-0.315-0.155- \ldots -0.284)^2$			
$= 20.106$	$\times \quad (22)^2$	$=$	9731.43
	Total		**9855.06**

Rule 6

$C_{\eta_1} = (1477.94)/3$			
$= 492.65$	$\times (0.6)^2$	$=$	177.35
$C_{\eta_2} = (107.52)/20$			
$= 5.38$	$\times (0.16)^2$	$=$	0.14
$C_{\eta_3} = (531.67)/16$			
$= 33.23$	$\times (0.06)^2$	$=$	0.12
$C_{\eta_4} = (-0.096)^2/1+(-0.187)^2/1$			
$= 0.0419$	$\times \quad (23)^2$	$=$	23.38
$C_{\eta_5} = (-0.023)^2/1+(-0.041)^2/1$			
$= 0.00221$	$\times \quad (170)^2$	$=$	63.87
$C_{\eta_6} = (-0.315)^2/1+(-0.155)^2/4+ \ldots$			
$= 1.01249$	$\times \quad (76)^2$	$=$	5848.14
		Total	**6113.00**

Rule 7

$C_{\theta_1} = 1477.94$	(Same as C_{δ_1})	$\times (0.29)^2$	$=$	124.29
$C_{\theta_2} = 107.52$	(Same as C_{Δ_2})	$\times (0.28)^2$	$=$	8.43
$C_{\theta_3} = 531.67$	(Same as C_{Δ_3})	$\times (0.28)^2$	$=$	41.68
$C_{\theta_4} = (0.096-0.187-0.023-0.041-0.315- \ldots)^2$				
$= 23.34$		$\times (0.38)^2$	$=$	3.37
		Total		**177.77**

* The 0.204 and 0.434 values relate to the cans of green scrap created during the month and carried at the same factors as the UO_2 powder.

Rule 8

$C_{\beta_1} = [(38.444)(1)]^2 = 1477.94 \quad \times (0.32)^2 = 151.34$

$C_{\beta_2} = [(-10.369)(1/4)]^2(4) = 26.88 \quad \times (0.32)^2 = 2.75$

$C_{\beta_3} = [(-23.058)(1/2)]^2(2) = 265.84 \times (0.28)^2 = 20.84$

C_{β_4}*

Condition 1:

$$[(-0.155)(1/4)+(-0.118)(1/4)+(-0.184)(1/4)+(-0.190)(1/4)+(-0.299)(1/4)]^2 = 0.055932$$

Condition 2:

$$[(-0.315)(1)+(-0.287)(1)+(-0.130)(1)+(-0.224)(1)+(-0.333)(1)+(-0.277)(1)+(-0.155)(1/4)+(-0.118)(1/4)+(-0.184)(1/4)+(-0.190)(1/4)+(-0.299)(1/4)+(-0.114)(1/2)+(0.380)(1/2)]^2 = 4.200450$$

Condition 3:

$$[(-0.096)(1)+(-0.187)(1)+(-0.023)(1)+(-0.041)(1)+(-0.155)(1/2)+(-0.118)(1/2)+(-0.184)(1/2)+(-0.190)(1/2)+(-0.299)(1/2)+(-0.216)(1)+(-0.315)(1)+(-0.362)(1)+(-0.301)(1)+(-0.284)(1)+(-0.114)(1/2)+(-0.380)(1/2)]^2 = 6.446521$$

By step e, $C_{\beta_4} = 0.055932+4.200450+6.446521$

$= 10.7029 \quad \times (0.45)^2 = 2.17$†

177.10

Rule 9

$C_{\omega_1} = (38.444)^2/3 = 492.65 \quad \times (0.6)^2 = 177.35$

$C_{\omega_2} = (-10.369)^2/20 = 5.38 \quad \times (0.32)^2 = 0.55$

$C_{\omega_3} = (-23.058)^2/16 = 33.23 \quad \times (0.11)^2 = 0.40$

* DP-1, 2, 4, 5, A-1 to A-5, and A-14 to A-16 will not enter in because they cancel out in the MUF calculation before LE–MUF is found.

† As a check, the sum of all the multipliers over all conditions must equal the total numbers of factors based on the method in question. In this case this is 22.

C_{ω_4}* $= (-0.096)^2/1 + (-0.187)^2/1 + \ldots$

$= 1.05889 \quad \times (2.0)^2 = 4.24$

Total **182.54**

Rule 10†

C_{γ_1}‡ $= (14.286 + 14.303 + 6.576 + 21.055 - 20.802 - 35.232)^2$

$= (0.186)^2 = 0.034596 \quad \times (0.19)^2$ **0.00**

Rule 11

Condition 1 (UF_6):

$[(0.060)(1/5) + (0.126)(1/5)]^2 = 0.001384$§

Condition 2 (UO_2 powder):

$[(0.060)(2/5) + (0.126)(2/5)]^2 = 0.005536$

Condition 3 (UO_2 pellets):

$[(0.060)(2/5) + (0.126)(2/5)]^2 = 0.005536$

$C_{\pi_1} = 0.001384 + 0.005536 + 0.005536$

$= 0.012456 \quad \times (0.2)^2 =$ **0.00**

Rule 12

$C_{\mu_1} = (0.060)^2/5 + (0.126)^2/5$

$= 0.003895 \quad \times (0.3)^2 =$ **0.00**

Rule 13

$C_{\gamma_1} = (0.060 + 0.126)^2 = 0.034596 \quad \times (0.7)^2 =$ **0.02**

Rule 14

$C_{\alpha_1} = (0.060 + 0.126)^2(1) = 0.034596 \quad \times (1.1)^2 =$ **0.04**

Rule 15

$C_{\nu_1} = (0.060)^2/5 + (0.126)^2/5$

$= 0.003895 \quad \times (5.0)^2 =$ **0.10**

The error components for the 15 rules are summarized in Table 6.11. It is apparent from this table that the uncertainties in the percent ^{235}U

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* $C_{\omega_4} = C_{\eta_4} + C_{\eta_5} + C_{\eta_6}$.

† There is only one material type, by definition. See last paragraph in Sec. 6.1.2.

‡ Use the totals at the bottom of Table 6.9.

§ 0.060 = 14.286 + 6.576 − 20.802 for 3.3% ^{235}U and 0.126 = 14.303 + 21.055 − 35.232 for 4.2% ^{235}U.

factors have negligible effect on the variance of MUF. The reason for this is that in this example the same factors are used for beginning inventories, receipts, and ending inventories. In effect, the uranium MUF, which is close to zero, is multiplied by the ^{235}U factor for a given enrichment. It is intuitively clear that even large uncertainties in this factor would contribute very little additional to the variance of the ^{235}U MUF. This would not be the case, of course, if one factor were used for receipts and another for product. Different factors are clearly required if any blending of different enrichments takes place, and the variance of MUF would increase accordingly.

Before continuing with the next example, we should comment at this point on the amount of computational effort required to calculate the standard deviation of MUF as just exemplified. Although the computational process may seem unwieldy, a number of arguments can be made to answer the objection that a simpler approach is needed.

1. Many systems of nuclear material accountability are computerized, at least to some degree. Calculations that seem unwieldy when performed on a desk calculator are no challenge to a computer. Further, the computational rules are easily programmed.

2. Even if a computer is not available, a number of shortcuts can be

TABLE 6.11 SUMMARY OF VARIANCE COMPONENTS
(Example 6.E)

Rule	Operation	Error type *	Variance, g^2 ^{235}U	
1	Weighing	LTS	403.38	
2		STS	0.00	
3		R	4.19	407.57
4	Sampling (uranium)	LTS	9855.06	
5		STS	0.00	
6		R	6113.00	15,968.06
7	Analysis (uranium)	LTS	177.77	
8		STS	177.10	
9		R	182.54	537.41
10	Sampling (^{235}U)	LTS	0.00	
11		STS	0.00	
12		R	0.00	0.00
13	Analysis (^{235}U)	LTS	0.02	
14		STS	0.04	
15		R	0.10	0.16
			Total	16,913.20 g^2

$$\sigma_{MUF} = \sqrt{16,913.20} = 130 \text{ g of } ^{235}U$$

* LTS, long-term systematic; STS, short-term systematic; R, random.

taken For example, for a given system certain error sources contribute a negligible amount to the overall uncertainty in MUF and can be ignored in routine calculation In the example just completed, the experienced individual will recognize immediately that rules 10 to 15 can be ignored

3 That a correct analysis requires some effort is no basis for analyzing data in a simpler but incorrect fashion This is not necessarily true when the degree of correctness is largely of academic importance In nuclear materials control applications, however, the simpler methods sometimes used not only are incorrect in principle but also may lead to results that are grossly in error and misleading

Example 6.F

(The data for this example are extracted from *Capability of a Typical Material Balance Accounting System for a Chemical Processing Plant*, by R A Schneider and D P Granquist, Report BNWL-1384, Battelle–Northwest, Richland, Wash , Pacific Northwest Laboratory, May, 1970 The authors quote "capability" and "performance" values for the measurement system The capability model represents the best performance that the measurement system is theoretically capable of achieving in an operating environment The performance model represents what might more generally be expected in practice from a high-quality measurement system The performance values are used in this example)

Consider the plutonium MUF in a chemical reprocessing facility for a given campaign The facility in question processes material at the rate of 1 tonne of uranium per batch, with one batch processed per day The campaign consists of 40 tonnes of uranium A plutonium content of 10,000 g of plutonium per tonne of uranium is assumed The pertinent material balance data are summarized in Table 6 12

Cladding waste is not included in this table Since it is treated in the accounting system as plant input and subtracted as plant waste, it cancels out in the MUF algebraic sum

The pertinent measurement methods are given in Table 6 13

TABLE 6 12 MATERIAL BALANCE DATA
(Example 6 F)

Material balance component	Batch size, kg of Pu	Batches per campaign	Total, kg of Pu
Input dissolver solution	10	40	400
Product $Pu(NO_3)_4$	22	18	396
Salt waste	0 25	16	4
Inventory (in-process)	0 20	10 *	2

* These 10 batches refer to 10 process vessels

TABLE 6 13 MEASUREMENT METHODS
(Example 6 F)

Process vessel	Volume or weight	Sampling	Analysis
Accountability tank	Dip-tube manometer and specific gravity	Circulating sampler	Isotopic dilution
Pu product receiver	Weight–specific gravity	Circulating sampler	Volumetric titration
Acid waste tank	Dip-tube manometer or recorder	Circulating sampler	Alpha counting
10 process vessels	Dip-tube manometer or recorder	Circulating sampler	Various

Using the notation of this chapter and the data of Schneider and Granquist, we find the parameter values given in Table 6 14 No short-term systematic-error components are given, they are assumed to be included in the long-term components

TABLE 6 14 ERROR STANDARD DEVIATIONS
(Example 6 F)

	Bulk Measurements	
Input	$\sigma_{\delta_1} = 0\ 0030$	$\sigma_{\epsilon_1} = 0\ 0030$
Product	$\sigma_{\delta_2} = 0\ 0010$	$\sigma_{\epsilon_2} = 0\ 0010$
Salt waste	$\sigma_{\delta_3} = 0\ 03$	$\sigma_{\epsilon_3} = 0\ 02$
Inventory	σ_{δ_i}* =	$\sigma_{\epsilon_i} = 0\ 05$ for all $i = 4,$, 13
	Sampling	
Input	$\sigma_{\Delta_1} = 0\ 0020$	$\sigma_{\eta_1} = 0\ 0030$
Product	$\sigma_{\Delta_2} = 0\ 0020$	$\sigma_{\eta_2} = 0\ 0050$
Salt waste	$\sigma_{\Delta_3} = 0\ 06$	$\sigma_{\eta_3} = 0\ 06$
Inventory	σ_{Δ_j}* =	$\sigma_{\eta_j} = 0\ 05$ for all $j = 4,$, 13
	Analysis	
Input	$\sigma_{\theta_1} = 0\ 0025$	$\sigma_{\omega_1} = 0\ 01$
Product	$\sigma_{\theta_2} = 0\ 0030$	$\sigma_{\omega_2} = 0\ 0070$
Salt waste	$\sigma_{\theta_3} = 0\ 10$	$\sigma_{\omega_3} = 0\ 20$
Inventory	σ_{θ_k}* =	σ_{ω_k}† $= 0\ 05$ for all $k = 4,$, 13

* The values of σ_{δ_i} σ_{Δ_j}, and σ_{θ_k} for the in process vessels are immaterial The algebraic sums in question will be zero when rule I is applied to the in process vessels assuming these vessels have the same amounts of material in beginning and ending inventories

† One comment on the analytical methods is in order The analytical methods used to measure the percent plutonium in the process vessels are no doubt the same for some different vessels For example σ_{ω_4} may equal $\sigma_{\omega_{11}}$ This poses no problems since the σ_{ω_l} s are random components It would create a problem for the systematic components σ_{θ_l} but their effects cancel anyway Thus it is acceptable to treat σ_{ω_l} values as distinct qualities for $l = 4$ 13 (i e , for the process vessels)

This example is much simpler than the one for the fuel fabrication facility. The principal reason for this is that, with a chemical reprocessing facility, there are far fewer instances in which assigned values are correlated. Common element factors, which are a major cause of correlations in a fuel fabrication plant, do not normally exist in a chemical reprocessing facility since each batch is measured. Also, in this particular example different analytical methods are assumed used for the major material balance components and all short-term systematic-error variances are included in the long-term variances. The rules for finding the variance of MUF are still applicable, of course, but are far simpler in application.

Let us now use these rules as appropriate to calculate the variance of the plutonium MUF.

Rule 1			**Product:** $C\sigma^2$, kg² of Pu
$C_{\delta_1} = (400)^2 = 160{,}000$	$\times (0.0030)^2$	=	1.4400
$C_{\delta_2} = (396)^2 = 156{,}816$	$\times (0.0010)^2$	=	0.1568
$C_{\delta_3} = (4)^2 = 16$	$\times (0.03)^2$	=	0.0144
		Total	**1.6112**
Rule 3			
$C_{\epsilon_1} = (10)^2(40) = 4000$	$\times (0.0030)^2$	=	0.0360
$C_{\epsilon_2} = (22)^2(18) = 8712$	$\times (0.0010)^2$	=	0.0087
$C_{\epsilon_3} = (0.25)^2(16) = 1$	$\times (0.02)^2$	=	0.0004
For each process vessel,			
$C_{\epsilon_i} = (0.20)^2(2)^* = 0.08$	$(i = 4, 5, \ldots, 13)$		
For all 10 process vessels,			
$(10)(0.08) = 0.80$	$\times (0.05)^2$	=	0.0020
		Total	**0.0471**
Rule 4			
$C_{\Delta_1} = (400)^2 = 160{,}000$	$\times (0.0020)^2$	=	0.6400
$C_{\Delta_2} = (396)^2 = 156{,}816$	$\times (0.0020)^2$	=	0.6273
$C_{\Delta_3} = (4)^2 = 16$	$\times (0.06)^2$	=	0.0576
		Total	**1.3249**

* The 2 factor is a result of the measurement being made on both the beginning and the ending inventory.

Rule 6

			$C\sigma^2$, kg² of Pu
$C_{\eta_1} = (10)^2(40) = 4000$	$\times (0.0030)^2$	=	0.0360
$C_{\eta_2} = (22)^2(18) = 8712$	$\times (0.0050)^2$	=	0.2178
$C_{\eta_3} = (0.25)^2(16) = 1$	$\times (0.06)^2$	=	0.0036
$C_{\eta_j} = (0.20)^2(2) = 0.08$	$j = 4, 5, \ldots, 13$		
For all j,			
$(10)(0.08) = 0.80$	$\times (0.05)^2$	=	0.0020
		Total	**0.2594**

Rule 7

$C_{\theta_1} = (400)^2 = 160{,}000$	$\times (0.0025)^2$	=	1.0000
$C_{\theta_2} = (396)^2 = 156{,}816$	$\times (0.0030)^2$	=	1.4113
$C_{\theta_3} = (4)^2 = 16$	$\times (0.10)^2$	=	0.1600
		Total	**2.5713**

Rule 9

$C_{\omega_1} = (10)^2(40) = 4000$	$\times (0.01)^2$	=	0.4000
$C_{\omega_2} = (22)^2(18) = 8712$	$\times (0.0070)^2$	=	0.4269
$C_{\omega_3} = (0.25)^2(16) = 1$	$\times (0.20)^2$	=	0.0400
$C_{\omega_k} = (0.20)^2(2) = 0.08$	$k = 4, 5, \ldots, 13$		
For all k,			
$(10)(0.08) = 0.80$	$\times (0.05)^2$	=	0.0020
		Total	**0.8689**

The results are summarized in Table 6.15.

TABLE 6.15 SUMMARY OF VARIANCES
(Example 6.F)

Rule	Description	Variance, kg² of Pu	Percent of total
1	Systematic bulk measurement	1.6112	24.1
3	Random bulk measurement	0.0471	0.7
4	Systematic sampling	1.3249	19.8
5	Random sampling	0.2594	3.9
7	Systematic analysis	2.5713	38.5
9	Random analysis	0.8689	13.0
	Total	6.6828	100.0
		$\sigma_{MUF} = 2.59$ kg of Pu	

In this particular example, in view of the statistical independence of the various components of the material balance, it is also possible to break down the variance in other ways. For example, see Table 6.16.

TABLE 6.16 COMPONENTS OF VARIANCE OF MUF
(Example 6.F)

Material balance component	Systematic error, kg^2 of Pu	Random error, kg^2 of Pu
Input	3.0800 (46.1%)	0.4720 (7.1%)
Product	2.1954 (32.9%)	0.6534 (9.8%)
Waste	0.2320 (3.5%)	0.0440 (0.7%)
Inventory	0	0.0060 (0.1%)
Total	5.5074 (82.4%)	1.1754 (17.6%)

Total = 6.6828 kg^2 of Pu

Example 6.G

(This example was provided by R. A. Schneider.)

In a given plutonium-scrap-recovery facility, the month-end inventory holdings in seven process vessels are determined. The volume of the contents of each tank is measured, and each tank is sampled and analyzed for percent plutonium. The total plutonium inventory is calculated from these data.

In Table 6.17 the calculated plutonium in each tank is given, along with the random-error standard deviations due to the volume determination, sampling for percent plutonium, and percent plutonium analysis. Find the random-error standard deviation of the total plutonium inventory of 3415 g.

TABLE 6.17 PLUTONIUM INVENTORY DATA
(Example 6.G)

Process vessel	Plutonium, g	σ_{ϵ_i}	σ_{η_j}	σ_{ω_k}
1	100	0.01	0.01	0.02
2	200	0.02	0.01	0.02
3	10	0.05	0.07	0.05
4	1800	0.005	0.001	0.005
5	1000	0.005	0.001	0.005
6	5	0.10	0.10	0.10
7	300	0.03	0.00	0.04
Total	3415			

The rules of Table 6.2 are applied. Since the problem is concerned only with random-error variances, only rules 3, 6, and 9 are pertinent. Further, because single determinations are made throughout, $C_\epsilon = C_\eta = C_\omega$ for each process vessel. Therefore the calculations are conveniently presented in tabular form (Table 6.18).

TABLE 6.18 CALCULATION OF VARIANCE OF INVENTORY
(Example 6.G)

Process vessel	$C_\epsilon = C_\eta = C_\omega$	$(\sigma_\epsilon^2 + \sigma_\eta^2 + \sigma_\omega^2)$	Product
1	$(100)^2$	0.0006	6.00
2	$(200)^2$	0.0009	36.00
3	$(10)^2$	0.0099	0.99
4	$(1800)^2$	0.000051	165.24
5	$(1000)^2$	0.000051	51.00
6	$(5)^2$	0.03	0.75
7	$(300)^2$	0.0025	225.00
		Variance Pu MUF	484.98 g^2
		σ_{MUF} 22.0 g	

Example 6.H

Reference is made to example 6.E, which dealt with the ^{235}U MUF in the fuel fabrication facility. Suppose now that the ^{235}U content in the ADU scrap containers is measured by a nondestructive assay (NDA) instrument rather than by wet chemistry. How does the calculation of the variance of MUF change? Assume that a linear calibration curve describes the relation between counts observed and ^{235}U content for the NDA instrument and that the same calibration curve is used for all ADU containers.

First, note that the ADU values will not be included in application of rules 1 to 15 in Tables 6.2 and 6.3. Rather, the methods of Sec. 3.3.8 will be applied to find the systematic- and random-error variances that must be added to those found by application of rules 1 to 15 to the other items in the MUF equation.

In applying the methods of Sec. 3.3.8, assume that the equation for the calibration curve relating predicted grams of ^{235}U, x, to counts observed, y, is

$$x = 100 + 0.05y$$

In the notation of Eq. 3.15, this means $\alpha' = 100$ and $\beta' = 0.05$.

Also, assume that the following values were calculated during the calibration:

$$\hat{\sigma}_\epsilon^2 = 20{,}160 \qquad \text{(from Eq. 3.24)}$$

$$R = 0.048 \qquad \text{(from Eq. 3.23)}$$

$$\frac{\Sigma x_i^2}{n} = \frac{2{,}040{,}000}{8} = 255{,}000$$

$$\bar{x} = 450$$

$$\hat{\beta} = 1/\hat{\beta}' = 1/0.05 = 20 \qquad \text{(from Eq. 3.18)}$$

$$\hat{\alpha} = -\hat{\alpha}'\hat{\beta} = -(100)(20) = -2000 \qquad \text{(from Eq. 3.19)}$$

The y values (total counts) corresponding to the amounts of ^{235}U in the ADU containers are required as final input. ADU cans AD-1 to AD-5 and AD-14 to AD-16 are ignored since they were all in both beginning and ending inventories. Table 6.19 gives the required data. (All values affect the MUF equation as negative values since all are in ending inventory only. The sign is ignored in this calculation.)

With these data we can apply rules 10 and 11 of Sec. 3.3.8 to find the systematic- and random-error variances for the sum of the ^{235}U contents in the ADU containers. (If some of the containers were in beginning inventory but not in ending inventory, then rules 13 and 14 would apply, with some of the c_i being $+1$ and some being -1.)

Rule 10

From Eq. 3.26, with $\bar{y} = 2982$ replacing y_0 and multiplying the expression by $k^2 = 324$,

$$\hat{\sigma}_s^2 = \frac{(0.048)(324)}{400}\left[255{,}000 + \frac{(2982+2000)^2}{400} - \frac{2(2982+2000)(450)}{20}\right]$$

$$= 3610 \text{ g}^2 \text{ of } ^{235}U$$

TABLE 6.19 OBSERVED COUNT DATA FOR ADU CANS
(Example 6.H)

Can No.	y_i, counts	x_i, g of ^{235}U	Can No.	y_i, counts	x_i, g of ^{235}U
A-6	4300	315	A-18	3540	277
A-7	1100	155	A-19	1800	190
A-8	3740	287	A-20	4300	315
A-9	600	130	A-21	5240	362
A-10	360	118	A-22	3980	299
A-11	2480	224	A-23	4020	301
A-12	2320	216	A-24	280	114
A-13	4660	333	A-25	5600	380
A-17	1680	184	A-26	3680	284

Rule 11

Multiplying Eq. 3.28 by $k = 18$ gives the random-error variance.

$$\hat{\sigma}_R^2 = \frac{(18)(20{,}160)}{400} = 907 \text{ g}^2 \text{ of } {}^{235}\text{U}$$

In comparing the variance of MUF with that found by the wet-chemistry approach, note (with reference to example 6.E) that most of the variance attributable to ADU scrap came from $C_{\Delta_6}\sigma_{\Delta_6}^2$ and $C_{\eta_6}\sigma_{\eta_6}^2$ because of sampling of the containers for percent uranium. The total variance due to these sources was $(9731 + 5848) = 15{,}579$ g^2 of ^{235}U. This variance would now be excluded and would be replaced by $(3610 + 907)$ or 4517 g^2 of ^{235}U.

Finally, if more than one calibration curve were involved, each would be handled separately by the methods of Sec. 3.3.8 or 3.3.10 and the variances added. This assumes independence of the curves, which is a reasonable assumption if they relate to different NDA instruments and if the calibrating standards are well defined. In other situations this assumption may be violated to some degree, and the estimated parameters for the calibration curves may not be statistically independent of one another. The situation is analogous to a long- and short-term systematic error, with the short-term error related to the systematic-error variance associated with each calibration and the long-term error to a persistent systematic error that affects all calibration curves. The long-term error variance is difficult to estimate in the calibration situation, however. It is affected by uncertainties in the standards and by persistent biases in the NDA instrument involved. In the modeling done in Secs. 3.3.8 and 3.3.10, we assumed that the calibrating standards are assigned known values and this problem is avoided. If we have some real concern about the validity of this assumption in a given application, we can, by technical judgment, assign additional variances to the parameter. These variances would then affect all calibration curves as a long-term systematic-error variance, whereas the short-term error variances would be estimated separately for each calibration. This problem area requires further study.

Example 6.I

A number of the preceding examples have been concerned with calculating the variance of MUF for specific facilities. In particular, example 6.E deals with a UO_2 fabrication facility, 6.F with a chemical reprocessing facility, and 6.G with a plutonium scrap recovery plant.

This final example relates to a single campaign in a PuO_2–UO_2 fabrication plant. It differs from the preceding examples primarily in that it represents the type of analysis that would be performed before the campaign to anticipate measurement problems that might arise and to identify actions that could be taken to alleviate their effects.

Because of the difference in motivation, this analysis is more detailed than one performed simply to assess the significance of a given observed MUF. In particular, the frequency of material balance closings is studied with respect to effects on the variance of MUF. In this connection, attention is directed to both the incremental MUF for a given time period and the MUF accumulated from the start of the campaign. In addition, although not shown here, in an a priori analysis such as this, we would perform parametric studies to investigate the effects of different measurement intensities on the variance of MUF. This amount of detail is helpful when we are performing studies for the purpose of guiding future actions.

Note that, although this is considerably more detailed than the previous examples cited, no additional statistical techniques are involved.

The campaign under study involves the processing of 32 batches of 3.65% PuO_2–96.35% UO_2 pellets, each batch containing 312 g of PuO_2. The 32 containers of PuO_2 powder are characterized prior to blending with UO_2 powder. The campaign lasts 10 weeks. During the first week all receipts are characterized, sealed, and stored in the vault for quality-control hold. During the second week all 32 batches are processed through blending and slugging and are again stored in the vault as individual batches. Pellet pressing begins during the third week, and thereafter the processing proceeds at a rate of five batches per week.

Material Flow. Table 6.20 summarizes the material status at the end of each week of this campaign.

Generation of Scrap. For this campaign, scrap is accumulated as indicated in Table 6.21. No further green scrap is generated after week 3, because all operations on green powder and pellets will have been completed. In this discussion we assume that all the scrap listed in Table 6.21 is contained and stored and is not recycled.

TABLE 6.20 MATERIAL STATUS BY WEEK (EXCLUDING SCRAP)
(Example 6.I)

	Equivalent batches at end of week									
Location	1	2	3	4	5	6	7	8	9	10
Vault (PuO_2)	32									
Vault (prepress)		32								
Vault (presinter)			28	23	18	13	8	3		
Line 2 (furnace)			1	1	1	1	1	1		
Line 3* (grinding, inspection)			1	1	1	1	1	1	1	
Vault (preloading)			2	7	7	7	7	7	5	
Rod form					5	10	15	20	26	32

* Two boat loads are ready for grinding, and three trays are ready for inspection–pretreatment.

Error Structure. The error structure assumed in this analysis is given in Table 6.22. The entries are percent standard deviations. In this table the short-term and long-term systematic-error standard deviations are identified to permit valid analysis in the situation in which the biases may shift. In this particular analysis, however, it is assumed that the biases remain constant over the course of the campaign.

Calculations for LE–MUF (Plutonium). To illustrate how LE–MUF is calculated, we show the steps in this calculation for LE–MUF accumulated from the start of the campaign through the end of week 4. Calculation of LE–MUF requires that each component in the MUF equation be identified by the scale on which the net weight is determined and by the plutonium factor used to convert net weight to grams of plutonium. The first figure in the third colum of Table 6.23 indicates the number of weighings made to arrive at the total net weight for each MUF component, and the last column of that table shows the number of analyses associated with each calculated plutonium factor. It is assumed that each analysis is made on a different sample so that the number of analyses equals the number of samples.

To illustrate the calculation of LE–MUF by applying the rules of Table 6.2, we will consider four typical error sources: Scale 2, systematic and random, and sampling of MO pellets, systematic and random.

Rules from Table 6.2

Scale 2

Systematic (Rule 1):
Find the algebraic sum of plutonium weight for all components weighed on scale 2, square the sum, and multiply by the square of the appropriate Table 6.22 entry.

TABLE 6.21 ACCUMULATED SCRAP (GRAMS OF PuO_2)
(Example 6.I)

End of week	Green	Grinder swarf	Hard	Dirty
1	0	0	0	0
2	50	0	0	3
3	100	37	134	8
4	100	100	357	14
5	100	162	580	20
6	100	225	803	26
7	100	287	1026	32
8	100	349	1249	38
9	100	400	1428	44
10	100	400	1428	50

TABLE 6.22 ERROR STRUCTURE* (PERCENT STANDARD DEVIATION)
(Example 6.I)

Operation	Type of error	
Weighing		
Scale type	*Systematic* (δ)	*Random* (ϵ)
1. Mettler P 160	0.01	0.01
2. Mettler P 1200	0.01	0.01
3. Mettler P 11	0.01	0.01
4. Mettler P 11	0.01	0.01
Sampling for percent of plutonium		
Material	*Systematic* (Δ)	*Random* (η)
1. PuO_2 powder	0.05	0.15
2 MO powder	0.03	0.08
3. MO pellets	0.03	0.10
4. Swarf	0.3	1
5. Dirty scrap	5	15

Analysis for percent of plutonium

Method	*Short-term systematic* (β)	*Long-term systematic* (θ)	*Random* (ω)
1. Ceric sulfate titration (PuO_2)	0.06	0.04	0.25
2. Controlled potential coulometry (main stream)	0 06	0.04	0.25
3. Controlled potential coulometry (scrap)	5	2.5	20

Sampling for fissile isotope

Material	*Systematic* (λ)	*Random* (μ)
1. PuO_2 powder	0.015	0.005
2. MO powder	0.015	0.008
3. MO pellets	0.015	0.002

Analysis for fissile isotope

Method	*Short-term systematic* (α)	*Long-tern systematic* (γ)	*Random* (ν)
1. Mass spectrometer	0.022	0.031	0.10

* See Table 5.1 for the error notation.

$$(-0.088-0.005-0.271-6.284)^2(1)(10^{-8}) = 44(10^{-8}) \quad \text{kg}^2 \text{ of Pu}$$

Random (Rule 3):
Square each net plutonium weight for all weighing performed on scale 2, sum the squares, and multiply by the square of the appropriate Table 6.22 entry.

$$[4(0.022)^2+1(0.005)^2+8(0.0399)^2+23(0.2732)^2](1)(10^{-8}) = 2(10^{-8})$$
kg^2 of Pu

TABLE 6 23 ACCUMULATED MUF COMPONENTS AT THE END OF WEEK 4
(Example 6 I)

Component *	Scale	Pu, kg †	Factor	Basis ‡
Receipts	1	32(0 2749) = 8 796	1	6
Green scrap	2	4(0 022) = 0 088	2	32
Swarf	3	2(0 044) = 0 088	3	2
Hard scrap	3	14(0 0225) = 0 315	4	7
Dirty scrap (green)	2	1(0 005) = 0 005	5	1
Dirty scrap (hard)	3	1(0 007) = 0 007	6	1
Boats in furnace	2	8(0 0339) = 0 271	2	32
Boats in line 3	4	2(0 0339) = 0 068	4	7
Trays in line 3	3	3(0 068) = 0 204	4	7
In vault (presinter)	2	23(0 2732) = 6 284	2	32
In vault (preload)	3	21(0 0690) = 1 448	4	7
		MUF = 0 018 kg of Pu		

* All entries except receipts are in ending inventory

† The first figure indicates the number of weighings made to arrive at the total net weight for each MUF component

‡ Number of analyses associated with each calculated plutonium factor

Sampling MO Pellets (Factor 4)

Systematic (Rule 4)

Find the algebraic sum of all plutonium weights for components based on factor 4, square the sum, and multiply by the square of the appropriate Table 6 22 entry

$$(-0\ 315 - 0\ 068 - 0\ 204 - 1\ 448)^2 9(10^{-8}) = 37(10^{-8}) \quad \text{kg}^2 \text{ of Pu}$$

Random (Rule 6)

Find the algebraic sum as for the systematic error, square the sum, divide by the number of samples used in estimating plutonium factor 4, and multiply by the square of the appropriate Table 6 22 entry

$$[(-0\ 315 - 0\ 068 - 0\ 204 - 1\ 448)^2/7](100)(10^{-8}) = 60(10^{-8}) \quad \text{kg}^2 \text{ of Pu}$$

Further detailed calculations are not shown, because the application of the rules of Table 6 2 has been thoroughly illustrated in this chapter

LE–MUF Components by Week. The LE–MUF components accumulated through the end of each week in the campaign are shown in Tables 6 24 and 6 25 Table 6 24 gives the systematic components and Table 6 25 the random components The entries underlined are those just calculated

Note that, as of the end of week 9, the accumulated MUF exceeds LE–MUF This occurs because no hoods have been cleaned out, and no solid

TABLE 6 24 ACCUMULATED LE-MUF SYSTEMATIC-VARIANCE COMPONENTS (GRAMS^2 OF PLUTONIUM)
(Example 6 I)

Operation	End of week									
	1	2	3	4	5	6	7	8	9	10
Weighing										
Scale 1	0	0 77	0 77	0 77	0 77	0 77	0 77	0 77	0 77	0 77
Scale 2	0	0 77	0 64	0 44	0 28	0 15	0 07	0 01	0 00	0 00
Scale 3	0	0	0 00	0 04	0 12	0 23	0 38	0 56	0 74	0 75
Scale 4	0	0	0 00	0 00	0 00	0 00	0 00	0 00	0 00	0 00
Sampling										
PuO_2 powder	0	19 34	19 34	19 34	19 34	19 34	19 34	19 34	19 34	19 34
MO powder	0	6 94	5 77	3 97	2 51	1 38	0 58	0 13	0 00	0 00
Swarf	0	0	0 01	0 07	0 18	0 35	0 58	0 85	1 12	1 12
MO pellets	0	0	0 05	0 37	1 00	1 93	3 17	4 71	6 16	6 15
Dirty scrap (green)	0	0	0 06	0 06	0 06	0 06	0 06	0 06	0 06	0 06
Dirty scrap (hard)	0	0	0	0 12	0 36	0 81	1 32	1 96	2 72	3 80
Analysis										
PuO_2 powder	0	40 23	40 23	40 23	40 23	40 23	40 23	40 23	40 23	40 23
MO (clean)	0	40 11	39 97	39 88	39 78	39 68	39 65	39 56	39 49	39 43
MO (dirty)	0	0	0 08	0 45	0 90	1 65	2 45	3 40	4 51	6 05
Total	0	108 16	106 92	105 74	105 53	106 58	108 60	111 58	115 14	117 70

TABLE 6 25 ACCUMULATED LE–MUF RANDOM-VARIANCE COMPONENTS (GRAMS² OF PLUTONIUM)
(Example 6 I)

Operation	End of week									
	1	2	3	4	5	6	7	8	9	10
Weighing										
Scale 1	0	0 02	0 02	0 02	0 02	0 02	0 02	0 02	0 02	0 02
Scale 2	0	0 02	0 02	0 02	0 01	0 01	0 01	0 00	0 00	0 00
Scale 3	0	0	0 00	0 00	0 00	0 00	0 00	0 00	0 01	0 01
Scale 4	0	0	0 00	0 00	0 00	0 00	0 00	0 00	0 00	0 00
Sampling										
PuO_2 powder	0	29 01	29 01	29 01	29 01	29 01	29 01	29 01	29 01	29 01
MO powder	0	4 94	1 28	0 88	0 56	0 31	0 13	0 03	0 00	0 00
Swarf	0	0	0 11	0 39	0 51	0 49	0 53	0 59	0 77	0 62
MO pellets	0	0	0 26	0 60	0 92	1 26	1 60	1 94	2 14	2 14
Dirty scrap (green)	0	0	0 56	0 56	0 56	0 56	0 56	0 56	0 56	0 56
Dirty scrap (hard)	0	0	0	1 10	3 24	7 29	11 90	8 82	12 25	17 11
Analysis										
PuO_2 powder	0	80 59	80 59	80 59	80 59	80 59	80 59	80 59	80 59	80 59
MO (clean)	0	48 21	14 18	12 32	11 25	10 90	11 35	12 49	13 50	13 50
MO (dirty)	0	0	1 00	2 96	6 76	13 96	21 36	16 68	22 76	31 40
Total	0	162 79	127 03	128 45	133 43	144 40	157 06	150 73	161 61	174 96
Random+Systematic, g^2	0	270 95	233 95	234 19	238 96	250 98	265 66	262 31	276 75	292 66
Standard deviation, g	0	16 5	15 3	15 3	15 5	15 8	16 3	16 2	16 6	17 1
Accumulated MUF, g	0	9	16	18	22	25	28	32	35	35
MUF, % of receipts	0	0 10	0 18	0 20	0 25	0 28	0 32	0 36	0 40	0 40
LE–MUF (2σ)	0	33 0	30 6	30 6	31 0	31 6	32 6	32 4	33 2	34 2
LE–MUF, % of receipts	0	0 38	0 35	0 35	0 35	0 36	0 37	0 37	0 38	0 39

wastes have been measured. In view of the slight amount by which MUF exceeds LE–MUF and in anticipation of the end of the campaign in another week (which calls for hood cleanout), no action would be taken except to begin hood cleanout in those operations which will process no additional material and to obtain measurements of the scrap thus accumulated. It is anticipated that an estimated 13 g of plutonium will be found in the hood sweepings; this would reduce the MUF to 22 g and increase LE–MUF to 34.5 g. It is also assumed that later measurement of solid waste discards by NDA assay will further reduce the MUF to 14 g and will increase LE–MUF to 35.4 g. (The increase in LE–MUF is not large in spite of the large measurement-error variance associated with the measurement of solid wastes. This is due to the very small amount of plutonium in these wastes.)

Table 6.23 gives the number of samples and analyses on which the six plutonium factors were based as of the end of week 4. These data accumulate as the campaign proceeds, and Table 6.26 gives the number of samples and analyses on which the plutonium factors are based throughout the campaign. A time lag of a few days in analytical results is included.

LE–MUF for Fissile Plutonium. There is no reason to believe that the percent of fissile plutonium will change during the campaign if hoods are cleaned out thoroughly before the start of the campaign. This assumption is checked for validity by analyzing the material at the receipt point, after blending, and after sintering. In anticipation that the assumption is valid, we apply a common fissile plutonium factor. Then we calculate the MUF for fissile plutonium by multiplying the MUF for total plutonium by this

TABLE 6.26 NUMBERS OF SAMPLES AND ANALYSES ON PLUTONIUM FACTORS THROUGHOUT THE CAMPAIGN
(Example 6.I)

	Plutonium factor					
End of week	1	2	3*	4	5	6
1						
2	6	10				
3	6	32	1	2	1	
4	6	32	2	7	1	
5	6	32	4-3	12	1	1
6	6	32	8-4	17	1	1
7	6	32	12-5	22	1	1
8	6	32	16-6	27	1	2
9	6	32	16-6	32	1	2
10	6	32	20-7	32	1	2

* After week 4, samples are composited. In hyphenated entries (e.g., 4-3), the first figure is the number of samples and the second figure is the total number of analyses.

common factor. Propagation of errors in this situation shows that the error in estimating the common fissile plutonium factor has negligible effect on the LE–MUF; thus, on a percentage basis, the LE–MUF is essentially the same for fissile plutonium as for total plutonium.

LE–MUF on an Incremental Basis. Thus far, LE–MUF has been calculated for accumulated MUF over the campaign. We may also wish to calculate MUF and LE–MUF on an incremental basis. The results of such an analysis are presented here. Details of the analysis are not shown since it is similar to that performed on accumulated MUF. The results pertain to an equilibrium period of operation, e.g., during weeks 4 to 8, as seen in Table 6.20.

The MUF and LE–MUF are shown for a 1-week, 2-week, 3-week, and 4-week basis in Tables 6.27 and 6.28. In Table 6.27 it is assumed that constant plutonium factors apply to all material processed during the equilibrium period. In this event, the random errors affecting the uncertainties in the common plutonium factors behave like systematic errors as they affect the LE–MUF. In Table 6.28 it is assumed that a separate

TABLE 6.27 MUF AND LE–MUF DURING EQUILIBRIUM ASSUMING COMMON PLUTONIUM FACTORS (GRAMS OF PLUTONIUM)
(Example 6.I)

Time interval	Long-term systematic error (LE)	Random error (LE)	LE–MUF	MUF
1 week	1.5	2.7	3.1	3.5
2 weeks	2.9	5.5	6.2	7.0
3 weeks	4.3	8.3	9.3	10.5
4 weeks	5.8	11.0	12.4	14.0

TABLE 6.28 MUF AND LE–MUF DURING EQUILIBRIUM ASSUMING DIFFERENT PLUTONIUM FACTORS FOR EACH BATCH (GRAMS OF PLUTONIUM)
(Example 6.I)

Time interval	Long-term systematic error (LE)	Random error (LE)	LE–MUF	MUF
1 week	1.5	5.2	5.4	3.5
2 weeks	2.9	7.3	7.8	7.0
3 weeks	4.3	9.0	10.0	10.5
4 weeks	5.8	10.4	11.9	14.0

plutonium factor is calculated for each batch processed, and the errors truly behave as random errors. The effects of both procedures are seen in the tables.

6.1.4 Basis

The rules for finding the variance for the general algebraic sum are derived by application of the results of Chaps. 4 and 5. Rather than attempting to derive the rules for a completely general case, we derive the results for example 6.C to illustrate the basis for the rules. This example was chosen because it includes the various kinds of situations that might exist.

With reference to the example, the sum S, whose variance is to be found, is $S=S_1+S_2-S_3-S_4+S_5-S_6+S_7+S_8+S_9+S_{10}$. Using the multiplicative model of Sec. 5.2, we can write the 10 observed element weights as follows:

$$\begin{aligned} S_1&=W_1\delta_1\phi_{11}\epsilon_{11}p_1 & S_6&=W_6\delta_3\phi_{31}\epsilon_{33}p_1\\ S_2&=W_2\delta_1\phi_{11}\epsilon_{12}p_1 & S_7&=W_7\delta_3\phi_{32}\epsilon_{34}p_3\\ S_3&=W_3\delta_2\phi_{21}\epsilon_{21}p_2 & S_8&=W_8\delta_1\phi_{11}\epsilon_{13}p_3\\ S_4&=W_4\delta_3\phi_{31}\epsilon_{31}p_3 & S_9&=W_9\delta_3\phi_{32}\epsilon_{35}p_2\\ S_5&=W_5\delta_3\phi_{31}\epsilon_{32}p_1 & S_{10}&=W_{10}\delta_2\phi_{21}\epsilon_{22}p_3 \end{aligned}$$

The p's are observed element factors. From the data of the example, we can write p_1 as follows (noting that it is the average of eight analyses):

$$\begin{aligned} p_{11}&=P_1\Delta_1\theta_1\psi_{11}\eta_{11}\beta_{11}\omega_{11} & p_{15}&=P_1\Delta_1\theta_1\psi_{11}\eta_{13}\beta_{12}\omega_{15}\\ p_{12}&=P_1\Delta_1\theta_1\psi_{11}\eta_{11}\beta_{11}\omega_{12} & p_{16}&=P_1\Delta_1\theta_1\psi_{11}\eta_{13}\beta_{12}\omega_{16}\\ p_{13}&=P_1\Delta_1\theta_1\psi_{11}\eta_{12}\beta_{11}\omega_{13} & p_{17}&=P_1\Delta_1\theta_1\psi_{11}\eta_{14}\beta_{12}\omega_{17}\\ p_{14}&=P_1\Delta_1\theta_1\psi_{11}\eta_{12}\beta_{12}\omega_{14} & p_{18}&=P_1\Delta_1\theta_1\psi_{11}\eta_{14}\beta_{12}\omega_{18} \end{aligned}$$

Then

$$p_1=\frac{P_1\Delta_1\theta_1\psi_{11}}{8}\{\eta_{11}(\beta_{11}\omega_{11}+\beta_{11}\omega_{12})+\eta_{12}(\beta_{11}\omega_{13}+\beta_{12}\omega_{14})+\ \ldots$$

$$+\eta_{14}(\beta_{12}\omega_{17}+\beta_{12}\omega_{18})\}$$

Similarly, p_2 is derived. This is based on 20 samples, with each group of four samples composited and with two analyses performed on each composite, for a total of 10 analyses. With p_{21} representing the first four samples, first analysis on composite; p_{22} representing the first four samples, second analysis on composite; and p_{23} representing the second four samples, first analysis on composite, etc., these 10 results are written:

$$p_{21}=P_2\Delta_2\theta_1\psi_{21}\left(\frac{\eta_{21}+\eta_{22}+\eta_{23}+\eta_{24}}{4}\right)\beta_{12}\omega_{19}$$

$$p_{22}=P_2\Delta_2\theta_1\psi_{21}\left(\frac{\eta_{21}+\eta_{22}+\eta_{23}+\eta_{24}}{4}\right)\beta_{12}\omega_{1,10}$$

$$p_{23}=P_2\Delta_2\theta_1\psi_{21}\left(\frac{\eta_{25}+\eta_{26}+\eta_{27}+\eta_{28}}{4}\right)\beta_{13}\omega_{1,11}$$

. . . .
. . . . . .
. . . .

$$p_{2,10}=P_2\Delta_2\theta_1\psi_{22}\left(\frac{\eta_{2,17}+\eta_{2,18}+\eta_{2,19}+\eta_{2,20}}{4}\right)\beta_{13}\omega_{1,18}$$

Then,

$$p_2=\frac{P_2\Delta_2\theta_1}{40}\{\psi_{21}(\eta_{21}+\eta_{22}+\eta_{23}+\eta_{24})(\beta_{12}\omega_{19}\beta_{12}\omega_{1,10})+\ \ldots$$

$$+\psi_{22}(\eta_{2,17}+\eta_{2,18}+\eta_{2,19}+\eta_{2,20})(\beta_{13}\omega_{1,17}+\beta_{13}\omega_{1,18})\}$$

Similarly,

$$p_3=\frac{P_3\Delta_2\theta_2\psi_{22}}{20}\{\beta_{21}(\eta_{2,21}\omega_{21}+\ldots+\eta_{2,28}\omega_{28})$$

$$+\beta_{22}(\eta_{2,29}\omega_{29}+\eta_{2,30}\omega_{2,10})$$

$$+\beta_{23}(\eta_{2,31}\omega_{2,11}+\ \ldots\ +\eta_{2,40}\omega_{2,20})\}$$

Let us now apply Eq. 4.6. The partial derivatives with respect to each random variable must be evaluated at the means of the random variables, which are all one. Since the values of W_i and P_i ,which are constants and not random variables, are not known they will be replaced by their estimates (note that the estimate of W_iP_i is S_i).

Basis for Rule 1

$$\frac{\partial S}{\partial \delta_1}=(S_1+S_2+S_8)$$

$$\frac{\partial S}{\partial \delta_2}=(-S_3+S_{10})$$

$$\frac{\partial S}{\partial \delta_3}=(-S_4+S_5-S_6+S_7+S_9)$$

Basis for Rule 2

$$\frac{\partial S}{\partial \phi_{11}}=(S_1+S_2+S_8)$$

$$\frac{\partial S}{\partial \phi_{21}}=(-S_3+S_{10})$$

$$\frac{\partial S}{\partial \phi_{31}}=(-S_4+S_5-S_6)$$

$$\frac{\partial S}{\partial \phi_{32}}=(S_7+S_9)$$

Basis for Rule 3

$$\frac{\partial S}{\partial \epsilon_{11}} = S_1$$

$$\frac{\partial S}{\partial \epsilon_{12}} = S_2$$

$$\frac{\partial S}{\partial \epsilon_{13}} = S_8$$

$$\frac{\partial S}{\partial \epsilon_{21}} = -S_3$$

$$\vdots \qquad \vdots$$

$$\frac{\partial S}{\partial \epsilon_{35}} = S_9$$

Basis for Rule 4

$$\frac{\partial S}{\partial \Delta_1} = (S_1+S_2+S_5-S_6)$$

$$\frac{\partial S}{\partial \Delta_2} = (-S_3-S_4+S_7+S_8+S_9+S_{10})$$

Basis for Rule 5

$$\frac{\partial S}{\partial \psi_{11}} = (S_1+S_2+S_5-S_6)$$

$$\frac{\partial S}{\partial \psi_{21}} = \frac{24}{40}(-S_3+S_9)$$

$$\frac{\partial S}{\partial \psi_{22}} = \frac{16}{40}(-S_3+S_9)+(-S_4+S_7+S_8+S_{10})$$

Basis for Rule 6

$$\frac{\partial S}{\partial \eta_{1i}} = \frac{2}{8}(S_1+S_2+S_5-S_6) \qquad (i=1, 2, \ldots, 4)$$

$$\frac{\partial S}{\partial \eta_{2i}} = \frac{2}{40}(-S_3+S_9) \qquad (i=1, 2, \ldots, 20)$$

$$= \frac{1}{20}(-S_4+S_7+S_8+S_{10}) \qquad (i=21, 22, \ldots, 40)$$

Basis for Rule 7

$$\frac{\partial S}{\partial \theta_1} = (S_1 + S_2 - S_3 + S_5 - S_6 + S_9)$$

$$\frac{\partial S}{\partial \theta_2} = (-S_4 + S_7 + S_8 + S_{10})$$

Basis for Rule 8

$$\frac{\partial S}{\partial \beta_{11}} = \frac{3}{8}(S_1 + S_2 + S_5 - S_6)$$

$$\frac{\partial S}{\partial \beta_{12}} = \frac{5}{8}(S_1 + S_2 + S_5 - S_6) + \frac{8}{40}(-S_3 + S_9)$$

$$\frac{\partial S}{\partial \beta_{13}} = \frac{32}{40}(-S_3 + S_9)$$

$$\frac{\partial S}{\partial \beta_{21}} = \frac{8}{20}(-S_4 + S_7 + S_8 + S_{10})$$

$$\frac{\partial S}{\partial \beta_{22}} = \frac{2}{20}(-S_4 + S_7 + S_8 + S_{10})$$

$$\frac{\partial S}{\partial \beta_{23}} = \frac{10}{20}(-S_4 + S_7 + S_8 + S_{10})$$

Basis for Rule 9

$$\frac{\partial S}{\partial \omega_{1i}} = \frac{1}{8}(S_1 + S_2 + S_5 - S_6) \qquad (i = 1, 2, \ldots, 8)$$

$$= \frac{4}{40}(-S_3 + S_9) \qquad (i = 9, 10, \ldots, 18)$$

$$\frac{\partial S}{\partial \omega_{2i}} = \frac{1}{20}(-S_4 + S_7 + S_8 + S_{10}) \qquad (i = 1, 2, \ldots, 20)$$

This development illustrates the bases for rules 1 to 9. The bases for rules 10 to 15 can be illustrated similarly. Because rules 10 to 15 so closely parallel 4 to 9, there is little need to discuss their derivation. The only point to note is that, when we deal with isotope weights rather than element weights, the various partial derivatives have means of the form $W_iP_iT_i$ rather than W_iP_i (T_i is the true isotopic factor). This is why "element weights" are replaced by "isotope weights" in the rules.

Chapter 7

INTERPRETATION OF MUF AND LE–MUF

OVERVIEW

In Chap. 6, rules were given for finding the variance of material unaccounted for (MUF), which can then be translated to limits of error–material unaccounted for (LE–MUF). (The results of Chap. 6 can be applied to any general sum, including MUF. In this chapter attention is restricted to MUF.) The two quantities MUF and LE–MUF are generally regarded as important indexes of material control performance. This chapter is concerned with the statistical interpretation of MUF as it relates to LE–MUF. (The term LE–MUF is not used in the succeeding discussion; rather, attention is focused on variance of MUF.)

Some clarification in terminology is helpful. First, a distinction must be made between an observed MUF and a true MUF. (When the term MUF is not preceded by the adjective "true," it is understood to be observed MUF). The observed MUF is a random variable that is an estimate of the true MUF. It is a random variable because its value is affected by errors of measurement. By properly combining the effects of these errors, we can calculate the measurement variance of MUF by the methods of Chap. 6. When we speak of the variance of MUF, we mean the measurement variance unless specifically stated otherwise. The variance is comprised of random and systematic components, and, if only the effects of one or the other type of error component is involved, the variance is referred to as either the random variance or the systematic variance of MUF.

The true MUF, on the other hand, is the actual amount of material unaccounted for, excluding the effects of measurement errors (i.e., in the absence of measurement errors, the observed MUF and the true MUF are identical). The true MUF is zero in an ideal situation. In actual practice, however, a nonzero true MUF may occur for a number of reasons, e.g., because of unmeasured inventory or process losses, stolen or diverted material, or operator mistakes in measurement or recording of data. If there were no measurement errors, the true MUF's might still vary somewhat from one material balance period to

the next because of these factors. This variation will be called the variance of the true MUF.

In an ideal situation the observed MUF and its variance are both zero. At the next level of idealism, the variance of MUF is zero, which means that the observed MUF represents exactly the true MUF, in which case there is proof positive that some real amount of material is unaccounted for. Whether this is an excessive amount is not primarily a problem in statistics. It has statistical overtones only if the criterion for making this judgment is based, in part at least, on experience data that sheds some light on the variance of the true MUF. The experience data are useful in this context only to the degree to which they were generated during operating periods in which acceptable control was exerted. The degree of control, of course, is a judgment that is devoid of statistical considerations.

Thus the significance of a given MUF is based on both statistical and nonstatistical considerations. To place in perspective the importance of the variance of MUF due to errors of measurement, we note that, although a zero variance does not negate the need for further judgments on the practical significance of an observed MUF value, if this variance is unduly large, there is little basis on which further judgment can be made. If the variance is large, we can only conclude that any true MUF that might exist is completely obscured by the inability to obtain a sufficiently good estimate of it. Thus it is important to exercise control over the variance of MUF. This may be done by the operator of a facility, who must maintain adequate control over his nuclear materials, or by an inspectorate agency, which must be satisfied that effective control does indeed exist.

The significance of a single, isolated MUF is considered in Sec. 7.1. In Sec. 7.2 attention is directed at combinations or sequences of MUF's, either over material balance areas (MBA's) or over time within a given MBA, or both. The concept of minimum variance MUF, although perhaps logically a part of Sec. 7.2, deserves special attention and is treated in Sec. 7.3. Finally, in Sec. 7.4 some thought is given to the role of material balance closings, unaccompanied by actual physical inventories, as they may relate to MUF calculations.

7.1 SIGNIFICANCE OF A SINGLE, ISOLATED MUF

7.1.1 Problem and Assumptions

For a given MBA the amount of some specified special nuclear material (SNM) in beginning inventory at some point in time is estimated by measurements. Similarly, at the end of an arbitrary time

period, the amount in ending inventory is also estimated by measurements. Inputs to the MBA are measured within the time interval, as are certain outputs from the system. (In common terminology the inputs are called receipts, and the outputs are called shipments and measured discards.) By algebraically summing, with the appropriate signs, the estimates of the amounts of material in beginning and ending inventories, inputs, and outputs, we can calculate the MUF. Similarly, by using the methods of Chap. 6, we can find the measurement standard deviation of this quantity. The problem, in general terms, is to examine the statistical significance of the observed, or estimated, MUF.

A number of specific questions within this general problem area are listed here and are answered, in turn, in Sec. 7.1.2.

Question 7.A. Given an observed MUF and its variance, is there evidence that the true MUF is greater than some specified value?

Question 7.B. Given an observed MUF and its variance, within what interval does the true MUF lie with a specified degree of confidence?

Question 7.C. What intensity of measurements must be performed to detect a given true MUF with a specified probability?

It is assumed that the MUF random variable is normally distributed and is unbiased in the sense that its expected value is the true MUF. It is also assumed that the error variances used in calculating the variance of the estimated MUF are known quantities. These assumptions, although often not strictly valid in practice, are judged to be reasonably valid in most applications. If there is real concern about treating some poorly estimated error variance as a known constant in a given application, we can use Satterthwaite's formula (Eq. 4.9) to calculate the degrees of freedom for the variance of MUF. In this event we apply the Student's t distribution rather than the normal distribution. The approach to judging the significance of MUF is very much the same as that used assuming normality. (See example 7.E.)

7.1.2 Solution

Let the observed MUF be denoted by the random variable X and its standard deviation by σ. Denote the true MUF by M. The random variable X is assumed to be normally distributed with mean M and standard deviation σ. The three questions posed in Sec. 7.1.1 are considered individually.

Question 7.A. This is a question in statistical hypothesis testing

(see Sec. 2.8). In that terminology the question can be restated as follows: Find a constant, c, such that, if an observed MUF, x, exceeds c, the hypothesis H_0: $M \leq M_0$ is rejected. Rejection of H_0 is equivalent to concluding that the true MUF is greater than M_0 by some amount not specified. (The inequality sign indicates that this is a one-sided test of significance. This is reasonable since we are usually interested in detecting positive MUF's, which indicate real unaccounted for material. The observance of too large a negative MUF is quite a different matter and implies that some statistically significant amount of material was "created," possibly as the result of some mistake. An isolated case of a significant negative MUF is of no real concern unless it is quite large in absolute value, in which case steps should be taken to identify the reasons for it.)

Answer 7.A. A significance level, α, is chosen (α is also called the probability of committing a type I error, i.e., of rejecting the hypothesis when it is true). From Table 7.1, a constant, c_α, is found as a function of α. The hypothesis H_0 is rejected if $x > (M_0 + c_\alpha\sigma)$.

TABLE 7.1* c_α VERSUS α

α	c_α	α	c_α	α	c_α
0.50	0	0.05	1.65	0.005	2.58
0.25	0.68	0.025	1.96†	0.0025	2.81
0.10	1.29	0.01	2.33	0.001	3.09

* This table is extracted from Appendix A.

† A decision rule often used is to reject H_0 if MUF > LE-MUF (i.e., if $x > 2\sigma$). This is equivalent to setting $M_0 = 0$ and $\alpha = \sim 0.025$. Thus, operating under this rule, we would declare that some true amount of material is unaccounted for about 2.5% of the time with no real basis; i.e., the significantly large MUF would be caused solely by errors of measurement with this expected frequency.

Question 7.B. This is a question in confidence-interval estimation (see Sec. 2.7). In that terminology the question can be restated as follows: Construct a 100 $(1-2\alpha)$ % confidence interval on the parameter M.

Answer 7.B. The confidence coefficient $100\,(1-2\alpha)$ % is chosen. The desired confidence interval is then $(x \pm c_\alpha\sigma)$, where c_α is related to α in Table 7.1. (Note that a confidence interval of the form MUF ± LE–MUF is equivalent to a 95% confidence interval on M.)

Question 7.C. This question is also related to hypothesis testing. The null hypothesis is H_0: $M \leq M_0$. An alternative hypothesis is also specified, H_1: $M = M_1$. In addition to specifying α, we also specify a

value of β, where $(1-\beta)$ is the probability of rejecting H_0 when H_1 is true. The problem is to find the value for σ which results in the specified value of β. (Note that a given value for σ can be attained in many different ways. Thus a solution for σ will not uniquely determine how many measurements of each type should be made. Within a given system, sensitivity studies are required to determine the effects of varying measurement intensities on σ.)

Answer 7.C. The required value for σ is

$$\sigma = \frac{M_1 - M_0}{c_\alpha + c_\beta} \tag{7.1}$$

For this value of σ, H_0 is rejected when $x > c$, where

$$c = \frac{M_0 c_\beta + M_1 c_\alpha}{c_\alpha + c_\beta} \tag{7.2}$$

In these equations c_α comes from Table 7.1; c_β also comes from this table with α replaced by β.

7.1.3 Examples

Example 7.A

In a fuel-fabrication-facility MBA, the calculated MUF for a given time period is 12 kg of uranium. Its standard deviation, σ, is 5 kg of uranium. At the 1% level of significance, do we have reason to believe that some true amount of material is unaccounted for?

This is question 7.A, with $\alpha = 0.01$, $x = 12$, $\sigma = 5$, and $M_0 = 0$. From answer 7.A and Table 7.1, the decision rule is to reject the hypothesis if x is greater than 2.33σ. Since 12 is greater than (2.33)(5), H_0 is rejected, and it is concluded that M is greater than zero, i.e., that some true amount of material is unaccounted for.

Example 7.B

For the data of example 7.A, what is the best estimate of the true amount of MUF, and what are the 95% confidence limits on this true amount?

The best estimate is $x = 12$ kg of uranium. From answer 7.B, the 95% confidence limits are found from $(x \pm c_\alpha\sigma)$, where $\alpha = 0.025$,* which gives $c_\alpha = 1.96$ (from Table 7.1).

The required confidence interval is

$$12 \pm (1.96)(5) = 12 \pm 9.8$$

* This follows from setting $100(1-2\alpha)\% = 95\%$ and solving for α.

Thus, with 95% confidence, between 2.2 and 21.8 kg of uranium are unaccounted for.

Example 7.C

For the data of example 7.A, at the 10% level of significance, is there statistical evidence that an amount in excess of 6 kg of uranium is actually unaccounted for?

This is question 7.A, with $\alpha = 0.10$, $x = 12$, $\sigma = 5$, and $M_0 = 6$. From answer 7.A, the decision rule is to reject the hypothesis if x is greater than [6 + (1.29) (5)] or 12.45. Since 12 is less than 12.45, we conclude that there is no statistical evidence of missing material in excess of 6 kg of uranium.

Example 7.D

The process in the previous examples is expected to yield a true MUF of 4 kg of uranium per unit time interval. This is considered tolerable over some period of time between thorough plant cleanouts and measurement of solid wastes. If the true MUF for a given time interval exceeds 10 kg of uranium, however, it is considered important to detect this and to investigate the causes. The following risks are established:

$\alpha = 0.025$ = probability of concluding that the true MUF > 4 kg of uranium when in fact it is 4 kg of uranium

$\beta = 0.05$ = probability of concluding that the true MUF $\leq$ 4 kg of uranium when in fact it is 10 kg of uranium

How small must σ be to meet these risk criteria, and what is the rule for deciding when a true MUF exceeds 4 kg of uranium?

This is question 7.C, with $M_0 = 4$, $M_1 = 10$, $c_\alpha = 1.96$, and $c_\beta = 1.65$.

Then, from Eq. 7.1,

$$\sigma = \frac{10-4}{1.96+1.65} = 1.66$$

and, from Eq. 7.2,

$$c = \frac{[(4)(1.65)]+[(10)(1.96)]}{1.96+1.65} = 7.26$$

Thus sufficient measurements of the right kind must be performed to produce a value for σ less than or equal to 1.66 kg of uranium. The rule is to conclude that M is greater than 4 if the observed MUF exceeds 7.26 kg of uranium.

Example 7.E

In the previous examples we assumed that σ is a constant value rather than a random variable. In most applications this is considered a reasonable approach. There may be instances, however, when it is advisable to relax this assumption, as this example will illustrate.

Reference is made to example 6.E. The variance of MUF, σ^2, was found to be 16,913 g^2 of ^{235}U. Of this total variance, 9731 g^2 was due to the systematic error in sampling ammonium diuranate (ADU) and 5848 g^2 to the random error in this sampling process. Suppose that these error variances are poorly estimated, having been based on an experiment in which only 2 degrees of freedom were associated with $\hat{\sigma}^2_{\Delta_6}=(22)^2$ and 6 degrees of freedom with $\hat{\sigma}^2_{\eta_6}=(76)^2$. Let $\hat{\sigma}^2$ denote the estimated variance of MUF and σ_r^2, based on an infinite number of degrees of freedom, designate the sum of all other variances exclusive of the ADU sampling error variances.* Then $\hat{\sigma}^2$ can be calculated from

$$\hat{\sigma}^2=20.106\ \hat{\sigma}^2_{\Delta_6}+1.01249\ \hat{\sigma}^2_{\eta_6}+\sigma_r^2$$

The coefficients 20.106 and 1.01249 are the values for C_{Δ_6} and C_{η_6}, respectively.

Formula 4.9 is applied to give the degrees of freedom, n_0, associated with $\hat{\sigma}^2$.

$$n_0=\frac{(16913)^2}{[(20.106)^2(22)^4/2]+[(1.01249)^2(76)^4/6]+(\sigma_r^4/\infty)}=5.4$$

Suppose that the 1% level of significance is chosen, how large must the observed MUF be to conclude that the true MUF exceeds zero? By analogy with question 7.A, we conclude that M is greater than zero if x is greater than $c_{0.01}\sigma$. For known σ, $c_{0.01}$ is 2.33 (from Table 7.1). For estimated σ, based on 5.4 degrees of freedom, $c_{0.01}$ is read from a table of Student's t distribution (Appendix C). At 5 degrees of freedom, $c_{0.01}$ is 3.36 and, at 6 degrees of freedom, 3.14. Then, by linear interpolation, which is adequate for this approximate solution, $c_{0.01}$ is 3.27 at 5.4 degrees of freedom. Thus, if $x > 3.27 \times \sqrt{16913}$, or 425 g of ^{235}U, it is concluded that the true MUF exceeds zero.

It may be advisable to regard the standard deviation of MUF as an estimate rather than a known value when the dominant sources of variation correspond to error variances that are poorly estimated or characterized. Both of these conditions must exist. Of course, if most or all of the error variances are poorly characterized regardless of their

* That there is no caret (^) on σ_r^2 indicates that this term is regarded as a known constant rather than an estimated value.

individual impacts on the variance of MUF, an analogous situation would exist.

7.1.4 Basis

The bases for solutions to the specific questions of Sec. 7.1.2 are developed in the framework of statistical hypothesis testing and interval estimation (see Secs. 2.7 and 2.8). These bases are considered for the questions raised in Sec. 7.1.2.

Question 7.A. The null hypothesis is H_0: $M \leq M_0$, and the one-sided alternative hypothesis is H_1: $M > M_0$.

A type I error is committed if H_0 is rejected when $M = M_0$. This error is committed with a probability α. Thus the decision rule is to reject H_0 when x, the observed MUF, exceeds c', where c' is determined from

$$\Pr\,(x > c' \mid M = M_0) = \alpha$$

The observation, x, is transformed to a normally distributed variable with zero mean and unit standard deviation by subtraction of the mean, M_0, and division by the standard deviation, σ. This permits the use of a table of the normal distribution to determine c'.

$$\Pr\left(\frac{x - M_0}{\sigma} > \frac{c' - M_0}{\sigma}\right) = \alpha$$

which gives

$$\frac{c' - M_0}{\sigma} = c_\alpha$$

where c_α comes from a table of the normal distribution (Appendix A).

Therefore the rule is to reject H_0 when

$$\frac{x - M_0}{\sigma} > c_\alpha \qquad \text{or} \qquad x > (M_0 + c_\alpha \sigma)$$

Question 7.B. This is a problem in interval estimation in which a $100\ (1 - 2\alpha)\%$ confidence interval is constructed on the true MUF M. Two values, c_1 and c_2, are chosen such that

$$\Pr\,(c_1 < M < c_2) = (1 - 2\alpha)$$

where c_1 and c_2 are random variables. There are an infinite number of combinations of c_1 and c_2 which will satisfy the equation. It is con-

ventional to select a unique set by the equal tail probability approach; i.e., the probability equation is rewritten as two equations:

$$\Pr\,(M<c_1)=\alpha \qquad \text{and} \qquad \Pr\,(M>c_2)=\alpha$$

This indicates that there is α probability in each tail.

Returning to the original equation, we use the fact that $(x-M)/\sigma$ is normally distributed with zero mean and unit standard deviation. Then

$$\Pr\left(\frac{x-c_1}{\sigma}>\frac{x-M}{\sigma}>\frac{x-c_2}{\sigma}\right)=1-2\alpha$$

which gives

$$\frac{x-c_1}{\sigma}=c_\alpha \qquad \text{and} \qquad \frac{x-c_2}{\sigma}=-c_\alpha$$

with c_α as defined in Table 7.1. Therefore

$$c_1=x-c_\alpha\sigma \qquad \text{and} \qquad c_2=x+c_\alpha\sigma$$

so that the confidence interval is

$$x-c_\alpha\sigma<M<x+c_\alpha\sigma \qquad \text{or} \qquad M=(x\pm c_\alpha\sigma)$$

Question 7.C. This problem is concerned with the power of a statistical test, i.e., with the probability of rejecting the null hypothesis when it is false. The null hypothesis is H_0: $M \leq M_0$. With an α significance level, H_0 is rejected when true with probability α. If c denotes the critical value which, if exceeded by x, results in rejection of H_0,

$$\Pr\,(x>c\,|\,M=M_0)=\alpha$$

Also, at some specified alternative value, M_1, H_0 is rejected with probability $(1-\beta)$. Stated equivalently, accept H_0 with probability β where β is the probability of committing the type II error, i.e., of accepting H_0 when H_1 is true.

This leads to the equation

$$\Pr\,(x>c\mid M=M_1)=(1-\beta)$$

This and the previous equation must be solved simultaneously for c and σ. When we transform to random variables with zero means and unit standard deviations, the equations become

$$\Pr\left(\frac{x-M_0}{\sigma}>\frac{c-M_0}{\sigma}\right)=\alpha \qquad \text{and} \qquad \Pr\left(\frac{x-M_1}{\sigma}>\frac{c-M_1}{\sigma}\right)=(1-\beta)$$

The value of $(1 - \beta)$ will normally exceed 0.50, in which case the right-hand side of the second inequality will be a negative number. This can be written conveniently as $-c_\beta$, which is numerically equal to c_α of Table 7.1 when α is replaced by β. Thus the equations reduce to

$$\frac{c-M_0}{\sigma} = c_\alpha \qquad \text{and} \qquad \frac{c-M_1}{\sigma} = -c_\beta$$

Solving them for c and σ gives

$$\sigma = \frac{M_1-M_0}{c_\alpha+c_\beta} \qquad \text{and} \qquad c = \frac{M_0c_\beta+M_1c_\alpha}{c_\alpha+c_\beta}$$

which are Eqs. 7.1 and 7.2, respectively.

7.2 COMBINATIONS AND SEQUENCES OF MUF'S

7.2.1 Problem and Assumptions

Thus far attention has been restricted to making inferences using a single observed MUF. The resulting information is somewhat limited since the inferences are restricted to one point in space and at one point in time.

In practice, for a given MBA a sequence of MUF's is generated, with the MUF being calculated each time a material balance is closed. Also, at a given point in time or as a sequence over time, MUF's from different MBA's can be summed algebraically to reflect total experience over these MBA's. This section is concerned, in general terms, with making inferences using sequences of MUF's over time or using a single MUF formed by summing MUF's over different MBA's and/or different material balance periods.

In particular, the following problems are considered.

Question 7.D. When individual MUF's are summed, what is the variance of the resulting sum?

Question 7.E. What information can be deduced about errors of measurement and about the behavior of the true MUF's by observing a sequence of MUF's?

Question 7.F. How can a given observed MUF for one time period be used to predict the MUF for the next time period? How can the result be used in constructing a control chart for MUF's?

Question 7.G. With what frequency should material balances be closed to effect the "best" control over SNM?

The assumptions for an individual MUF are the same as those in Sec. 7.1.1. Each observed MUF is regarded as the sum of three components: a beginning inventory, an ending inventory, and a difference between measured inputs to and outputs from the MBA in question. In this section, the error model can be simplified. Each component is assumed to be comprised of three parts: a true value, a systematic error, and a random error. It is further assumed that, for the sequence of MUF's, the systematic-error structure does not change over time throughout the data set and that an equilibrium condition exists in the sense that inventory levels and throughputs per unit time remain reasonably constant. These latter assumptions are somewhat idealistic, but in many instances they may be reasonably valid. In making inferences from sequences of MUF's, we are often more interested in the macrostructure than in the microstructure, and even moderate departures from the assumptions may have little effect on the macrostructure.

7.2.2 Solution

The four questions are considered in turn.

Question 7.D. When individual MUF's are summed, what is the variance of the resulting sum?

Answer 7.D. This question is important because of the interest (1) in calculating an overall MUF either over MBA's (when combining MUF's over different MBA's, we must include shipper–receiver differences) or over material balance periods for a single MBA and (2) in using the methods of Sec. 7.1 to make inferences about the corresponding true MUF. To make the inferences, we must know the variance of the combined MUF. The variance in question cannot be found by summing the variances of the individual MUF's comprising the sum. This is true because the individual MUF's are likely to be correlated for a number of reasons. Rather than attempt to identify and evaluate all the possible correlations, we simply regard all the MBA's as a single master MBA and all the material balance periods as a single period. All movements of material into this master MBA are then regarded as inputs and all movements out as outputs. In calculating the variance of the overall MUF, we are not concerned about movements of material between the individual MBA's within the master MBA. Further, the only inventories affecting the variance in question are the beginning inventory for all MBA's for time period 1 and the corresponding ending inventory for the last time period. The rules of Chap. 6 for finding the variance of an algebraic sum are then applied to these data for the master MBA over the entire material balance

period. Thus no new results beyond those given in Chap. 6 are required to find the solution to this problem.

Question 7.E. What information can we deduce about errors of measurement and about the behavior of the true MUF's by observing a sequence of MUF's?

Answer 7.E. The observed MUF data are of the form $x_1, x_2, \ldots, x_n$, with x_j being the MUF for time period j. Under the assumptions stated in Sec. 7.2.1, each x_j, with mean M_j, has the same random-error variance associated with determining an inventory, σ_η^2, and the same random-error variance associated with the difference (inputs minus outputs), σ_ϵ^2. (Note that the Greek letters are assigned meanings different from those in Chap. 6.) These random-error variances are assigned values by the methods of the previous chapters, taking into account the random errors of measurement due to bulk determination, sampling, and analysis. Let σ_M^2 denote the variance between the true MUF's, i.e., between the M_j values. Let $\sigma_{M_j,M_{j+1}}$ denote the covariance between any two successive true MUF's. (It is common for successive true MUF's to be negatively correlated. This is because hidden inventory items in one period of time can be measured during the next time period. Also, mistakes committed during one time period can be detected and corrected subsequently. It is noted that, if σ_M^2 is zero, so is $\sigma_{M_j,M_{j+1}}$.) Then these parameters can be estimated by

$$\hat{\sigma}_M^2 = \frac{2n(s_{j,j+1} - s_x^2) + (n^2+2)s_x^2}{n(n-2)} - 2\sigma_\eta^2 - \sigma_\epsilon^2 \tag{7.3}$$

$$\hat{\sigma}_{M_j,M_{j+1}} = \frac{s_x^2 + n s_{j,j+1}}{n-2} + \sigma_\eta^2 \tag{7.4}$$

where

$$s_x^2 = \frac{\sum_{j=1}^{n} x_j^2 - \left[\left(\sum_{j=1}^{n} x_j\right)^2 \Big/ n\right]}{n-1} \tag{7.5}$$

[which is the variance of the x_j values (see Eq. 2.61)] and

$$s_{j,j+1} = \sum_{j=1}^{n-1} \frac{x_j x_{j+1}}{n-1} - \frac{\left(\sum_{j=1}^{n} x_j\right)^2}{n^2} \tag{7.6}$$

If the true MUF is assumed constant from one interval to the next (i.e., if $M_j = M$ for all j), then the sequence of MUF data can be used to obtain estimates of σ_η^2 and σ_ϵ^2 which can be compared with estimates derived by the methods of Chap. 6. A significant discrepancy would

indicate that either the values assigned to σ_η^2 and/or σ_ε^2 are incorrect or the assumption of a constant true MUF is invalid. Under the assumption of a constant true MUF, σ_η^2 and σ_ε^2 are estimated by

$$\hat{\sigma}_\eta^2 = \frac{s_x^2 + n s_{j,j+1}}{2-n} \tag{7.7}$$

$$\hat{\sigma}_\epsilon^2 = \frac{(n^2+2)s_x^2 + 2n(n+1)s_{j,j+1}}{n(n-2)} \tag{7.8}$$

Question 7.F. How can a given observed MUF for a given time period be used to predict the MUF for the next time period? How can the result be used in constructing a control chart for MUF's?

Answer 7.F. This question is meaningful because there is a correlation between successive observed MUF's whether the true MUF's are correlated or not and has pertinence if we want to construct a control chart on MUF's (see Sec. 2.8.2.). Because of this correlation, the expected value for a given MUF is not zero. Therefore it is difficult to construct a meaningful standard control chart on MUF's because the mean will shift from one time period to the next as a result of the correlation.

If ρ is the correlation coefficient between x_j and x_{j+1}, then

$$\rho = \frac{\hat{\sigma}_{M_j, M_{j+1}} - \sigma_\eta^2 + \sigma_\delta^2}{\hat{\sigma}_M^2 + 2\sigma_\eta^2 + \sigma_\delta^2 + \sigma_\epsilon^2} \tag{7.9}$$

where, in addition to the quantities already defined, σ_δ^2 is the systematic-error variance of a given difference between inputs and outputs.

For a given value of ρ, the conditional expected value of x_{j+1} is related to the observed value x_j by

$$E(x_{j+1} \mid x_j) = \rho(x_j - M) + M \tag{7.10}$$

In application M can be replaced by its estimate, $(\sum_{j=1}^{n} x_j)/n$. Since the mean of x_{j+1} depends on the value for x_j, the construction of a standard control chart for MUF's clearly leads to difficulties because the center control line is not constant. This problem can be circumvented by plotting $x_{j+1} - E(x_{j+1}|x_j)$ rather than x_{j+1} since this difference statistic will have zero mean. The variance of this difference is given by

$$\sigma_d^2 = \sigma_M^2(1+\rho^2) - 2\rho\sigma_{M_j, M_{j+1}} + 2\sigma_\eta^2(1+\rho+\rho^2) + \sigma_\delta^2(1-\rho)^2 + \sigma_\epsilon^2(1+\rho^2) \tag{7.11}$$

where ρ and M are regarded as known constants.

In application, we can base σ_M^2 and $\sigma_{M_j, M_{j+1}}$ on experience data, using Eqs. 7.3 and 7.4, and assuming that the data were collected over

a period of time during which acceptable control was exerted. Deeming this control acceptable requires making a judgment devoid of statistical considerations. If the degree of control is judged unacceptable, an alternative is to assign values to the parameters on the basis of what is judged to be attainable in an adequate control system.

Once σ_d is calculated, the standard control chart, say at 3σ limits, would have limit lines at $\pm 3\sigma_d$ with a central line at zero.

Question 7.G. With what frequency should material balances be closed?

Answer 7.G. This is related to question 7.D. From point of view of sensitivity of detection of a true MUF over a given interval of time, the frequency of closing material balances within that interval has no effect on the variance of MUF over the entire interval. Thus, over a 1-year period, for example, the variance of the annual MUF is the same whether one physical inventory or twelve inventories are taken.

This is the statistical answer to question 7.G, and it relates only to the error variance of the MUF over the entire interval of time. There is another consideration, however, which enters in. It deals with the timeliness of detection and subsequent correction of a situation that may be producing an unacceptably large MUF. If a material balance is closed only after a lengthy period of operation, it may be too late to take meaningful action. In the same sense, even though measurements made on movements of material within a given MBA in no way affect the size of the variance of the MUF for that MBA, they may be very helpful in isolating the sources creating a MUF. Thus nonstatistical considerations are the ones of greater importance when we are making decisions about how often to close material balances and how many measurement points should exist within an MBA.

7.2.3 Examples

Example 7.F

Monthly MUF data in grams of ^{235}U for a small-scale fuel fabrication facility are reported in Table 7.2.

TABLE 7.2 MONTHLY MUF DATA
(Example 7.F)

Month, j	MUF, x_j	Month, j	MUF, x_j	Month, j	MUF, x_j
1	149	4	178	7	−12
2	162	5	10	8	5
3	11	6	107	9	354

Assuming that the true MUF is the same from month to month, what are the estimates of σ_η^2 and σ_ε^2? These estimates are given by Eqs. 7.7 and 7.8. First s_x^2 and $s_{j,j+1}$ must be calculated from Eqs. 7.5 and 7.6.

From Eq. 7.5,

$$s_x^2 = \frac{(149)^2+(162)^2+\ldots+(354)^2-[(149+162+\ldots+354)^2/9]}{8} = 14{,}254$$

From Eq. 7.6,

$$s_{j,j+1} = \frac{(149)(162)+(162)(11)+\ldots+(5)(354)}{8} - \frac{(149+162+\ldots+354)^2}{81} = -7579$$

Then,

$$\hat{\sigma}_\eta^2 = \frac{(14{,}254)+(9)(-7579)}{-7} = 7708 \quad \text{g}^2 \text{ of } {}^{235}\text{U}$$

$$\hat{\sigma}_\varepsilon^2 = \frac{(83)(14{,}254)+(180)(-7579)}{63} = -2875 \quad \text{g}^2 \text{ of } {}^{235}\text{U}$$

The estimate of σ_ε^2, the variance of a given difference between inputs and outputs, is zero. Clearly a variance cannot be negative, although an estimate of a variance, being a random variable, could be.

One conclusion at this point might be that the measurement random variance of an inventory, σ_η^2, is the dominant contributor to the variance of MUF, with σ_ε^2 close to zero. Another possibility is that the assumption of a constant true MUF is not valid; i.e., there is a true MUF that varies from month to month. Assuming that values are assigned to σ_η^2 and σ_ε^2 based on the methods of Chap. 6, obtain estimates σ_M^2 and $\sigma_{M_j,M_{j+1}}$ from Eqs. 7.3 and 7.4. If σ_η = 40 g of ^{235}U and σ_ε = 20 g of ^{235}U, then,

$$\hat{\sigma}_M^2 = \frac{18(-7579-14{,}254)+83(14{,}254)}{63} - 3200 - 400 = 8941$$

or σ_M = 95 g of ^{235}U, which is the estimate of the standard deviation between true MUF's. Also

$$\hat{\sigma}_{M_j,M_{j+1}} = \frac{14{,}254+9(-7579)}{7} + 1600 = -6108$$

Given these results, what is the estimate of the MUF for the next

month? This is given by Eq. 7.10, with ρ given by Eq. 7.9. Assume that σ_δ = 15 g of ^{235}U. Then

$$\rho = \frac{-6108-1600+225}{8941+3200+225+400} = -0.59$$

The true monthly MUF, M, is estimated by

$$\frac{\sum_{j=1}^{n} x_j}{n} = 107 \quad \text{g of } ^{235}\text{U}$$

Therefore, by application of Eq. 7.10, the expected value for the observed MUF for the next month would be

$$E(x_{10} \mid x_9) = -0.59(354-107)+107 = -39 \quad \text{g of } ^{235}\text{U}$$

A control chart on MUF is calculated to illustrate how it would apply to future observed MUF's, assuming that the data of Table 7.2 were generated during an acceptable period of control. To construct the chart, we calculate σ_d^2 from Eq. 7.11:

$$\sigma_d^2 = (8941)(1.35)+(1.18)(-6108)+(2)(1600)(0.76)$$
$$+(225)(2.53)+(400)(1.35) = 8404 \quad \text{g}^2 \text{ of } ^{235}\text{U}$$

which gives

$$\sigma_d = 92 \quad \text{g of } ^{235}\text{U}$$

The 3σ control limits are then $0 \pm 3\ (92) = 0 \pm 276$ g of ^{235}U. Consider how this would be applied to the last three months' data of Table 7.2. For month 7,

$$E(x_7 \mid x_6) = -0.59(107-107)+107 = 107$$
$$x_7 = -12$$
$$x_7 - E(x_7 \mid x_6) = -12-107 = -119$$

(the plotted point, which lies between -276 and $+276$, and is hence in control).

For month 8,

$$E(x_8 \mid x_7) = -0.59(-12-107)+107 = 177$$
$$x_8 = 5$$
$$x_8 - E(x_8 \mid x_7) = 5-177 = -172$$

(the plotted point, which lies between -276 and $+276$, and is hence in control).

For month 9,

$$E(x_9 \mid x_8) = -0.59(5-107)+107 = 167$$

$$x_9 = 354$$

$$x_9 - E(x_9 \mid x_8) = 354-167 = 187$$

(again in control).

Example 7.G

The monthly MUF data for a diffusion plant, given in Table 2.1, Chap. 2, are analyzed to provide estimates of the parameters. For a diffusion plant the assumption of a constant true MUF from month to month is not valid. Because of condensation of UF_6 in a cold spot in the cascade, for example, a significant portion of an inventory may not be measured in a given month, but it would be in measurable form at the next month's inventory. This is an excellent example of a variance in true MUF from month to month and a corresponding strong negative correlation between successive monthly MUF's.

The problem is to obtain estimates of σ_M^2 and $\sigma_{M_j,M_{j+1}}$. To do this, we must assign values to σ_η and σ_ε. Assume for purposes of this example that $\sigma_\eta = 1000$ units and $\sigma_\varepsilon = 400$ units. Then, to evaluate σ_M^2 and $\sigma_{M_j,M_{j+1}}$, we must calculate s_x^2 and $s_{j,j+1}$ from Eqs. 7.5 and 7.6

$$s_x^2 = \frac{(-358)^2+\ldots+(3618)^2-[(-358+\ldots+3618)^2/144]}{143} = 9{,}422{,}042$$

$$s_{j,j+1} = \frac{(-358)(-3287)+\ldots+(-376)(3618)}{143} - \frac{(-358+\ldots+3618)^2}{(144)^2}$$

$$= -3{,}599{,}163$$

Then, from Eqs. 7.4 and 7.5,

$$\hat{\sigma}_M^2 = \frac{288(-3{,}599{,}163-9{,}422{,}042)+20{,}738(9{,}422{,}042)}{20{,}448} - 2{,}000{,}000-160{,}000$$

$$= 7{,}212{,}271 \qquad \sigma_M = 2686 \quad \text{units}$$

$$\sigma_{M_j,M_{j+1}} = \frac{9{,}422{,}042+144(-3{,}599{,}163)}{142} + 1{,}000{,}000 = -2{,}583{,}503 \quad \text{units}^2$$

To estimate the MUF for the next month, we apply Eq. 7.10. First, replace M by its estimate, the average monthly MUF of 156 units (this

value was found in Sec. 2.1). Assume that σ_δ, the systematic-error standard deviation for a difference between inputs and outputs, is 100 units. Then calculate ρ from Eq. 7.11:

$$\rho = \frac{-2{,}583{,}503 - 1{,}000{,}000 + 10{,}000}{7{,}212{,}271 + 2{,}000{,}000 + 10{,}000 + 160{,}000} = -0.38$$

Then $E(x_{145}|x_{144}) = -0.38(3618 - 156) + 156 = -1160$ units.

A control chart for MUF is calculated assuming that the base data were collected during a state of satisfactory control and that the parameter values assigned to σ_η, σ_ε, and σ_δ are correct. The variance of a plotted difference between an observed MUF and its expected value is σ_d^2; from Eq. 7.11,

$$\sigma_d^2 = (7{,}212{,}271)(1.1444) + (0.76)(-2{,}583{,}503) + (2{,}000{,}000)(0.7644) + (225)(1.9044) + (160{,}000)(1.1444) = 8{,}002{,}593$$

which gives

$$\sigma_d = 2829 \quad \text{units}$$

The appropriate 3σ control lines on the difference statistic are then $\pm$ 8487 units. Apply these limits to the data for year 7 from Table 2.1, Chap. 2. Results are given in Table 7.3.

TABLE 7.3 CONTROL CHART DATA FOR DIFFUSION PLANT MUF (Example 7.G)

Month, $j+1$	x_j	x_{j+1}	$E(x_{j+1} \mid x_j)$*	$x_{j+1} - E(x_{j+1} \mid x_j)$†	Within ±8487?
73	−5,317	−694	2236	−2,930	Yes
74	−694	933	479	454	Yes
75	933	−1,350	−139	−1,211	Yes
76	−1,350	637	728	−91	Yes
77	637	−1,305	−27	−1,278	Yes
78	−1,305	1,318	711	607	Yes
79	1,318	−779	−286	−493	Yes
80	−779	−351	511	−862	Yes
81	−351	2,354	349	2,005	Yes
82	2,354	11,311	−679	11,990	No
83	11,311	−13,775	−4083	−9,692	No
84	−13,775	1,384	5450	−4,066	Yes

* From Eq. 7.10.

† These values would be plotted on the control chart.

7.2.4 Basis

The model forming the basis for the results is written as follows: Let y_{j-1} be the beginning inventory for time period j and y_j be the ending inventory. Let w_j be the difference, inputs minus outputs. Then, the observed MUF, x_j, is

$$x_j = y_{j-1} + w_j - y_j \tag{7.12}$$

Assume that y_j is comprised of a true inventory, μ_j, a systematic measurement error, γ (the same for all j), and a random measurement error, η_j (the Greek letters are assigned meanings different from those in the previous chapters):

$$y_j = \mu_j + \gamma + \eta_j \tag{7.13}$$

Similarly, w_j is written:

$$w_j = \nu_j + \delta + \epsilon_j \tag{7.14}$$

In these models the facts that γ and δ are assumed to be constants for all j imply that the amounts of material in inventory are reasonably constant throughout the total time period involved, as are the amounts of material represented by the differences between inputs and outputs. In an equilibrium environment these are reasonable assumptions.

From Eqs. 7.12 to 7.14,

$$x_j = (\mu_{j-1} - \mu_j) + \nu_j + (\eta_{j-1} - \eta_j) + \delta + \epsilon_j \tag{7.15}$$

Each error random variable is assumed to have zero mean. The variance of δ is denoted by σ_δ^2, the variance by η_j by σ_η^2 for all j, and the variance of ϵ_j by σ_ϵ^2 for all j. Note that x_j does not involve γ, the bias in estimating an inventory.

For this model the expected value of x_j is

$$E(x_j) = (\mu_{j-1} - \mu_j) + \nu_j = M_j \tag{7.16}$$

and the expected value of the mean, $\bar{x}$, is

$$E(\bar{x}) = \frac{\mu_0 - \mu_n}{n} + \bar{\nu} \tag{7.17}$$

where ν is the average difference between inputs and outputs over the n time periods. If the true inventory at the beginning of the sequence,

μ_0, is equal to that at the end of the sequence μ_n, the average of the observed MUF's is simply the average value of the inputs minus the outputs for a unit time period. Since μ_0 and μ_n will be nearly equal in an equilibrium operating situation, a situation assumed to exist, it is reasonable to regard $\bar{x}$ as an estimate of the average true difference between inputs and outputs for a given unit time period. In any event, $\bar{x}$ approaches $\bar{v}$ as n gets large, regardless of the size of the difference, $\mu_0 - \mu_n$.

Next, consider the sample variance, s_x^2, defined by Eq. 2.61. The expected value of s^2 is found by application of Eq. 4.2. The derivation is simpler if s^2 is written in an equivalent form.

$$s_x^2 = \frac{(n-1)\sum_j x_j^2 - 2\sum_{j<k} x_j x_k}{n(n-1)} \tag{7.18}$$

where there are n terms in the first sum and $n(n-1)/2$ terms in the second. To find $E(s_x^2)$, we must evaluate $E(x_j^2)$. First, from Eqs. 7.15 and 7.16,

$$E(x_j^2) = E(M_j^2) + 2\sigma_\eta^2 + \sigma_\delta^2 + \sigma_\epsilon^2 \tag{7.19}$$

Also,

$$\begin{aligned} E(x_j x_k) &= E(M_j M_k) - \sigma_\eta^2 + \sigma_\delta^2 \qquad (k = j+1) \\ &= E(M_j M_k) + \sigma_\delta^2 \qquad (k > j+1) \end{aligned} \tag{7.20}$$

The expected value of s_x^2 in Eq. 7.18 is found in Eqs. 7.19 and 7.20:

$$\begin{aligned} E(s_x^2) &= E\left(\frac{\sum M_j^2}{n}\right) + 2\sigma_\eta^2 + \sigma_\delta^2 + \sigma_\epsilon^2 - 2E\left[\sum_{j<k} \frac{M_j M_k}{n(n-1)}\right] + \frac{2\sigma_\eta^2}{n} - \sigma_\delta^2 \\ &= \sigma_M^2 + 2\sigma_\eta^2\left(1 + \frac{1}{n}\right) + \sigma_\epsilon^2 - \frac{2\sigma_{M_j, M_{j+1}}}{n} \end{aligned} \tag{7.21}$$

where σ_M^2 denotes the variance among the true MUF's, and $\sigma_{M_j, M_{j+1}}$ is the covariance between successive true MUF's.

Next consider the sample covariance between successive MUF's, denoted by $s_{j,j+1}$. This is defined as follows in this application:

$$s_{j,j+1} = \sum_{j=1}^{n-1} \frac{x_j x_{j+1}}{n-1} - \frac{\left(\sum_{j=1}^{n} x_j\right)^2}{n^2} \tag{7.22}$$

This can also be written

$$s_{j,j+1}=\frac{(n^2-2n+2)\sum_{j=1}^{n-1}x_jx_{j+1}}{n^2(n-1)}-\frac{\sum_{j=1}^{n}x_j^2}{n^2}-\frac{2\sum_{j=1}^{n-2}\sum_{k=j+2}^{n}x_jx_k}{n^2} \tag{7.23}$$

where there are $[(n-1)(n-2)]/2$ terms in the double summation. Using Eqs. 7.19 and 7.20, we find the expected value of $s_{j,j+1}$.

$E(s_{j,j+1})$ reduces to

$$E(s_{j,j+1})=\frac{(n^2-2n+2)\sigma_{M_jM_{j+1}}}{n^2}-\frac{(n^2+2)}{n^2}\sigma_\eta^2-\frac{\sigma_\epsilon^2}{n}-\frac{\sigma_M^2}{n} \tag{7.24}$$

Equations 7.21 and 7.24 are solved simultaneously for $\sigma_M{}^2$ and $\sigma_{M_j,M_{j+1}}$ to give Eqs. 7.3 and 7.4.

Now, assume that the true MUF is constant for all time periods, so that $M_j = M$ for all j. Then σ_M and $\sigma_{M_j,M_{j+1}}$ are both zero, and Eqs. 7.21 and 7.24 can be solved simultaneously for $\sigma_\eta{}^2$ and $\sigma_\epsilon{}^2$ to give their estimates based on the experience MUF data.

Solving

$$s_x^2=2\sigma_\eta^2\left(1+\frac{1}{n}\right)+\sigma_\epsilon^2$$

and

$$s_{j,j+1}=-\frac{(n^2+2)\sigma_\eta^2}{n^2}-\frac{\sigma_\epsilon^2}{n}$$

gives the solutions

$$\sigma_\eta^2=\frac{s_x^2+ns_{j,j+1}}{2-n} \tag{7.25}$$

$$\hat{\sigma}_\epsilon^2=\frac{(n^2+2)s_x^2+2n(n+1)s_{j,j+1}}{n(n-2)} \tag{7.26}$$

where the carets (^) denote that these are estimated quantities. These are Eqs. 7.7 and 7.8.

Next, consider the basis for ρ in Eq. 7.9. The correlation coefficient between two random variables is defined by Eq. 2.55 to be the ratio of their covariance and the product of their standard deviations. In this instance, since both the random variables x_j and x_{j+1} have the same standard deviation, the denominator is simply the variance of x_j. This is given by Eq. 7.19. Also, the covariance between x_j and x_{j+1} is given

by Eq. 7.20, and ρ in Eq. 7.9 follows immediately. Equation 7.10 is a direct consequence of the relation between the means of two random variables with a correlation coefficient ρ.

Finally, the variance of $[x_{j+1} - E(x_{j+1}|x_j)]$ is found. This reduces to finding the variance of $(x_{j+1} - \rho x_j)$ if ρ and M can be regarded as known constants. Write, from Eqs. 7.15 and 7.16,

$$x_{j+1}-\rho x_j=(M_{j+1}-\rho M_j)+(\eta_j-\eta_{j+1}-\rho\eta_{j-1}+\rho\eta_j)+(\delta-\rho\delta)+(\epsilon_{j+1}-\rho\epsilon_j) \tag{7.27}$$

and the variance, σ_d^2, follows immediately by application of Eq. 4.3:

$$\sigma_d^2=\sigma_M^2(1+\rho^2)-2\rho\sigma_{M_j,M_{j+1}}+\sigma_\eta^2[(1+\rho)^2+1+\rho^2]+\sigma_\delta^2(1-\rho)^2+\sigma_\epsilon^2(1+\rho^2) \tag{7.28}$$

which is formula 7.11.

7.3 THE MINIMUM VARIANCE MUF

7.3.1 Problem and Assumptions

As shown in the previous section, for a given material balance period, the uncertainty in MUF is directly affected by the uncertainties in the measured beginning and ending inventories. Inventories are very difficult to measure, especially in some types of facilities. When this is true and when, in addition, the uncertainty in the inventory is a major contributor to the uncertainty in MUF, it may be enlightening to complement the traditional MUF with another MUF-like statistic. This statistic replaces the measured beginning inventory by a weighted average of previously measured inventories plus totaled inputs to and outputs from the MBA in question. (This idea, originally suggested by C. A. Bennett several years ago, was thoroughly developed by K. B. Stewart in a series of papers on the subject. His results have been extended to include the possibility of nonzero true MUF's and of a nonzero systematic-error variance. To my knowledge there has been little application of the method in practice, and its practicality has not been demonstrated for routine use.)

The problem is stated specifically as follows: Given a series of measured inventories plus inputs and outputs, how can these data be combined to provide the estimate of the inventory having minimum variance, and how can this estimate be used to estimate the MUF? This problem is solved by use of the model given in Sec. 7.2.

7.3.2 Solution

The notation is the same as in Sec. 7.2.4; i.e., y_{j-1} is the measured beginning inventory for time period j, y_j is the ending inventory, and w_j is the difference (inputs minus outputs). Let I_j be the minimum variance estimate of the ending inventory for time period j. Then I_j is given by the recursion formula:

$$I_j = P_{j-1}y_j + (1-P_{j-1})(I_{j-1}+w_j) \tag{7.29}$$

with $I_o = y_o$, where

$$P_{j-1} = \left(1+\frac{1}{p_{j-2}+c}\right)^{-1} \qquad \begin{pmatrix} j=1, 2, 3, \ldots \\ p_{-1}=1 \end{pmatrix} \tag{7.30}$$

where the limiting value of P_{j-1} as $j \to \infty$ is $[-c+\sqrt{(c+2)^2-4}]/2$ and where

$$c = \frac{\sigma_\epsilon^2}{\sigma_\eta^2} \tag{7.31}$$

Application of the results requires a knowledge of c, which would be an estimate based on past data. A perfect knowledge is not necessary.

The random-error variance of I_j, denoted by V_j, is

$$V_j = p_{j-1}\sigma_\eta^2 \tag{7.32}$$

The minimum variance MUF for period j, denoted by x'_j, is defined as in Eq. 7.12, except that the beginning inventory, y_{j-1}, is replaced by I_{j-1}.

$$x'_j = I_{j-1} + w_j - y_j \tag{7.33}$$

The random-error variance of x'_j is

$$V_r(x'_j) = \sigma_\eta^2(1+p_{j-2}) + \sigma_\epsilon^2 \tag{7.34}$$

The systematic variance of x'_j is given by the recursion formula:

$$V_s(x'_j) = L_j^2\sigma_\delta^2$$

where

$$L_j = 1+(1-p_{j-2})L_{j-1}$$

In addition to having minimum variance, x'_j has another property of some interest and practical importance. As shown earlier in Eq. 7.20,

when all true MUF's are constant, the covariance between two successive MUF's is $(-\sigma_\eta^2 + \sigma_\delta^2)$, where σ_η^2 is the random-error variance for a given inventory and σ_δ^2 is the systematic-error variance for a given difference (input minus output). When σ_δ^2 is assumed to be zero or, more realistically, to be small relative to σ_η^2, this covariance is given by $-\sigma_\eta^2$. For the minimum variance MUF, x'_j, the covariance in question is zero when σ_δ^2, the systematic-error variance, is zero. Thus successive minimum variance MUF's have more meaning when viewed individually under these assumptions since each such MUF is statistically independent of the preceding and succeeding MUF's. For nonzero σ_δ^2 the covariance between x_j and x_{j+1} is given by $L_j L_{j+1} \sigma_\delta^2$.

When the true MUF for each time period is zero, x'_j has an expected value of zero. Suppose, however, that the true MUF for period j is M_j. Then the minimum variance MUF, x'_j, has an expected value given by the recursion formula:

$$E(x'_j) = M_j + (1 - p_{j-2})E(x'_{j-1}) \tag{7.36}$$

The covariance between successive MUF's then becomes

$$\operatorname{cov}(x'_j, x'_{j+1}) = \sigma_{M_j, M_{j+1}} + L_j L_{j+1} \sigma_\delta^2 \tag{7.37}$$

7.3.3 Examples

Example 7.H

Given the data in arbitrary units for 10 months of operation, find the minimum variance MUF's and their random-error variances when $\sigma_\varepsilon^2 = 0.10$ and $\sigma_\eta^2 = 1.0$. Compare these results with the MUF's calculated by Eq. 7.12. Data are given in Table 7.4.

TABLE 7.4 DATA FOR EXAMPLE 7 H

Month, j	Beginning inventory, y_{j-1}	Inputs − Outputs, x_j	Ending inventory, y_j
1	20 51	−0 02	19 85
2	19 85	0 11	20 88
3	20 88	−0 44	20 16
4	20 16	0 02	19.41
5	19 41	−0.18	18 87
6	18 87	−0 10	17 96
7	17 96	−0 28	19 78
8	19 78	0 51	19 54
9	19 54	−0 10	20 49
10	20 49	−0.30	19 03

The standard MUF's are computed first by use of Eq. 7.12:

$$x_1 = 20.51 + (-0.02) - 19.85 = 0.64$$
$$x_2 = 19.85 + (0.11) - 20.88 = -0.92$$
$$x_3 = 20.88 + (-0.44) - 20.16 = 0.28$$
$$x_4 = 0.77$$
$$x_5 = 0.36$$
$$x_6 = 0.81$$
$$x_7 = -2.00$$
$$x_8 = 0.75$$
$$x_9 = -1.05$$
$$x_{10} = 1.16$$

For a constant true MUF, each MUF has a random-error variance of $(\sigma_\varepsilon^2 + 2\sigma_\eta^2) = 0.10 + 2.00 = 2.10$ and a standard deviation of $\sqrt{2.10} = 1.45$ units. Because σ_η^2 is large relative to σ_ε^2, there is a large negative correlation between successive MUF's. These are plotted in Fig. 7.1.

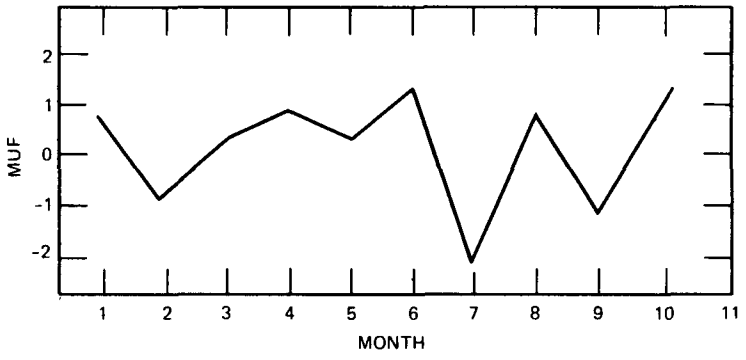

FIGURE 7.1 Plot of standard MUF data.

The tendency toward nonrandomness is apparent in the figure, especially for the last few months. This pattern is caused by the negative covariance, $-\sigma_\eta^2$, between successive observed MUF's (this assumes that $\sigma_\delta^2 = 0$).

Next, consider the minimum variance estimates of each month's ending inventory and the minimum variance MUF's. We must calculate the p values from Eq. 7.30 recognizing that c in Eq. 7.31 is 0.10/1.0 or 0.1:

$$p_0 = \frac{1}{1+[1/(1+0.1)]} = 0.5238$$

$$p_1 = \frac{1}{1+[1/(0.5238+0.1)]} = 0.3842$$

$$p_2 = \frac{1}{1+[1/(0.3842+0.1)]} = 0.3262$$

$$p_3 = 0.2988$$

$$p_4 = 0.2851$$

$$p_5 = 0.2780$$

$$p_6 = 0.2743$$

$$p_7 = 0.2724$$

$$p_8 = 0.2713$$

$$p_9 = 0.2708$$

The inventory estimates, I_j, are then given by Eq. 7.29:

$$I_0 = 20.51$$

$$I_1 = (0.5238)(19.85) + (0.4762)(20.51 - 0.02) = 20.15$$

$$I_2 = (0.3842)(20.88) + (0.6158)(20.15 + 0.11) = 20.50$$

$$I_3 = (0.3262)(20.16) + (0.6738)(20.50 - 0.44) = 20.09$$

$$I_4 = 19.90$$

$$I_5 = 19.48$$

$$I_6 = 18.98$$

$$I_7 = 19.00$$

$$I_8 = 19.52$$

$$I_9 = 19.26$$

Then, from Eq. 7.33, the minimum variance MUF's are:

$$x'_1 = 20.51 - 0.02 - 19.85 = 0.64$$

$$x'_2 = 20.15 + 0.11 - 20.88 = -0.62$$

$$x'_3 = 20.50 - 0.44 - 20.16 = -0.10$$

$$x'_4 = 20.09 + 0.02 - 19.41 = 0.70$$

$$x'_5 = 0.85$$

$$x'_6 = 1.42$$

$$x'_7 = -1.08$$
$$x'_8 = -0.03$$
$$x'_9 = -1.07$$
$$x'_{10} = -0.07$$

These have random-error variances and standard deviations as follows (from Eq. 7.34):

$$V_r(x'_1) = 1.0(1+1)+0.1 = 2.10 \qquad \sigma_{x'_1} = 1.449$$
$$V_r(x'_2) = 1.0(1+0.5238)+0.1 = 1.6238 \qquad \sigma_{x'_2} = 1.274$$
$$V_r(x'_3) = 1.0(1+0.3842)+0.1 = 1.4842 \qquad \sigma_{x'_3} = 1.218$$
$$V_r(x'_4) = 1.0(1+0.3262)+0.1 = 1.4262 \qquad \sigma_{x'_4} = 1.194$$
$$\vdots \qquad\qquad \vdots$$
$$V_r(x'_{10}) = 1.0(1+0.2713)+0.1 = 1.3713^* \qquad \sigma_{x'_{10}} = 1.171$$

By comparison, the standard MUF has a standard deviation of 1.449 units. Thus, under the conditions of this example, the minimum variance MUF is more sensitive to detecting real losses.

Example 7.I

Assume that the true MUF's for $n = 4$ time periods are all $M = 1$ unit. Further assume that $\sigma_\delta^2 = 0.10$, $\sigma_\varepsilon^2 = 0.10$, and $\sigma_\eta^2 = 1.0$. Compare the standard MUF, x_j, with the minimum variance MUF, x'_j.

First, consider the standard MUF, which has a mean of 1 unit and a variance of $\text{var}(x_j) = 2\sigma_\eta^2 + \sigma_\delta^2 + \sigma_\varepsilon^2 = 2.20$, or a standard deviation of 1.48 units. The minimum variance MUF, x'_j has a mean value given by Eqs. 7.36, 7.30, and 7.31. By use of the recursion formulas,

$$E(x'_1) = M_1 = 1.0$$
$$E(x'_2) = M_2 + (1-p_0)(1.0) = 1.0 + (0.4762)(1.0) = 1.4762\dagger$$
$$E(x'_3) = M_3 + (1-p_1)(1.4762) = 1.0 + (0.6158)(1.4762) = 1.9090$$
$$E(x'_4) = M_4 + (1-p_2)(1.9090) = 1.0 + (0.6738)(1.9090) = 2.2863 \quad \text{units}$$

The variance of x'_4 is given by Eqs. 7.34 and 7.35. First, consider the random-error variance:

$$V_r(x'_4) = 1.0(1+0.3262)+0.10 = 1.4262$$

---

* The limiting value of p_{j-1} as $j \to \infty$ is $[-0.1 + \sqrt{(2.1)^2 - 4}]/2 = 0.270$, which yields a limiting variance of 1.370.

† p_0, p_1, etc., are taken from example 7.H since c has the same value in both examples.

The systematic variance must be calculated recursively. From Eq. 7.35,

$$L_1 = 1 \rightarrow V_s(x'_1) = (1)^2(0.10) = 0.10$$

$$L_2 = 1 + 0.4762 = 1.4762 \rightarrow V_s(x'_2) = (1.4762)^2(0.10) = 0.218$$

$$L_3 = 1 + (0.6158)(1.4762) = 1.9090 \rightarrow V_s(x'_3) = (1.9090)^2(0.10) = 0.364$$

$$L_4 = 1 + (0.6738)(1.9090) = 2.2863 \rightarrow V_s(x'_4) = (2.2863)^2(0.10) = 0.523$$

Therefore the total variance of x'_4 is (1.4262 + 0.523) = 1.949, which gives a standard deviation of 1.40 units.

To recapitulate, for this example:

Standard MUF has a mean of 1.2 units and a standard deviation of 1.48 units.

Minimum variance MUF has a mean of 2.74 units and a standard deviation of 1.40 units.

It is apparent that, for this particular set of data, the minimum variance MUF is much more sensitive in detecting the true unaccounted for material, since it has a much larger mean value and a smaller standard deviation. Lest the wrong impression is left, however, we should note that, if the standard MUF were accumulated in this example, its mean would be 4 (1.0), or 4.0 units, and its standard deviation would be $\sqrt{2\sigma_\eta^2 + 4\sigma_\varepsilon^2 + 16\sigma_\delta^2} = 2.00$ units, which compares very favorably with the results for the minimum variance MUF.

Example 7.J

Consider the diffusion plant data of example 7.G. For these data, and assuming the true MUF's were constant, c of Eq. 7.31 is

$$c = \frac{2{,}205{,}265}{3{,}583{,}503} = 0.615$$

The minimum variance MUF has a random-error variance given by Eq. 7.34. This requires determination of p_{n-2} for month n. The limiting value of p_{n-2} as n approaches infinity is

$$\frac{-c + \sqrt{(c+2)^2 - 4}}{2} = \frac{-0.615 + \sqrt{2.8382}}{2} = 0.535$$

(see definition following Eq. 7.30).

Thus, by Eq. 7.34, the random-error variance of the minimum variance MUF is

$$V_r(x'_j) = 3{,}583{,}503(1.535) + 2{,}205{,}265 = 7{,}705{,}942 \text{ units}^2$$

which gives a standard deviation of 2776 units, as compared with the 3061 units found for the standard MUF. Although this reduction is not large, in this application the real benefit comes from the fact that successive MUF's are now uncorrelated and a control chart can be easily constructed. (This assumes that σ_S^2, the systematic-error variance of a given inputs-minus-outputs value is negligibly small and that successive true MUF's are uncorrelated.) For such a chart the mean is 156 units for all months and the limits are of the form $\pm k\,(2776)$.

7.3.4 Basis

The results of Sec. 7.3 are derived by use of the model of Sec. 7.2, and specifically Eqs. 7.13 and 7.14.

The basic idea behind the minimum variance inventory and minimum variance MUF is that under certain conditions each ending inventory can be estimated from some previous ending inventory plus additions to and removals from the process since that date. For example, at some starting point, with y_0 designating beginning inventory, with a series of inventory estimates $(y_1, y_2, \ldots, y_n)$, and with a series of inputs minus outputs $(w_1\ w_2, \ldots, w_n)$, we can define a corresponding series of z's:

$$\begin{aligned} z_n &= y_n \\ z_{n-1} &= y_{n-1} + w_n \\ z_{n-2} &= y_{n-2} + w_{n-1} + w_n \\ &\cdots \\ z_0 &= y_0 + w_1 + w_2 + \cdots + w_n \end{aligned} \tag{7.38}$$

If the process is stable, with no true MUF's and with negligible biases, each z_j is an estimate of the ending inventory for time period n. Calling this I_n, we can write

$$I_n = \sum_{j=0}^{n} \alpha_j z_j \tag{7.39}$$

where the α_j's sum to 1 and are chosen to minimize the random variance of I_n.

It is convenient to develop the formula for I_n with a recursion relation since the α_j's clearly depend on how many terms are included in the sum. Consider the data for the initial few periods of operation:

Beginning inventory

$$z_{00}=y_0$$

Period 1

$$z_{10}=y_0+w_1$$

$$z_{11}=y_1$$

Period 2

$$z_{20}=y_0+w_1+w_2 \tag{7.40}$$

$$z_{21}=y_1+w_2$$

$$z_{22}=y_2$$

At the end of period 1, there are two estimates of the ending inventory, z_{10} and z_{11}. A weighted average to give I_1 can be written:

$$I_1=p_0z_{11}+(1-p_0)z_{10}=p_0y_1+(1-p_0)(y_0+w_1) \tag{7.41}$$

where p_0 is chosen to minimize the random-error variance of I_1, designated by V_1. From Eqs. 7.13 and 7.14, and including only the random-error variances,

$$V_1=p_0^2\sigma_\eta^2+(1-p_0)^2(\sigma_\eta^2+\sigma_\epsilon^2) \tag{7.42}$$

Let

$$c=\frac{\sigma_\epsilon^2}{\sigma_\eta^2} \tag{7.43}$$

Then

$$V_1=\sigma_\eta^2[p_0^2+(1-p_0)^2(1+c)] \tag{7.44}$$

We can minimize V_1 with respect to p_0 by equating the partial derivative of V_1 with respect to p_0 to zero and solving for p_0:

$$p_0=\frac{1+c}{2+c}=\frac{1}{1+[1/(1+c)]} \tag{7.45}$$

For this value of p_0, V_1 is found to be

$$V_1=\sigma_\eta^2\left[\frac{(1+c)^2}{(2+c)^2}+\frac{1}{(2+c)^2}(1+c)\right]=\frac{(1+c)}{(2+c)}\sigma_\eta^2=p_0\sigma_\eta^2 \tag{7.46}$$

Equations 7.41, 7.45, and 7.46 form the bases for Eqs. 7.29, 7.30, and 7.32, respectively, for $n = 1$.

Having demonstrated that Eq. 7.29 holds for $n = 1$, we will prove by induction that this equation holds for any value of n. Proof by induction requires demonstrating that, if some statement holds for n, it also holds for $n + 1$. Since Eq. 7.29 is known to hold for $n = 1$, once we demonstrate that it holds for $n + 1$, it will then follow that it holds for $n = 2$, $n = 3$, etc. (i.e., for any n).

Thus in the inductive proof assume that

$$I_n = p_{n-1} y_n + (1 - p_{n-1})(I_{n-1} + w_n) \tag{7.47}$$

where

$$p_{n-1} = \frac{1}{1 + [1/(p_{n-2} + c)]} \tag{7.48}$$

with

$$c = \frac{\sigma_\epsilon^2}{\sigma_\eta^2} \tag{7.49}$$

and the random variance of I_n, V_n, is given by

$$V_n = p_{n-1} \sigma_\eta^2 \tag{7.50}$$

Given these results, we are then required to show that

$$I_{n+1} = p_n y_{n+1} + (1 - p_n)(I_n + w_{n+1}) \tag{7.51}$$

where

$$p_n = \frac{1}{1 + [1/(p_{n-1} + c)]} \tag{7.52}$$

Proof: Assume that I_{n+1} is in the form of Eq. 7.51 and prove that the solution for p_n is given by Eq. 7.52:

$$I_{n+1} = p_n y_{n+1} + (1 - p_n)[p_{n-1} y_n + (1 - p_{n-1})(I_{n-1} + w_n) + w_{n+1}]$$

The random-error variance of I_{n+1} is given by

$$\begin{aligned} V_{n+1} = {} & p_n^2 \sigma_\eta^2 + p_{n-1}^2 (1 - p_n)^2 \sigma_\eta^2 + (1 - p_{n-1})^2 p_{n-2} (1 - p_n)^2 \sigma_\eta^2 \\ & + (1 - p_n)^2 (1 - p_{n-1})^2 c \sigma_\eta^2 + (1 - p_n)^2 c \sigma_\eta^2 \end{aligned}$$

Then, equating $(\partial V_{n+1} / \partial p_n)$ to zero, using the fact (from Eq. 7.48) that

$$p_{n-2} = \frac{p_{n-1}(c + 1) - c}{(1 - p_{n-1})} \tag{7.53}$$

and solving for p_n yields

$$\frac{\partial V_{n+1}}{\partial p_n} = \sigma_\eta^2\{2p_n - 2(1-p_n)[p_{n-1}^2 + (1-p_{n-1})(cp_{n-1}+p_{n-1}-c) + c(1-p_{n-1})^2 + c]\} = 0$$

or

$$p_n - (1-p_n)(p_{n-1}+c) = 0$$

from which

$$p_n = \frac{p_{n-1}+c}{p_{n-1}+c+1} = \frac{1}{1+[1/(p_{n-1}+c)]} \tag{7.54}$$

which is identical to Eq. 7.52 and completes the proof.

Also, it was asserted that, when $\sigma_\delta^2 = 0$ and $M_j = M$ for all j, then x'_n and x'_{n+1} have zero covariance. This is proved as follows:

$$\begin{aligned} x'_n &= I_{n-1} + w_n - y_n \\ x'_{n+1} &= I_n + w_{n+1} - y_{n+1} \\ &= p_{n-1}y_n + (1-p_{n-1})(I_{n-1}+w_n) + w_{n+1} - y_{n+1} \end{aligned}$$

The covariance is

$$\begin{aligned} \operatorname{cov}(x'_n, x'_{n+1}) &= (1-p_{n-1})V_{n-1} + (1-p_{n-1})\operatorname{var}(w_n) - p_{n-1}\operatorname{var}(y_n) \\ &= \sigma_\eta^2[(1-p_{n-1})p_{n-2} + c(1-p_{n-1}) - p_{n-1}] \end{aligned}$$

But

$$p_{n-1} = \frac{p_{n-2}+c}{p_{n-2}+c+1} \tag{7.55}$$

Therefore

$$\operatorname{cov}(x'_n, x'_{n+1}) = \frac{p_{n-2}+c-p_{n-2}-c}{p_{n-2}+c+1} = 0$$

which completes the proof.

Finally, consider the effect on I_n and x'_n when the assumption of a stable process is not valid. Specifically, suppose that the true MUF for period j is not zero and that σ_δ^2 and σ_γ^2, the systematic-error variances, are not zero. Then, consider the ending inventory estimates,

$$I_1 = p_0 y_1 + (1-p_0)(y_0 + w_1)$$

$$I_2 = p_1 y_2 + (1-p_1)[p_0 y_1 + (1-p_0)(y_0 + w_1) + w_2]$$

$$I_3 = p_2 y_3 + (1-p_2)\{p_1 y_2 + (1-p_1)[p_0 y_1 + (1-p_0)(y_0 + w_1) + w_2] + w_3\}$$

etc.

The corresponding minimum variance MUF's are

$$x'_1 = y_0 + w_1 - y_1 \qquad x'_3 = I_2 + w_3 - y_3$$

$$x'_2 = I_1 + w_2 - y_2 \qquad x'_4 = I_3 + w_4 - y_4$$

etc.

Then, from Eqs. 7.13 and 7.14, with the error random variables all having zero means, the expected value of x'_j is

$$E(x'_1) = (\mu_0 + \nu_1 - \mu_1) = M_1$$

To find $E(x'_2)$, write

$$\begin{aligned} x'_2 &= p_0 y_1 + (1-p_0)(y_0 + w_1) + w_2 - y_2 \\ &= p_0 y_1 + (1-p_0)(x'_1 + y_1) + w_2 - y_2 \end{aligned}$$

Then,

$$\begin{aligned} E(x'_2) &= p_0 \mu_1 + (1-p_0)(M_1 + \mu_1) + \nu_2 - \mu_2 \\ &= M_2 + (1-p_0)M_1 = M_2 + (1-p_0)E(x'_1) \end{aligned}$$

Similarly,

$$E(x'_3) = M_3 + (1-p_1)E(x'_2)$$

Clearly, for general n,

$$E(x'_n) = M_n + (1-p_{n-2})E(x'_{n-1}) \tag{7.56}$$

which is Eq. 7.36.

By comparison with the standard MUF (which has expected value M_n), note that, when there are nonzero true MUF's the x'_j estimate of the MUF has an expected value that moves further and further from zero. This is not necessarily a poor characteristic since we would like to detect such conditions.

Even though $E(x'_n)$ may deviate from zero by a value greater than $E(x_n)$, however, its variance is also larger. From Eq. 7.50, its random-error variance is

$$V_r(x'_n) = p_{n-2}\sigma_\eta^2 + \sigma_\epsilon^2 + \sigma_\eta^2 = \sigma_\epsilon^2 + \sigma_\eta^2(1 + p_{n-2}) \tag{7.57}$$

This is Eq. 7.34.

The systematic variance, $V_s(x'_n)$, is expressed by the recursion formula:

$$V_s(x'_n) = L_n^2 \sigma_\delta^2$$

where

$$L_n = 1 + (1 - p_{n-2}) L_{n-1} \tag{7.58}$$

This follows when we note that, retaining only the nonrandom-error terms, we can write x'_1, x'_2, etc., as follows:

$$x'_1 = M_1 + \delta$$
$$x'_2 = M_2 + \delta[(1 - p_0) + 1]$$
$$x'_3 = M_3 + \delta[(1 - p_1)(1 - p_0) + (1 - p_1) + 1]$$
$$x'_4 = M_4 + \delta[(1 - p_2)(1 - p_1)(1 - p_0) + (1 - p_2)(1 - p_1) + (1 - p_2) + 1]$$
$$\cdot$$
$$\cdot$$
$$\cdot$$

or
$$x'_1 = M_1 + L_1\delta$$
$$x'_2 = M_2 + [(1 - p_0)L_1 + 1]\delta = M_2 + L_2\delta$$
$$x'_3 = M_3 + [(1 - p_1)L_2 + 1]\delta = M_3 + L_3\delta$$
$$x'_4 = M_4 + [(1 - p_2)L_3 + 1]\delta = M_4 + L_4\delta$$
$$\cdot$$
$$\cdot$$
$$\cdot$$

Further, the covariance between x'_n and x'_{n+1} is easily seen to be

$$\text{cov}(x'_n, x'_{n+1}) = \sigma_{M_n, M_{n+1}} + L_n L_{n+1} \sigma_\delta^2 \tag{7.59}$$

which is zero only if the covariance between successive true MUF's is zero and if σ_δ^2 is zero.

7.4 MATERIAL BALANCE CLOSINGS

7.4.1 Problem and Assumptions

Thus far in the discussion of MUF's an essential requirement has been that the applicable time period over which the MUF is calculated be closed on both ends by physical inventories. Conceptually this is a necessary requirement since it can be argued that, without taking

a physical inventory, we cannot know the amount of material in inventory. However, situations exist in which the need for a complete physical inventory in the traditional sense may be mitigated.

Consider the situation in which items are measured as they are placed in inventory. This occurs in a fuel fabrication facility, for example. The entire inventory of the plant, of course, does not consist of such measured quantities, because of hidden inventories, such as hood hold-ups. Whenever a physical inventory is taken, it is the practice to containerize and measure as much of the hidden inventory as possible, with production necessarily being interrupted in the process.

Suppose, now, that hidden inventories represent a relatively small part of the total inventory and suppose that it has been verified that the items as measured and placed in inventory were accounted for on a piece-count basis and their contents have not been disturbed (this can be verified through the use of tamper-indicating seals). Verifications can be made on a spot-check basis when inventory listings are produced on the basis of floor transactions. Spot checks can be made on randomly selected portions of the inventory occasionally to assure that the inventory listings are valid. (The need for timeliness in this instance would probably require a computerized accounting system, except in very small facilities.) Under these conditions it may be technically feasible to effect control over the material by closing the material balance on the basis of measured additions to the process, measured removals from the process, and measured items in inventory, where this last information is derived from the floor-transaction data.

The resulting MUF-like quantity is not MUF in the accepted sense of the term since it includes hidden unmeasured inventories to a larger extent than does the MUF calculated as the result of a physical inventory. With relatively small hidden inventories, however, it can provide assurance that gross unaccounted-for losses are not occurring. Such a material balance closing could be effected frequently, and the build-up of this MUF-like quantity could be evaluated against the combination of known measurement errors plus reasonable expected accumulations of hidden inventories. With proper guidelines it could be used to trigger the need for a partial or a complete physical inventory.

In this section we consider the problem of how to judge objectively whether a given material balance closing indicates a satisfactory state of control.

7.4.2 Solution

For time period j the MUF-like quantity referred to in the previous discussion is designated x_j^*, which is identical with the

traditional MUF, x_j, only if there are no known hidden inventories involved. Otherwise, x_j^* is the sum of x_j and these hidden inventories.

By way of clarification, a hidden inventory item is an unmeasured inventory item, not one whose presence is unknown or undetected. In a chemical reprocessing facility, for example, it is known that at any point in time the various vessels and pipes contain material and are part of the inventory. Unless they are measured, they are a part of the hidden inventory. Since such material collectively represents a major part of the inventory in a chemical reprocessing facility, the concept under discussion in this section does not appear to be applicable to this type of facility.

A reasonable decision is to trigger action when x_j^* exceeds some critical quantity. The action could range from cleanout of the suspect hood and recomputation of x_j^* after including the contents as part of the measured inventory to a complete physical inventory. The specific action to take would depend on the circumstances of the given situation; e.g., a gradual buildup in x_j^* over successive balance periods would tend to indicate the need for a complete inventory, whereas a sudden blip, traceable to a given step of the process, might call at least for a hood cleanout as the initial course of action.

Let the critical quantity be c_j^* such that, when x_j^* exceeds c_j^*, some (unspecified) action is taken. It is reasonable to write c_j^* in the form

$$c_j^* = A_j + c_\alpha(\sigma_{1_j}^2 + \sigma_{2_j}^2)^{1/2} \tag{7.60}$$

where A_j = an assigned constant, dependent on total throughput through the various stages and representative of the material expected to become hidden

c_α = a constant that depends on the probability of calling for action when, in fact, it is not warranted. (c_α depends on the significance level, α, or the probability of committing a type I statistical error)

$\sigma_{1_j}^2$ = variance of x_j^* attributed to measured quantities

$\sigma_{2_j}^2$ = variance of A_j

These quantities are determined as follows: A_j is based on a compilation of past data for various segments of the hidden inventory tempered by engineering judgment on the reasonableness of the data. In Table 7.1 c_α is found for given α. We can calculate $\sigma_{1_j}^2$ by the methods of Chap. 6 for finding the variance of an algebraic sum and can evaluate $\sigma_{2_j}^2$ when A_j is found by assigning a value to the variance

of each segment of the hidden inventory and summing. These assigned values are also based on past data tempered by engineering judgment.

7.4.3 Examples

Example 7.K

During a 4-week period, six material balance closings were made in a fuel fabrication facility. During this interval less than 0.003% of the inventory was shipped out of the MBA, and there were no receipts. Therefore x_j^* is simply the difference in measured inventory from one time period to the next.

The data and pertinent calculations are shown in Table 7.5. Details leading to the calculation of the A_j, σ_{1_j}, and σ_{2_j} are not shown. We chose $c_\alpha = 1.96$, corresponding to $\alpha = 0.025$.

TABLE 7.5 DATA FOR MATERIAL BALANCE CLOSINGS
(Example 7.K)

Date	Measured inventory, kg of ^{235}U	x_j^*	A_j	σ_{1_j}	σ_{2_j}	c_j^*	$x_j^* > c_j^*$ (?)
7-1	213.617						
7-10	213.439	0.178	0.4	0.3	0.10	1.020†	No
7-17	211.232	2.207	1.2	0.6	0.40	2.613‡	No
7-19	211.202	0.030	0.2	0.2	0.08	0.622	No
7-20	209.984	1.218	1.0	0.1	0.15	1.353	No
7-21	212.687	−2.703	0.1	0.7	0.03	1.473	No
7-26	213.318	−0.631	0.3	0.8	0.10	1.880	No

† $c_1^* = 0.4 + 1.96\sqrt{(0.3)^2 + (0.10)^2} = 1.020$
‡ $c_2^* = 1.2 + 1.96\sqrt{(0.6)^2 + (0.40)^2} = 2.613$

On an individual x_j^* basis, since in no instance is x_j^* greater than c_j^*, there is no cause for concern or action. The data should also be analyzed on a cumulative basis, however, to see if an excessive leakage of material has resulted. These calculations are shown in Table 7.6. The A_j's sum directly to form the cumulative sum. The cumulative value for σ_{2_j} is found by extracting the square root of the sum of squares for the individual σ_{2_j} values, but this is not the case for σ_{1_j}, which reflects the uncertainties in the measured inventories. Rather, σ_{1_j} is found by always regarding the 7-1 inventory as the beginning inventory and the inventory for the closing date as the ending inventory, as appropriate, and disregarding the inventories within the balance period. The methods of Chap. 6 are again applied.

TABLE 7.6 CUMULATIVE DATA
(Example 7.K)

Balance period	x_j^*	A_j	σ_{1_j}	σ_{2_j}	c_j^*	$x_j^* > c_j^*$ (?)
7–1 to 7–10	0.178	0.4	0.30	0.10	1.020	No
7–1 to 7–17	2.385	1.6	0.55	0.41	2.945	No
7–1 to 7–19	2.415	1.8	0.50	0.42	3.080	No
7–1 to 7–20	3.633	2 8	0.52	0.45	4.148	No
7–1 to 7–21	0.930	2.9	0.75	0.45	4.614	No
7–1 to 7–26	0.299	3.2	0.83	0.46	5.060	No

That x_j^* in no case exceeds the critical value for the cumulative case indicates that the hidden inventories are under control. The increase in the measured inventory between 7–20 and 7–21 and again between 7–21 and 7–26 is attributed to a partial cleanout at various stages in the process and the corresponding transfer of material from a hidden to a measured inventory status.

7.4.4 Basis

No new statistical concepts are presented in Sec. 7.4. Refer to Chap. 6 to determine σ_{1_j}. The basis for the test criterion, $x_j^* > c_j^*$, is found in Sec. 7.1.4.

Chapter 8

ANALYSIS OF PAIRED DATA

OVERVIEW

In Chaps. 6 and 7, attention is focused on material unaccounted for (MUF), an important index of performance that measures the effectiveness of a nuclear materials control system within a given material balance area (MBA) or within a facility. It is also important to provide assurance that nuclear materials moving between facilities are properly accounted for. This is not really a separate and distinct problem, because errors associated with measuring inputs to a facility and outputs from it lead directly to errors in MUF. In fact, over an extended period of time, the errors in input and output measurements are of controlling importance, as compared with errors in measuring inventories, in determining the errors of MUF. (This point is made in Chap. 7.)

To a degree dependent upon the particular material involved, in addition to other factors, facility inputs and outputs are measured by two parties—the one who ships the material and the one who receives it. For a given shipment of materials, the shipper's value will tend to disagree with the receiver's value because of measurement uncertainties associated with both values, if for no other reason. This difference is commonly called a shipper–receiver difference.

This chapter is concerned with statistical significance of a shipper–receiver difference, i.e., with resolving the question of whether or not an observed difference can be explained by measurement errors. If it cannot, there are a number of possible explanations; e.g., one or both parties may have intentionally or unintentionally biased his results, or the material may have been altered en route. Perhaps the most common explanation, however, is that the pertinent measurement-error variances are understated by either the shipper or the receiver, or both. Whatever the explanation, detection of a significant shipper–receiver difference is an indication that some kind of investigaton as to its cause is in order.

Up to this point in the discussion, it would seem that the chapter should properly be entitled "Analysis of Shipper–Receiver Data."

The subject matter is broader than this, however, not only its statistical aspects but also as applied to other nuclear materials control problems. Shipper–receiver data consist of measurements reported by two parties on the same items, where the parties may or may not use the same analytical techniques. In its broader aspects, any time two measurements are made on samples of the same material, the data are of the same type as shipper–receiver data. For example, a container of uranium-bearing scrap can be sampled and measured for ^{235}U content by wet-chemistry techniques, and the same container can be measured by a nondestructive assay instrument. Or, during an audit inspection, the inspector produces a result for a given item which can be compared with the facility's value for that item. Therefore, even though this chapter is motivated primarily by the need to analyze shipper–receiver data, the statistical techniques have broader application, as will be illustrated in some of the examples. Thus it is appropriate to indicate this generality of application in the chapter title. (For convenience in exposition, the topic is dealt with in the shipper–receiver frame of reference. The reader should keep in mind the broader aspects of the problem.)

With actual shipper–receiver data, the primary interest is generally in the average difference between the shipper and the receiver values. The same is often true for other data of this type; biases between measurement methods, between a facility and an audit measurement, etc., are of concern. This topic is treated in Sec. 8.2. To make this evaluation, we must know the measurement-error variances. Although some of this information may be supplied with the data, its validity is on occasion open to question. In this connection the data themselves can be used to make inferences about the random components of the measurement variances. This is of particular interest in analyzing all kinds of paired data because it suggests still another method of attacking the very important materials control problem, that of estimating measurement-error variances. This is the subject of Sec. 8.1. Finally, Sec. 8.3 is concerned with evaluating shipper–receiver data over several shipments or, in the broader aspects, with making inferences from paired data collected under more than one set of conditions.

8.1 INFERENCES ON MEASUREMENT VARIANCES

8.1.1 Problem and Assumptions

It is assumed that the data are paired, with values being reported for each of the n items by two parties (parties may be shipper and receiver, analytical methods 1 and 2, analysts A and B, facility and audit

teams, sampling methods 1 and 2, etc.). For modeling purposes the parties are called the shipper and the receiver although, as was pointed out in the Overview, the results have wider applicability. Each reported value is made up of three components, the true value for the item in question, the systematic-error component, and the random-error component. The error components are, in turn, made up of contributions from various sources, which may or may not be identified. To interpret the results of the analysis properly, we must make this identification, at least to some degree. This point is best illustrated by an example. Suppose that a shipment consists of containers of plutonium oxide with an assigned value of total plutonium associated with each container. There is no way of telling from the data alone how these values were assigned to the containers. Was each container weighed, sampled, and analyzed for percent plutonium? Or was the entire shipment of powder characterized for percent plutonium by drawing and analyzing samples and assigning the average percent plutonium to the shipment? In the former case, the variance due to sampling and analysis manifests itself as the random-error variance although the systematic error still plays a role. In the latter case, however, the uncertainty in the average percent plutonium factor appears as a systematic error, and, as a result, there is less scatter in the data themselves. Any scatter in the data would be explained by the random error in determining the net weights. The systematic errors are assumed to be constant for both parties for this entire set of n items; this assumption is very important (see example 8.A). It is further assumed that the random variables are normally distributed.

In equation form, if we let s_i be shipper value for item i and r_i be the receiver value, the model is

$$s_i = x_i + \delta + \epsilon_i \tag{8.1}$$

$$r_i = x_i + \Delta + \eta_i \qquad (i = 1, 2, \ldots, n) \tag{8.2}$$

where x_i is the true value of item i, having a variance of σ_x^2, which represents the random variance between the true amounts for the items; δ and Δ are the systematic errors for the shipper and receiver, respectively (they are assumed to have been drawn from distributions having zero means and variances of σ_δ^2 and σ_Δ^2, respectively); and ϵ_i and η_i are the random errors, each normally distributed with zero means and variances of σ_ϵ^2 and σ_η^2, respectively. If δ and/or Δ have nonzero means, then we can speak of a bias between the two sets of data, a bias which perhaps is introduced intentionally.

The data are used to make inferences about σ_ϵ^2 and σ_η^2. Some specific questions are posed:

Question 8.A. Do the random measurement-error variances differ for the shipper and the receiver?

Question 8.B. A value is assigned to the sum of the variances $\sigma_\varepsilon^2 + \sigma_\eta^2$. Do the data support this value as being valid?

Question 8.C. The shipper and the receiver assign values to σ_ε^2 and σ_η^2, respectively. Do the data support these values jointly as being valid?

Question 8.D. The receiver assigns a value to σ_η^2, but the shipper does not assign a value to σ_ε^2. Do the data support this value for σ_η^2 as being valid? (It is a simple matter to reverse the roles of σ_ε^2 and σ_η^2.)

In the terminology of statistical hypothesis testing, the preceding questions can be regarded as tests of the hypotheses:

Question 8.A. H_{01}: $\sigma_\varepsilon^2 = \sigma_\eta^2$ against the alternative that $\sigma_\varepsilon^2 \neq \sigma_\eta^2$

Question 8.B. H_{02}: $(\sigma_\varepsilon^2 + \sigma_\eta^2) = \sigma_{mo}^2$ against the alternative that $(\sigma_\varepsilon^2 + \sigma_\eta^2) \neq \sigma_{mo}^2$

Question 8.C. H_{03}: $\sigma_\varepsilon^2 = \sigma_{\varepsilon 0}^2$ and $\sigma_\eta^2 = \sigma_{\eta 0}^2$ against the alternative that $\sigma_\varepsilon^2 \neq \sigma_{\varepsilon 0}^2$ or $\sigma_\eta^2 \neq \sigma_{\eta 0}^2$, or both

Question 8.D. H_{04}: $\sigma_\eta^2 = \sigma_{\eta 0}^2$ against the alternative that $\sigma_\eta^2 \neq \sigma_{\eta 0}^2$

Depending on the answers to these questions, the remaining question is:

Question 8.E. What values should be used for σ_ε^2 and σ_η^2 in making inferences about the mean difference?

8.1.2 Solution

In answering any of these questions, we first calculate the variances among the s_i values and among the r_i values by Eq. 2.61 and the covariances between the s_i and r_i values. (The covariance is given by $\{\sum s_i r_i - [(\sum s_i \sum r_i)/n]\}/(n-1)$, where each sum runs from 1 to n.) Designate these quantities by S_s^2, S_r^2, and S_{sr}, respectively. The answers to the specific questions are then found by making the calculations indicated in the following steps.

Question 8.A

Step a. Calculate

$$S_u^2 = S_s^2 + S_r^2 + 2S_{sr} \tag{8.3}$$

$$S_v^2 = S_s^2 + S_r^2 - 2S_{sr} \tag{8.4}$$

$$S_{uv} = S_s^2 - S_r^2 \tag{8.5}$$

Step b. Calculate

$$r=\frac{S_{uv}}{S_u S_v} \tag{8.6}$$

Step c. Calculate

$$t=r\sqrt{(n-2)/(1-r^2)} \tag{8.7}$$

Step d. If t exceeds in absolute value the critical value of Student's t distribution with $(n-2)$ degrees of freedom, $t_{1-(\alpha/2)}$, at the α significance level, conclude that σ_ε^2 and σ_η^2 are not equal (from Appendix C; this is set up as a two-sided test of the hypotheses.)

Question 8.B

Step a. Calculate S_v^2 from Eq. 8.4.

Step b. Form the ratio

$$R=\frac{(n-1)S_v^2}{\sigma_{m0}^2} \tag{8.8}$$

where σ_{m0}^2 is the hypothesized value for the sum $(\sigma_\varepsilon^2+\sigma_\eta^2)$

Step c. At the α level of significance, reject the hypothesis if $R<\chi_{\alpha/2}^2$ or if $R>\chi_{1-(\alpha/2)}^2$, where $\chi_{\alpha/2}^2$ and $\chi_{1-(\alpha/2)}^2$ are read from Appendix B with $(n-1)$ degrees of freedom.

Question 8.C. (The solutions to this question and to question 8.D are both based on large-sample theory. The question of how large the sample size must be to result in tests that are reasonably valid has not been investigated.)

Step a. Denoting the hypothesized values by $\sigma_{\varepsilon 0}^2$ and $\sigma_{\eta 0}^2$, calculate

$$\hat{\sigma}_x^2=\frac{S_s^2\sigma_{\eta 0}^4+2S_{sr}\sigma_{\varepsilon 0}^2\sigma_{\eta 0}^2+S_r^2\sigma_{\varepsilon 0}^4}{(\sigma_{\varepsilon 0}^2+\sigma_{\eta 0}^2)^2}-\frac{\sigma_{\varepsilon 0}^2\sigma_{\eta 0}^2}{\sigma_{\varepsilon 0}^2+\sigma_{\eta 0}^2} \tag{8.9}$$

Step b. Calculate

$$\ln L(\hat{\Omega})=-n-0.5n\ln(S_s^2S_r^2-S_{sr}^2) \tag{8.10}$$

Step c. Calculate

$$\ln L(\hat{\omega}_3)=-0.5n\ln(\hat{\sigma}_x^2\sigma_{\varepsilon 0}^2+\hat{\sigma}_x^2\sigma_{\eta 0}^2+\sigma_{\varepsilon 0}^2\sigma_{\eta 0}^2)$$
$$-n\left[\frac{(\hat{\sigma}_x^2+\sigma_{\eta 0}^2)S_s^2-2\hat{\sigma}_x^2S_{sr}+(\hat{\sigma}_x^2+\sigma_{\varepsilon 0}^2)S_r^2}{2(\hat{\sigma}_x^2\sigma_{\varepsilon 0}^2+\hat{\sigma}_x^2\sigma_{\eta 0}^2+\sigma_{\varepsilon 0}^2\sigma_{\eta 0}^2)}\right] \tag{8.11}$$

Step d. Find

$$\lambda_3 = 2[\ln L(\hat{\Omega}) - \ln L(\hat{\omega}_3)] \tag{8.12}$$

Step e. If λ_3 exceeds $\lambda_3^{(\alpha)}$, conclude that either $\sigma_\varepsilon^2 \neq \sigma_{\varepsilon 0}^2$ or $\sigma_\eta^2 \neq \sigma_{\eta 0}^2$ or both. The value of $\lambda_3^{(\alpha)}$ depends on the significance level, α, and is given for various values of α in Table 8.1.

TABLE 8.1 CRITICAL VALUES OF $\lambda_3^{(\alpha)}$ FOR TEST OF H_{03}*

α	$\lambda_3^{(\alpha)}$	α	$\lambda_3^{(\alpha)}$
0.10	4.61	0.025	7.38
0.05	5.99	0.01	9.21

* These values are taken from Appendix B with 2 degrees of freedom.

Question 8.D

Step a. Solve Eqs. 8.13 and 8.14 simultaneously for $\hat{\sigma}_x^2$ and $\hat{\sigma}_\varepsilon^2$. (They can be solved most simply by assigning a value to $\hat{\sigma}_\varepsilon^2$ in Eq. 8.13, solving this for $\hat{\sigma}_x^2$, using this value in Eq. 8.14 to solve for $\hat{\sigma}_\varepsilon^2$, using this in Eq. 8.13 to solve for $\hat{\sigma}_x^2$, etc., until the values of $\hat{\sigma}_\varepsilon^2$ and $\hat{\sigma}_x^2$ no longer change. Experience indicates that convergence is quite rapid.)

$$\hat{\sigma}_x^2 = \frac{S_s^2\sigma_{\eta 0}^4 + 2S_{sr}\hat{\sigma}_\epsilon^2\sigma_{\eta 0}^2 + S_r^2\hat{\sigma}_\epsilon^4}{(\hat{\sigma}_\epsilon^2 + \sigma_{\eta 0}^2)^2} - \frac{\hat{\sigma}_\epsilon^2\sigma_{\eta 0}^2}{\hat{\sigma}_\epsilon^2 + \sigma_{\eta 0}^2} \tag{8.13}$$

$$\hat{\sigma}_\epsilon^2 = \frac{S_r^2\hat{\sigma}_x^4 - 2S_{sr}\hat{\sigma}_x^2(\hat{\sigma}_x^2 + \sigma_{\eta 0}^2) + S_s^2(\hat{\sigma}_x^2 + \sigma_{\eta 0}^2)^2}{(\sigma_{\eta 0}^2 + \hat{\sigma}_x^2)^2} - \frac{\sigma_{\eta 0}^2\hat{\sigma}_x^2}{\sigma_{\eta 0}^2 + \hat{\sigma}_x^2} \tag{8.14}$$

Step b. Find $\ln L(\hat{\Omega})$ from Eq. 8.10.

Step c. Find $\ln L\ (\hat{\omega}_4)$, using Eq. 8.11 with $\hat{\sigma}_\varepsilon^2$ from Eq. 8.14 replacing $\hat{\sigma}_{\varepsilon 0}^2$.

Step d. Find

$$\lambda_4 = 2[\ln L(\hat{\Omega}) - \ln L(\hat{\omega}_4)] \tag{8.15}$$

Step e. If λ_4 exceeds $\lambda_4^{(\alpha)}$, conclude that σ_η^2 does not equal its stated or hypothesized value, $\sigma_{\eta 0}^2$. The value of $\lambda_4^{(\alpha)}$ depends on the significance level, α, and is given for various values of α in Table 8.2.

TABLE 8.2 CRITICAL VALUES OF $\lambda_4^{(\alpha)}$ FOR TEST OF H_{04}*

α	$\lambda_4^{(\alpha)}$	α	$\lambda_4^{(\alpha)}$
0.10	2.71	0.025	5.02
0.05	3.84	0.01	6.63

* These values are taken from Appendix B with 1 degree of freedom.

Question 8.E. The several possible situations that may arise in choosing the values to assign to σ_ε^2 and σ_η^2 are detailed in Table 8.3.

TABLE 8.3 POSSIBLE SITUATIONS LEADING TO DIFFERENT ESTIMATES OF σ_ϵ^2 AND σ_η^2

Situation	Assigned values *	Hypothesis tested †	Result of test
A	None	None	
B	None	H_{01}	Rejected
C	None	H_{01}	Not rejected
D	Sum	H_{01} and H_{02}	Rejected
E	Sum	H_{01} and H_{02}	Rejected Not rejected
F	Sum	H_{01} and H_{02}	Not rejected Rejected
G	Sum	H_{01} and H_{02}	Not rejected
H	σ_η^2 or σ_ϵ^2 ‡	H_{04}	Rejected
I	σ_η^2 or σ_ϵ^2 ‡	H_{04}	Not rejected
J	Both	H_{03}	Rejected
K	Both	H_{03}	Not rejected

* "Sum" denotes $(\sigma_\epsilon^2 + \sigma_\eta^2)$. "Both" denotes $(\sigma_\eta^2$ and $\sigma_\epsilon^2)$

† Hypotheses are as follows H_{01} $\sigma_\epsilon^2 = \sigma_\eta^2$. H_{02} $(\sigma_\epsilon^2 + \sigma_\eta^2) = \sigma_{m0}^2$. H_{03} $\sigma_\eta^2 = \sigma_{\eta 0}^2$. H_{04} $\sigma_\eta^2 = \sigma_{\eta 0}^2$

‡ The case where the roles of σ_ϵ^2 and σ_η^2 are reversed is straightforward.

In Table 8.4 values are assigned σ_ε^2 and σ_η^2 corresponding to each situation (in some instances, as indicated, one situation can lead back to another).

TABLE 8.4 ACTIONS CORRESPONDING TO EACH SITUATION IN TABLE 8.3

Situation	Action	
A	$\sigma_\epsilon^2 = S_s^2 - S_{sr}$	(8.16)
	$\sigma_\eta^2 = S_r^2 - S_{sr}$	(8.17)
	If either is negative, call it zero, and the other is S_t^2 (from Eq. 8.4) If S_{sr} is negative, then	
	$\sigma_\epsilon^2 = S_s^2$	(8.18)
	$\sigma_\eta^2 = S_r^2$	(8.19)
B	Same as A	
C	$\sigma_\epsilon^2 = \sigma_\eta^2 = S_t^2/2$	
D	Same as A	
E	$\sigma_\epsilon^2 = \sigma_{m0}^2 \dfrac{S_s^2 - S_{sr}}{S_t^2}$	(8.20)
	$\sigma_r^2 = \sigma_{r0}^2 \dfrac{S_r^2 - S_{sr}}{S_t^2}$	(8.21)
F	Same as C	
G	$\sigma_\epsilon^2 = \sigma_\eta^2 = \sigma_{m0}^2/2$	
H	Same as A *	
I	$\sigma_\eta^2 = \sigma_{\eta 0}^2$	
	σ_ϵ^2 from Eq. 8.14	
J	Calculate $R_\epsilon = \ln(\sigma_\epsilon^2/\sigma_{\epsilon 0}^2)$	(8.22)
	and $R_\eta = \ln(\sigma_\eta^2/\sigma_{\eta 0}^2)$	(8.23)
	where σ_ϵ^2 and σ_η^2 come from Eqs. 8.16 and 8.17. If $\lvert R_\eta \rvert < \lvert R_\epsilon \rvert$ or if σ_ϵ^2 is negative, revert to situation H or I (i.e., ask question 8.D). If $\lvert R_\eta \rvert > \lvert R_\epsilon \rvert$ or if σ_η^2 is negative, revert to situation H or I with the roles of σ_ϵ^2 and σ_η^2 reversed	
K	$\sigma_\epsilon^2 = \sigma_{\epsilon 0}^2$	
	$\sigma_\eta^2 = \sigma_{\eta 0}^2$	

* Situation B or C may possibly apply if there is reason to believe that σ_ϵ^2 and σ_η^2 might be equal

8.1.3 Examples

Because of the wide variety of paired-data applications likely to be encountered, several different examples are given.

Example 8.A

(This example was provided by R. A. Schneider.)

When nitrate solution is being loaded into a recovery plant for further purification, samples are drawn from each container and analyzed for percent plutonium with two different analytical techniques. One analytical method is a direct assay, and the other requires that a correction factor be applied. Samples from 20 containers are analyzed in this way. Using the resulting data (given in Table 8.5) at the $\alpha = 0.05$ significance level, test the hypothesis that the analytical random-error variances are the same for both analytical methods.

TABLE 8.5 PLUTONIUM CONCENTRATION DATA (% OF Pu) (Example 8.A)

Container, i	Method 1, s_i	Method 2, r_i	Container, i	Method 1, s_i	Method 2, r_i
1	13.11	13.00	11	13.26	13.01
2	15.14	14.90	12	11.00	11.06
3	13.22	13.01	13	12.74	12.75
4	13.67	13.65	14	13.69	13.69
5	10.48	10.61	15	10.43	10.40
6	15.37	15.11	16	11.38	11.30
7	12.37	12.40	17	12.26	12.27
8	12.50	12.63	18	12.89	12.70
9	11.46	11.71	19	13.33	13.30
10	14.28	14.21	20	11.88	11.90

The question asked of the data is question 8.A, and the hypothesis is H_{01}: $\sigma_\varepsilon^2 = \sigma_\eta^2$. The steps to the solution of question 8.A are followed. First, calculate the variances, S_s^2 and S_r^2 and the covariance, S_{sr}. From Eq. 2.61,

$$S_s^2 = \frac{(13.11)^2 + \ldots + (11.88)^2 - [(13.11 + \ldots + 11.88)^2/20]}{19} = 1.891696$$

$$S_r^2 = \frac{(13.00)^2 + \ldots + (11.90)^2 - [(13.00 + \ldots + 11.90)^2/20]}{19} = 1.666079$$

From Sec. 8.1.2 (page 270),

$$S_{sr} = \{(13.11)(13.00) + \ldots + (11.88)(11.90) - [(13.11 + \ldots + 11.88)(13.00 + \ldots + 11.90)/20]\} / 19$$
$$= 1.769446$$

Then,

Question 8.A

Step a.

$$S_u^2 = 1.891696 + 1.666079 + 2(1.769446) = 7.096667$$
$$S_v^2 = 1.891696 + 1.666079 - 2(1.769446) = 0.018883$$
$$S_{uv} = 1.891696 - 1.666079 = 0.225617$$

Step b.

$$r = \frac{0.225617}{\sqrt{(7.096667)(0.018883)}} = 0.616$$

Step c.

$$t = 0.616\sqrt{18/0.6205} = 3.318$$

Step d. The critical value of Student's t distribution with 18 degrees of freedom is $t_{0.975} = 2.101$ (from Appendix C) with $\alpha = 0.05$. Since 3.318 exceeds 2.101, the hypothesis of equal random analytical-error variances is rejected.

With respect to the estimates of σ_ε^2 and σ_η^2, situation B of Table 8.3 applies. From Eqs. 8.16 and 8.17,

$$\sigma_\varepsilon^2 = 1.891696 - 1.769446 = 0.122250$$
$$\sigma_\eta^2 = 1.666079 - 1.769446 = -0.103367$$

Since σ_η^2 is negative, it would be assigned the value zero, and σ_ε^2 would be estimated by S_v^2.

$$\sigma_\varepsilon^2 = 0.018883$$

This completes the steps of the analysis. A disturbing note is indicated by the large negative estimate for σ_η^2, -0.103367. The reason for this becomes evident when the data of Table 8.5 are plotted. An important assumption in the analysis is that, if there is a bias between the values given by the two parties, it is constant over the data set in question. This is the result of the assumption that δ and Δ in Eqs. 8.1 and 8.2 are constants. This assumption can be checked for validity by plotting $(s_i - r_i)$ vs. r_i (or vs. s_i or the average of r_i and s_i). If the

assumption is true, this plot should indicate no relation between $(s_i - r_i)$ and r_i. The data are plotted in Fig. 8.1.

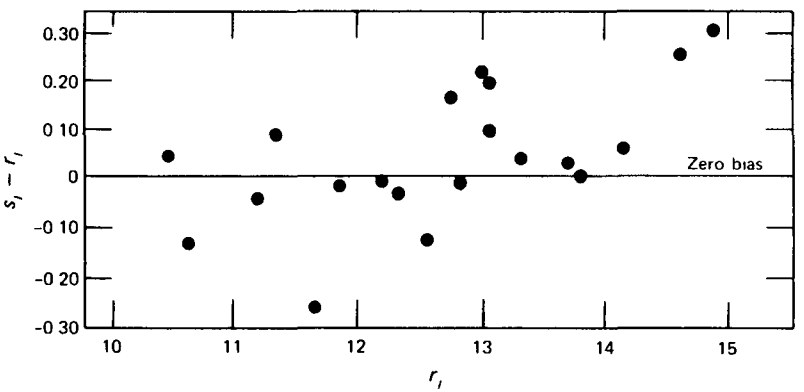

FIGURE 8.1 Plot of data in Table 8.5.

The relation between $(s_i - r_i)$ and r_i is evident. The s_i values (Table 8.5, Method 1) are relatively high at high plutonium concentrations and low at low concentrations. This accounts for the large negative estimate of σ_η^2. In view of this apparent nonconstant relative bias, the statistical analysis is not valid because the assumption of a constant bias is grossly violated. Physically the nonconstant bias might be explained as being due to the use of a wrong correction factor applied for Method 2. Perhaps the correction factor should be a function of the concentration.

For illustrative purposes the calculations for this example have been carried to completion even though the results are not valid. This was done to show how the calculations are made and, more important, to demonstrate the need to be aware of the assumptions made in the analysis. If there is any question at all about the validity of the assumptions, the first step should be to plot the data. Had this been done in this instance, the analysis would not have proceeded beyond that point. For further discussion of these data, see Example 8.J.

Example 8.B

In a Gulf report (R. L. Bramblett et al., Applications of Photo-induced Reactions to Nuclear Materials Safeguards Problems, Quarterly Progress Report, July 1–Sept. 30, 1971, USAEC Report GULF-RT-A-10914, Gulf Radiation Technology, Dec. 17, 1971), data are given for total amounts of ^{235}U for Power Burst Facility (PBF) UO_2 powder in

2-quart polyethylene bottles as reported by the manufacturer and as measured by the Isotopic Source Assay System (ISAS) unit. Omitting a few of the values with smaller amounts of ^{235}U to reduce the size of σ_x^2, and hence enhance the test sensitivity, we obtain the data listed in Table 8.6 for 22 bottles.

TABLE 8.6 ^{235}U IN PBF UO_2 POWDER (GRAMS)
(Example 8.B)

Container	Manufacturer value	ISAS	Container	Manufacturer value	ISAS
1	613	618	12	623	628
2	639	633	13	630	634
3	661	655	14	645	646
4	652	648	15	655	653
5	658	660	16	648	650
6	640	653	17	605	606
7	661	676	18	645	640
8	645	654	19	624	638
9	646	636	20	666	656
10	627	633	21	622	619
11	602	622	22	637	630

Suppose the manufacturer states that his random-error standard deviation is 3.2 g of ^{235}U (this was not stated in the document but is put forth for illustrative purposes only). Do the data substantiate this as valid? Operate at the $\alpha = 0.05$ level of significance. (We can verify that a plot of the data discloses no nonconstant bias between the two measurement methods, so the analysis can proceed.)

This is question 8.D. For simplicity, identify ISAS as the shipper and the manfacturer as the receiver, so that σ_η^2 is related to the manufacturer. The hypothesis, H_{04}: $\sigma_\eta^2 = (3.2)^2 = 10.24$, is tested for significance by application of the steps under question 8.D. First, we must calculate S_s^2, S_r^2, and S_{sr}.

$$S_s^2 = \frac{(618)^2+(633)^2+\ldots+(630)^2-[(618+633+\ldots+630)^2/22]}{21}$$
$$= 271.96$$

$$S_r^2 = \frac{(613)^2+(639)^2+\ldots+(637)^2-[(613+639+\ldots+637)^2/22]}{21}$$
$$= 329.19$$

$$S_{sr} = \{(618)(613)+(633)(639)+\ldots+(630)(637)$$
$$-[(618+\ldots+630)(613+\ldots+637)/22]\} / 21 = 265.58$$

Then apply the steps of question 8.D with $\sigma_{\eta 0} = 3.2$.

Question 8.D.

Step a. Solve simultaneously for $\hat{\sigma}_x^2$ and $\hat{\sigma}_\epsilon^2$ in Eqs. 8.13 and 8.14.

$$\hat{\sigma}_x^2 = \frac{271.96(3.2)^4 + 2(265.58)(3.2)^2\hat{\sigma}_\epsilon^2 + 329.19\hat{\sigma}_\epsilon^4}{(\hat{\sigma}_\epsilon^2 + 10.24)^2} - \frac{10.24\hat{\sigma}_\epsilon^2}{\hat{\sigma}_\epsilon^2 + 10.24}$$

$$= \frac{28{,}517.07 + 5439.08\hat{\sigma}_\epsilon^2 + 329.19\hat{\sigma}_\epsilon^4}{(10.24 + \hat{\sigma}_\epsilon^2)^2} - \frac{10.24\hat{\sigma}_\epsilon^2}{\hat{\sigma}_\epsilon^2 + 10.24} \tag{8.24}$$

$$\hat{\sigma}_\epsilon^2 = \frac{329.19\hat{\sigma}_x^4 - 2(265.58)\hat{\sigma}_x^2(\hat{\sigma}_x^2 + 10.24) + 271.96(\hat{\sigma}_x^2 + 10.24)^2}{(10.24 + \hat{\sigma}_x^2)^2}$$

$$- \frac{10.24\hat{\sigma}_x^2}{10.24 + \hat{\sigma}_x^2} \tag{8.25}$$

To solve, assign an initial value of 20 to $\hat{\sigma}_\epsilon^2$ (this value is selected arbitrarily but is judiciously based on some knowledge of what the value might be) and work iteratively on Eqs. 8.24 and 8.25 as follows:

In Eq. 8.24, let $\hat{\sigma}_\epsilon^2 = 20$ and solve for $\hat{\sigma}_x^2$. This gives
$$\hat{\sigma}_x^2 = 294.14 - 6.77 = 287.37$$

In Eq. 8.25, let $\hat{\sigma}_x^2 = 287.37$ and solve for $\hat{\sigma}_\epsilon^2$. This gives
$$\hat{\sigma}_\epsilon^2 = 66.00 - 9.89 = 56.11$$

In Eq. 8.24, let $\hat{\sigma}_\epsilon^2 = 56.11$ and solve for $\hat{\sigma}_x^2$. This gives
$$\hat{\sigma}_x^2 = 311.22 - 8.66 = 302.56$$

In Eq. 8.25, let $\hat{\sigma}_x^2 = 302.56$ and solve for $\hat{\sigma}_\epsilon^2$. This gives
$$\hat{\sigma}_\epsilon^2 = 66.18 - 9.90 = 56.28$$

In Eq. 8.24, let $\hat{\sigma}_\epsilon^2 = 56.28$ and solve for $\hat{\sigma}_x^2$. This gives
$$\hat{\sigma}_x^2 = 311.26 - 8.66 = 302.60\ *$$

In Eq. 8.25, let $\hat{\sigma}_x^2 = 302.60$ and solve for $\hat{\sigma}_\epsilon^2$. This gives
$$\hat{\sigma}_\epsilon^2 = 66.18 - 9.90 = 56.28\ *$$

Since this is the same value as in the previous iteration to four significant figures, the values marked with an asterisk are the solutions to Eqs. 8.24 and 8.25. Proceed to step b.

Step b. From Eq. 8.10,

$$\ln L(\hat{\Omega}) = -22 - 11 \ln[(271.96)(329.19) - (265.58)^2] = -130.37$$

Step c. From Eq. 8.11, with $\sigma_{\epsilon 0}^2$ replaced by $\hat{\sigma}_\epsilon^2 = 56.28$,

$$\ln L(\hat{\omega}_4) = -11 \ln [(302.60)(56.28)+(302.60)(10.24)+(56.28)(10.24)]$$

$$-22\left\{\frac{(302.60+10.24)(271.96)-2(302.60)(265.58)+(302.60+56.28)(329.19)}{2[(302.60)(56.28)+(302.60)(10.24)+(56.28)(10.24)]}\right\}$$

$$= -109.32-22.57 = -131.89$$

Step d. From Eq. 8.15,

$$\lambda_4 = 2\ (-130.37 + 131.89) = 3.04$$

Step e. From Table 8.1, at $\alpha = 0.05$, $\lambda_4^{(\alpha)} = 3.84$. Since 3.04 is less than 3.84, conclude that $\sigma_{\eta 0} = 3.2$ g of ^{235}U is consistent with the data. (The solution to question 8.D is based on large-sample-distribution theory. In this example n is 22. There is no intent to imply that this value of n is large enough to permit application of the large-sample theory. The question of how large n must be has not been investigated. A similar disclaimer is attached to other examples in this book involving application of the results of questions 8.D and 8.E.)

To continue with this example, what would be the values to use for σ_ε^2 and σ_η^2? This is question 8.E and situation I in Table 8.3. Therefore, from Table 8.4, the values are

$\sigma_\eta^2 = \sigma_{\eta 0}^2 = 10.24$ g^2 of ^{235}U $\quad$ $\sigma_\eta = 3.20$ g of ^{235}U

$\sigma_\epsilon^2 = 56.28$ g^2 of ^{235}U $\quad$ $\sigma_\epsilon = 7.50$ g of ^{235}U

Example 8.C

In this example, use the same data as in example 8.B but operate at the $\alpha = 0.10$ significance level. The calculations are the same as in example 8.B up to step e of question 8.D.

Question 8.D

Step e. From Table 8.2, at $\alpha = 0.10$, $\lambda_4^{(\alpha)} = 2.71$. Since 3.04 is greater than 2.71, conclude that σ_η^2 does not equal its stated value of 10.24 g^2 of ^{235}U.

With this conclusion, what would be the values to assign to σ_ε^2 and σ_η^2? This is question 8.E and situation H, which proceeds as situation A since there is no a priori reason to believe that σ_ε^2 and σ_η^2 would

be equal in this example, the methods being quite different. The values for σ_ε^2 and σ_η^2 are then given by Eqs. 8.16 and 8.17:

$$\sigma_\varepsilon^2 = 271.96 - 265.58 = 6.38 \qquad \sigma_\varepsilon = 2.53 \text{ g of } {}^{235}\text{U}$$

$$\sigma_\eta^2 = 329.19 - 265.58 = 63.61 \qquad \sigma_\eta = 7.98 \text{ g of } {}^{235}\text{U}$$

The almost complete reversal of results between these two examples illustrates the influence of a priori knowledge on the final estimates. The conclusion is quite different whether one uses the data to confirm a prior estimate or to provide an estimate exclusive of any prior knowledge.

Example 8.D

Assigned uranium weights in kilograms for ten cylinders of UF_6 are given in Table 8.7.

TABLE 8.7 NET WEIGHTS OF URANIUM IN UF_6 CYLINDERS (KG) (Example 8.D)

Cylinder	Shipper value (s_i)	Receiver value (r_i)
1	1471.22	1468.12
2	1470.98	1469.52
3	1470.82	1469.22
4	1470.46	1469.26
5	1469.42	1462.96
6	1468.98	1470.80
7	1469.10	1467.89
8	1470.22	1472.28
9	1470.86	1469.02
10	1470.38	1470.16

First, consider the question of whether the shipper and receiver have different random-error-measurement variances. This is question 8.A, Sec. 8.1.1, with the solution given under question 8.A of Sec. 8.1.2. Before following the steps of this solution, we find the values of S_s^2, S_r^2, and S_{sr}:

$$S_s^2 = \frac{(1471.22)^2 + \ldots + (1470.38)^2 - [(1471.22 + \ldots + 1470.38)^2/10]}{9}$$

$$= 0.6507$$

$$S_r^2 = \frac{(1468.12)^2 + \ldots + (1470.16)^2 - [(1468.12 + \ldots + 1470.16)^2/10)]}{9}$$

$$= 6.0177$$

$$S_{sr} = \{(1471.22)(1468.12) + \ldots + (1470.38)(1470.16) - [(1471.22 + \ldots)(1468.12 + \ldots)/10]\} / 9$$
$$= 0.4189$$

Then,

Question 8.A

Step a. From Eqs. 8.3 to 8.5,

$$S_u^2 = 0.6507 + 6.0177 + 2(0.4189) = 7.5062$$
$$S_v^2 = 0.6507 + 6.0177 - 2(0.4189) = 5.8306$$
$$S_{uv} = 0.6507 - 6.0177 = -5.3670$$

Step b. From Eq. 8.6,

$$r = \frac{-5.3670}{\sqrt{(7.5062)(5.8306)}} = -0.811$$

Step c. From Eq. 8.7,

$$t = -0.811\sqrt{\frac{8}{1-(0.811)^2}} = -3.92$$

Step d. At the 5% two-sided level of significance, the critical value of Student's t distribution with 8 degrees of freedom is $t_{0.975} = 2.306$. Since -3.92 exceeds this in absolute value, conclude that σ_ε^2 and σ_η^2 are not equal. (The reasons for this significant difference cannot be discerned from the data themselves; additional information is required. As one possible explanation, suppose the shipper assigned an average percent uranium to all ten cylinders, and the receiver drew a sample from each cylinder, analyzed it for percent uranium, and applied a different factor to each cylinder. Then the uncertainty in the factor would not be reflected in σ_ε^2 for the shipper but would affect the value of σ_η^2 for the receiver. If this is the case, it does not mean the shipper's values are necessarily better. Rather, the shipper's values would tend to have a larger systematic-error variance due to the common percent uranium factor. Thus the shipper's actual error may well be larger than the receiver's even though it appears to be smaller because only random errors are estimable from the data.) What, then, would be the values to use for σ_ε^2 and σ_η^2? This is question 8.E, situation B, with the estimates given by Eqs. 8.16 and 8.17:

$$\sigma_\varepsilon^2 = 0.6507 - 0.4189 = 0.2318$$

$$\sigma_\eta^2 = 6.0177 - 0.4189 = 5.5988$$

Example 8.E

Using the data of example 8.D, suppose the shipper and the receiver assert that their random-error standard deviations are

$$\sigma_{\varepsilon 0} = 1.0 \qquad \sigma_{\eta 0} = 1.5$$

Do the data support these values taken jointly? This is question 8.C of Sec. 8.1.1, with the solution given in Sec. 8.1.2 under question 8.C.

Question 8.C

Step a. From Eq. 8.9,

$$\hat{\sigma}_x^2 = \frac{(0.6507)(1.5)^4 + 2(0.4189)(1.0)^2(1.5)^2 + (6.0177)(1.0)^4}{(1.0+2.25)^2} - \frac{(1.0)(2.25)}{1.0+2.25} = 1.0601 - 0.6923 = 0.3678$$

Step b. From Eq. 8.10,

$$\ln L(\hat{\Omega}) = -10 - 5 \ln[(0.6507)(6.0177) - (0.4189)^2] = -16.596$$

Step c. From Eq. 8.11,

$$\ln L(\hat{\omega}_3) = -5 \ln[(0.3678)(1.0) + (0.3678)(2.25) + (1.0)(2.25)] - 10 \left\{ \frac{\begin{array}{r}(0.3678+2.25)(0.6507) - 2(0.3678)(0.4189) \\ + (0.3678+1.0)(6.0117)\end{array}}{2[(0.3678)(1.0) + (0.3678)(2.25) + (1.0)(2.25)]} \right\}$$

$$= -20.155$$

Step d. From Eq. 8.12,

$$\lambda_3 = 2(-16.596 + 20.155) = 7.118$$

Step e. Choose $\alpha = 0.05$ so $\lambda_3^{(\alpha)} = 5.99$ from Table 8.1. Since $7.118 > 5.99$, conclude that $\sigma_\varepsilon^2 \neq 1.0$ or $\sigma_\eta^2 \neq 1.5$, or both. That is, the joint hypothesis H_{02}: $\sigma_\varepsilon^2 = \sigma_{\varepsilon 0}^2$ and $\sigma_\eta^2 = \sigma_{\eta 0}^2$ is rejected.

To continue with this example, what values should be used for σ_ε^2 and σ_η^2? This is question 8.E and situation J. Then, from Eqs. 8.22 and 8.23, since σ_ε^2 and σ_η^2 were calculated from example 8.D to be 0.2318 and 5.5986, respectively.

$$R_\epsilon = \ln\left(\frac{0.2318}{1.0}\right) = -1.46 \qquad R_\eta = \ln\left(\frac{5.5898}{2.25}\right) = 0.91$$

Since R_η is smaller than R_ε in absolute value, ask question 8.D, with $\sigma_{\eta 0}^2 = (1.5)^2$. The hypothesis, $\sigma_\eta^2 = 2.25$ is tested. Follow the steps of question 8.D (see solution in Sec. 8.1.2):

Question 8.D

Step a. From Eq. 8.13 and 8.14, solve simultaneously,

$$\hat{\sigma}_x^2 = \frac{(0.6507)(1.5)^4 + 2(0.4189)(1.5)^2\hat{\sigma}_\epsilon^2 + (0.0177)\hat{\sigma}_\epsilon^4}{(\hat{\sigma}_\epsilon^2 + 2.25)^2} - \frac{2.25\hat{\sigma}_\epsilon^2}{\hat{\sigma}_\epsilon^2 + 2.25}$$

$$= \frac{3.2942 + 1.8851\hat{\sigma}_\epsilon^2 + 6.0177\hat{\sigma}_\epsilon^4}{(2.25 + \hat{\sigma}_\epsilon^2)^2} - \frac{2.25\hat{\sigma}_\epsilon^2}{2.25 + \hat{\sigma}_\epsilon^2}$$

and

$$\hat{\sigma}_\epsilon^2 = \frac{(6.0177)\hat{\sigma}_x^4 - 2(0.4189)\hat{\sigma}_x^2(\hat{\sigma}_x^2 + 2.25) + (0.6507)(\hat{\sigma}_x^2 + 2.25)^2}{(2.25 + \hat{\sigma}_x^2)^2}$$

$$- \frac{2.25\hat{\sigma}_x^2}{2.25 + \hat{\sigma}_x^2}$$

To solve, assign an initial value of 0.5 to σ_ε^2, and work iteratively on the two equations as follows:

In the $\hat{\sigma}_x^2$ equation, let $\hat{\sigma}_\varepsilon^2 = 0.5$ and solve for $\hat{\sigma}_\varepsilon^2$. This gives $\hat{\sigma}_x^2 = 0.7592 - 0.4091 = 0.3501$

In the $\hat{\sigma}_\varepsilon^2$ equation, let $\hat{\sigma}_x^2 = 0.3501$ and solve for $\hat{\sigma}_\varepsilon^2$. This gives $\hat{\sigma}_\varepsilon^2 = 0.6470 - 0.3030 = 0.3440$

In the $\hat{\sigma}_x^2$ equation, let $\hat{\sigma}_\varepsilon^2 = 0.3440$ and solve for $\hat{\sigma}_x^2$. This gives $\hat{\sigma}_x^2 = 0.6918 - 0.2984 = 0.3934$

In the $\hat{\sigma}_\varepsilon^2$ equation, let $\hat{\sigma}_x^2 = 0.3934$ and solve for $\hat{\sigma}_\varepsilon^2$. This gives $\hat{\sigma}_\varepsilon^2 = 0.6593 - 0.3349 = 0.3244$

Using this in the $\hat{\sigma}_x^2$ equation, we find
$\hat{\sigma}_x^2 = 0.6849 - 0.2835 = 0.4014$

Using this in the $\hat{\sigma}_\varepsilon^2$ equation, we find
$\hat{\sigma}_\varepsilon^2 = 0.6618 - 0.3406 = 0.3212$

Use $\hat{\sigma}_\varepsilon^2 = 0.32$ and $\hat{\sigma}_x^2 = 0.40$ as the solutions.

Step b. From Eq. 8.10,

$$\ln L(\hat{\Omega}) = -10 - 5 \ln[(0.6507)(6.0177) - (0.4189)^2] = -16.596$$

Step c. From Eq. 8.11, with 0.32 replacing $\sigma_{\epsilon 0}^2$,

$$\ln \mathbf{L}(\hat{\omega}_4) = -5 \ln[(0.40)(0.32) + (0.40)(2.25) + (0.32)(2.25)]$$

$$-10\left[\frac{(0.40+2.25)(0.6507) - 2(0.40)(0.4189) + (0.40+0.32)(6.0177)}{2[(0.40)(0.32)+(0.40)(2.25)+(0.32)(2.25)]}\right]$$

$$= -2.7924 - 16.3672 = -19.160$$

Step d. From Eq. 8.15,

$$\lambda_4 = 2(-16.596 + 19.160) = 5.128$$

Step e. From Table 8.2, at $\alpha = 0.05$,

$$\lambda_4^{(\alpha)} = 3.84 \text{ and } \lambda_4 > \lambda_4^{(\alpha)}$$

Therefore, reject the hypothesis that $\sigma_\eta^2 = 2.25$.

To recapitulate, thus far in the analysis, we have demonstrated that neither of the error parameter values supplied by the two parties are supported by the data. This is situation H, which corresponds to situation A. Since this was the situation in example 8.D the estimates of the error variances are the same as in that example,

$$\sigma_\epsilon^2 = 0.2318 \qquad \sigma_\eta^2 = 5.5988$$

Example 8.F

From the data in Table 8.8, which show percent of ^{235}U measured by two mass spectrometers, obtain estimates of the random-error variances for each instrument.

TABLE 8.8 PERCENT ^{235}U VALUES
(Example 8.F)

Sample	Instrument A (s_i)	Instrument B (r_i)	($s_i - r_i$)
1	1.0054	1.0116	−0.0062
2	1.0154	1.0070	0.0084
3	0.9889	0.9907	−0.0018
4	4 967	4.880	0.087
5	5 025	5.063	−0.038
6	4.926	4.892	0.034
7	2.064	2.055	0.009
8	2.007	2.029	−0.022
9	4.987	4.974	0.013
10	0.9988	1.0003	−0.0015
11	4.932	5.006	−0.074
12	3.471	3.508	−0.037
13	2.026	2.014	0.012
14	1.0084	0.9977	0.0107

When we inspect these results, we see that the differences in readings for the two mass spectrometers depend on the percent ^{235}U values. To illustrate, at about 1% ^{235}U, the five differences (in absolute value) are 0.0062, 0.0084, 0.0018, 0.0015, and 0.0107. At about 5% ^{235}U, the differences are 0.087, 0.038, 0.034, 0.014, and 0.074, which are clearly larger than those at 1% ^{235}U. The implication is that the random-error standard deviations probably should be expressed on a relative basis rather than an absolute basis. This is accomplished by transforming the data to logarithms before proceeding with the analysis (Table 8.9).

TABLE 8.9 LN PERCENT ^{235}U VALUES
(Example 8.F)

Sample	Instrument A (s_i)	Instrument B (r_i)	($s_i - r_i$)
1	0.0054	0.0115	−0.0061
2	0.0153	0.0070	0.0083
3	−0.0112	−0.0093	−0.0019
4	1.6028	1.5851	0.0177
5	1.6144	1.6220	−0.0076
6	1.5945	1.5876	0.0069
7	0.7246	0.7203	0.0043
8	0.6966	0.7075	−0.0109
9	1.6068	1.6042	0.0026
10	−0.0012	0.0003	−0.0015
11	1.5957	1.6106	−0.0149
12	1.2444	1.2550	−0.0106
13	0.7061	0.7001	0.0060
14	0.0084	−0.0023	0.0107

Note that, with these transformed data, the differences appear to be independent of the percent ^{235}U values. A data plot would confirm this conclusion.

The analysis then proceeds with the transformed data. The problem is to obtain estimates of σ_ε^2 and σ_η^2. Neither parameter has an assigned value. Although there is no reason to believe that the variances are truly different, the data are interrogated to test the hypothesis H_{01}. (In this example the test of H_{01} is not strictly valid because x is not normally distributed with variance σ_x^2. The estimates of the parameters σ_ε^2 and σ_η^2 are valid, however.) Ask question 8.A, Sec. 8.1.1.

First,

$$S_s^2 = \frac{(0.0054)^2 + \ldots + (0.0084)^2 - [(0.0054 + \ldots + 0.0084)^2/14]}{13}$$
$$= 0.508963$$

$$S_r^2 = \frac{(0.0115)^2 + \ldots + (-0.0023)^2 - [(0.0115 + \ldots - 0.0023)^2/14]}{13}$$
$$= 0.510309$$

$$S_{sr} = \{(0.0054)(0.0115) + \ldots + (0.0084)(-0.0023) - [0.0054 + \ldots)(0.0115 + \ldots)/14]\} / 13$$
$$= 0.509591$$

Then,

Question 8.A

Step a. From Eqs. 8.3 to 8.5,

$$S_u^2 = 0.508963 + 0.510309 + 2(0.509591) = 2.038454$$
$$S_v^2 = 0.508963 + 0.510309 - 2(0.509591) = 0.000090$$
$$S_{uv} = 0.508963 - 0.510309 = -0.001346$$

Step b. From Eq. 8.6,

$$r = -\frac{0.001346}{\sqrt{(2.038454)(0.000090)}} = -0.099$$

Step c. From Eq. 8.7,

$$t = -0.099\sqrt{(12)/[1 - (0.099)^2]} = -0.34$$

Step d. Since the absolute value of t does not exceed $t_{1-(\alpha/2)} = 2.179$ for $\alpha = 0.05$ and $n = 14$, conclude that there is no reason to believe that σ_ε^2 differs from σ_η^2.

To proceed then with question 8.E, situation C, the estimates of σ_ε^2 and σ_η^2 are identical and are both $S_r^2/2 = 0.000090/2$ or 0.000045, as indicated by Table 8.4. Expressed as standard deviations, these estimates are

$$\sigma_\epsilon = \sigma_\eta = \sqrt{0.000045} = 0.0067$$

This result applies to the logarithmically transformed data. As was seen in example 4.G, Chap. 4, the standard deviation of a logarithm is approximately equal to the relative standard deviation. Thus the relative random-error standard deviation of either instrument is estimated to be 0.0067 or 0.67% of the percent ^{235}U value.

8.1.4 Basis

The bases for the solutions of Sec. 8.1.2 are considered for each of the five questions raised.

Question 8.A

The mathematical model can be written

$$s_i = x_i + \delta + \epsilon_i \tag{8.26}$$

$$r_i = x_i + \Delta + \eta_i \tag{8.27}$$

where s_i and r_i are the observed shipper and receiver values, respectively, for item i; x_i is the true value for item i; δ and Δ are the systematic-error components; and ε_i and η_i are the random-error components. All random variables are assumed to be normally distributed with zero means (except that x_i has mean value μ_x and δ and/or Δ may have nonzero means as indicated previously) and variances of σ_x^2, σ_δ^2, σ_ε^2, σ_Δ^2, and σ_η^2.

Since δ and Δ are constants for a given set of data, they will not affect the observed variances of s and r, respectively. These observed variances, S_s^2 and S_r^2, are estimates of σ_x^2, σ_ε^2, and σ_η^2 as follows:

S_s^2 estimates $(\sigma_x^2 + \sigma_\varepsilon^2)$ $\qquad$ S_r^2 estimates $(\sigma_x^2 + \sigma_\eta^2)$

Also, the covariance,

$$S_{sr} \text{ estimates } \sigma_x^2$$

since x_i is common to both s_i and r_i and ε_i and η_i are assumed to be independently distributed.

Since S_s^2 estimates $(\sigma_x^2 + \sigma_\varepsilon^2)$ and S_r^2 estimates $(\sigma_x^2 + \sigma_\eta^2)$, it follows that $(S_s^2 - S_r^2)$ estimates $(\sigma_\varepsilon^2 - \sigma_\eta^2)$. But, by Eq. 8.5, $(S_s^2 - S_r^2)$ is identically S_{uv}, and steps b, c, and d of question 8.A are

the steps taken to test for significance of a correlation coefficient. The hypothesis $\rho_{uv} = 0$ is equivalent to the hypothesis $\sigma_\varepsilon^2 = \sigma_\eta^2$ where ρ_{uv} is the true correlation coefficient between u and v. Since $\rho_{uv} = 0$ is the hypothesis formally tested, rejection of this is tantamount to rejection of the hypothesis that $\sigma_\varepsilon^2 = \sigma_\eta^2$.

Question 8.B

The statistic used in testing the hypothesis that $(\sigma_\varepsilon^2 + \sigma_\eta^2)$ is equal to some specified value is the difference $(s_i - r_i)$. From Eqs. 8.26 and 8.27, it is evident that this difference is independent of x_i, the true value of the item being measured. The variance of $(s_i - r_i)$, which is equivalent to S_v^2 of Eq. 8.4 is therefore the estimate of $(\sigma_\varepsilon^2 + \sigma_\eta^2)$. In testing whether or not this estimate is significantly different from the hypothesized value, σ_{mo}^2, we apply the chi-square test based on Sec. 2.6.2.

Question 8.C

Equation 8.9 is the likelihood equation (see Sec. 2.7.1.) for σ_x^2 with $\sigma_{\varepsilon_0}^2$ and $\sigma_{\eta_0}^2$ given as hypothesized values. The terms $L(\hat{\Omega})$ and $L(\hat{\omega}_3)$ in Eqs. 8.10 and 8.11 are the likelihood functions maximized over the entire sample space and over the restricted space in which the hypothesis is true, respectively. The test of significance detailed by steps d and e is based on the likelihood ratio test and large-sample theory. An exact test of this hypothesis for small samples has not been developed, nor have studies been made to evaluate the adequacy of this large-sample test for smaller sample sizes.

Question 8.D

Equations 8.13 and 8.14 are the likelihood equations for σ_x^2 and σ_ε^2 with $\sigma_{\eta_0}^2$ given as the hypothesized value. Again $L(\hat{\Omega})$ and $L(\hat{\omega}_4)$ are the likelihood functions maximized over the appropriate spaces. Large-sample theory is again applied, with the same caution noted as in question 8.C.

Question 8.E

In sorting through the various best estimates of σ_ε^2 and σ_η^2, we note that, if both $\sigma_{\varepsilon_0}^2$ and $\sigma_{\eta_0}^2$ are given and if the hypothesis test does not reject them as being invalid, then these given values can be used. (Otherwise, there would be little point in testing the hypothesis to begin with. If we have little faith in the a priori values, we should not regard them as given values.) If only one value is given and accepted by the statistical test as valid, or if both are given but only one is accepted as valid, then that value, say $\sigma_{\eta_0}^2$, is used, and $\hat{\sigma}_\varepsilon^2$, given in Eq. 8.14, is used for σ_ε^2. This is the maximum likelihood estimate of σ_ε^2 for given $\sigma_{\eta_0}^2$.

If neither value is given, or if given values are rejected as invalid, the maximum likelihood estimates (given by Eqs. 8.16 and 8.17) are used. These estimates are averaged to give the same estimate for both parameters when there is no reason to believe that the values differ (special cases are included to avoid negative estimates of the variance components). The estimates given by Eqs. 8.20 and 8.21 are used when the sum $(\sigma_\varepsilon^2 + \sigma_\eta^2)$ is fixed at σ_{mo}^2 but when σ_ε^2 and σ_η^2 are believed to be different. The estimates are Eqs. 8.16 and 8.17, respectively, adjusted to sum to σ_{mo}^2.

8.2 INFERENCES ABOUT MEAN DIFFERENCES

8.2.1 Problems and Assumptions

The model and assumptions of Sec. 8.1.1 apply. Now, however, the problem is to make inferences about the population means rather than the measurement variances. Specifically, letting μ_s be the true mean for the shipper and μ_r for the receiver, we consider the following questions:

Question 8.F. Are these mean values significantly different? That is, test the hypothesis H_{01}': $\mu_s = \mu_r$ against the alternative $\mu_s \neq \mu_r$.

Question 8.G. What is the best estimate of μ_x, the true average value represented by the data, and what is the variance of this estimate? (Assume that the items measured represent the entire population of interest and not items sampled from this population. This question is particularly appropriate for actual shipper–receiver data.)

8.2.2 Solution

The answers to these questions are considered in turn.

Question 8.F

Step a. Determine values for σ_ε^2 and σ_η^2 by the analysis given in Sec. 8.1 and, specifically, in answer to question 8.E of Sec. 8.1.2.

Step b. Assuming that σ_δ^2 and σ_Δ^2, the systematic error variances, are given, calculate

$$\sigma_d^2 = (\sigma_\delta^2 + \sigma_\Delta^2) + \frac{\sigma_\epsilon^2 + \sigma_\eta^2}{n} \tag{8.28}$$

where n is the number of items with paired measurements.

If σ_δ^2 and σ_Δ^2 are not given, let them be zero (see the discussion following Table 8.10). If one value is given but not the other, either equate the second value to the given value, if it is reasonable to assume they have comparable systematic-error variances, or equate it to zero.

Step c. Calculate $\bar{s}$ and $\bar{r}$, the average values for the shipper and receiver.

Step d. Form the statistic $z = (\bar{s} - \bar{r})/\sigma_{\bar{d}}$ and conclude that $\mu_s \neq \mu_r$ if the absolute value of z exceeds the tabulated value $z_{1-(\alpha/2)}$ at the α level of significance.

The values in Table 8.10 are extracted from Appendix A by using a two-sided test of significance; σ_δ^2, σ_Δ^2, σ_ε^2, σ_η^2 are assumed to be constants. If we have no a priori knowledge about the values of σ_ε^2 and σ_η^2, and if the estimates are based on very few data points, this is a poor assumption. However, it is difficult to use Satterthwaite's formula (Eq. 4.9) and the t distribution because the effective degrees of freedom associated with estimates of σ_ε^2 and σ_η^2 derived from the methods of analysis used in this chapter are difficult to develop. They depend not only on the number of observations but also on the size of σ_x^2 relative to σ_ε^2 and/or σ_η^2. If we are concerned about using a poor estimate of one or both of these parameters, the simplest way to allow for this concern is to use a smaller value of α when applying the test. This is rather subjective but should be a satisfactory approach in practice.

TABLE 8.10 CRITICAL VALUES FOR TEST OF HYPOTHESIS $\mu_s = \mu_r$

α	$z_{1-(\alpha/2)}$
0.10	1.645
0.05	1.960
0.025	2.242
0.01	2.576

In answering question 8.F, we should keep in mind just what is implied by rejection or acceptance of the hypothesis that $\mu_s = \mu_r$. If σ_δ^2 and σ_Δ^2 are not known and are equated to zero, rejection of the hypothesis indicates that the two means are further apart than expected based on the knowledge about the random errors. The resulting significant difference is then explained by a combination of measurement biases and real differences in the material being measured, but there is no way to distinguish between these causes from the data. On the other hand, if known values of σ_δ^2 and σ_Δ^2 are included in the analysis, a

significant difference in the means implies that a real difference exists in the materials being measured (or that the assigned values of σ_δ^2 and σ_Δ^2 are not valid). Alternately, if it is known for certain that both parties are measuring the same quantities (i.e., that no changes have taken place in the material between the times of drawing the two samples or making the two measurements), then the mean difference provides information on the value of the combined systematic-error variances over and above that due to the effects of the random errors.

Question 8.G. The solution for question 8.G follows.

Step a. Determine values for σ_ε^2, σ_η^2, σ_δ^2, and σ_Δ^2 in question 8.F.

Step b. The estimate of μ_x is

$$\hat{\mu}_x = \frac{w_s\bar{s} + w_r\bar{r}}{w_s + w_r} \tag{8.29}$$

where

$$w_s = \left(\sigma_\delta^2 + \frac{\sigma_\varepsilon^2}{n}\right)^{-1} \tag{8.30}$$

and

$$w_r = \left(\sigma_\Delta^2 + \frac{\sigma_\eta^2}{n}\right)^{-1} \tag{8.31}$$

Step c. $\hat{\mu}_x$ has variance $(w_s + w_r)^{-1}$.

8.2.3 Examples

Example 8.G

For the data of example 8.B, is there a significant relative bias between the two measurement methods at the $\alpha = 0.01$ level of significance? This is question 8.F with the systematic-error variances not specified. The question is concerned with whether one or both measurements have systematic-error variances that are nonnegligible relative to the random errors.

Question 8.F. To answer this question, follow the steps to the solution of question 8.F in Sec. 8.2.2.

Step a. From example 8.B, the values derived from a priori information and from the data are

$$\sigma_\varepsilon^2 = 56.28 \qquad \sigma_\eta^2 = 10.24$$

Step b. With $\sigma_\delta^2=\sigma_\Delta^2=0$, σ_d^2 is given by Eq. 8.28:

$$\sigma_d^2=\frac{56.28+10.24}{22}=3.024$$

Step c. $$\bar{s}=\frac{613+639+\ldots+637}{22}=638.36$$

$$\bar{r}=\frac{618+633+\ldots+630}{22}=640.36$$

Step d. From Table 8.10, for $\alpha=0.01$, $z_{1-(\alpha/2)}=2.576$,

$$z=\frac{638.36-640.36}{\sqrt{3.024}}=-1.15$$

Since 1.15 is less than 2.576, conclude that the relative bias between the methods is not significantly different from zero.

Example 8.H

For the data of example 8.D, what is the best estimate of the total uranium in the shipment? Assume that the stated values for the systematic-error standard deviations are $\sigma_\delta = 0.80$ and $\sigma_\Delta = 1.20$. The steps that comprise the solution to question 8.G of Sec. 8.2.2 are followed.

Question 8.G

Step a. Given values are

$$\sigma_\delta^2=0.64 \quad \text{and} \quad \sigma_\Delta^2=1.44$$

From example 8.D

$$\sigma_\epsilon^2=0.23 \quad \text{and} \quad \sigma_\eta^2=5.60$$

Step b. $$w_s=\left(0.64+\frac{0.23}{10}\right)^{-1}=1.51$$

$$w_r=\left(1.44+\frac{5.60}{10}\right)^{-1}=0.50$$

$$\hat{\mu}_x=\frac{1.51\bar{s}+0.50\bar{r}}{1.51+0.50}=0.755\bar{s}+0.245\bar{r}$$

This gives the estimate of the average content per cylinder. For the ten cylinders, the estimate of the total content is

$$10\hat{\mu}_x = 10(0.755\bar{s} + 0.245\bar{r}) = 0.755 \sum s_i + 0.245 \sum r_i$$

From the data,

$$\sum s_i = 1471.22 + \ldots + 1470.38 = 14{,}702.44$$

$$\sum r_i = 1468.12 + \ldots + 1470.16 = 14{,}689.23$$

Then, the estimate of the total uranium content is

$$10\hat{\mu}_x = (0.755)(14{,}702.44) + (0.245)(14{,}689.23)$$
$$= 14{,}699.20 \quad \text{kg of U}$$

Step c. μ_x has variance $(w_s + w_r)^{-1} = (1.51 + 0.50)^{-1} = 0.4975$. Therefore, the total uranium, $10\hat{\mu}_x$, has variance $(10)^2 (0.4975) = 49.75$ kg^2 of uranium, giving a standard deviation of $\sqrt{49.75} = 7.05$ kg of uranium.

Example 8.I

In example 8.H, is there a significant difference at the $\alpha = 0.025$ level between the shipper and receiver values? This is question 8.F, with the steps in the solution as follows:

Question 8.F

Step a. From example 8.H,

$$\sigma_\epsilon^2 = 0.23 \quad \text{and} \quad \sigma_\eta^2 = 5.60$$

Step b. $$\sigma_d^2 = (0.64 + 1.44) + \frac{(0.23 + 5.60)}{10} = 2.666$$

Step c. $$\bar{s} = 1470.24 \quad \text{and} \quad \bar{r} = 1468.92$$

Step d. $$z = \frac{1470.24 - 1468.92}{\sqrt{2.663}} = 0.81$$

which is less than the critical $z_{1-(\alpha/2)}$ value of 2.242. Conclude that the difference is not significant. If, however, the difference had been statistically significant, what would be the explanation? In this particular example, because of the nature of the material involved, it would be reasonable to suspect that one or both parties had understated the size of their systematic-error variance. Another possibility, discounting any

alteration of the cylinder contents during shipment, is that some or all of the values at either end were inadvertently, or deliberately, altered for some reason. Or, as with all statistical tests, a type I error could have been committed in this instance. Whatever the explanation, the significant difference detected should lead to some type of action which, ideally, should be decided upon prior to the shipment. If no such action is taken, the statistical hypothesis test becomes little more than an exercise.

8.2.4 Basis

The basis for the solution to question 8.F in Sec. 8 2.3 is as follows: From the model (Eqs. 8.1 and 8.2), $\bar{s}$ and $\bar{r}$ both have expected values μ_x under the hypothesis that both parties are measuring the same quantities and that $E(\delta) = E(\Delta) = 0$. Further, assuming that the items being measured represent the entire population of interest,* as will normally be the case in a shipper–receiver situation, $\bar{s}$ and $\bar{r}$ have variances

$$\sigma_{\bar{s}}^2 = \sigma_\delta^2 + \frac{\sigma_\epsilon^2}{n} \tag{8.32}$$

and

$$\sigma_{\bar{r}}^2 = \sigma_\Delta + \frac{\sigma_\eta^2}{n} \tag{8.33}$$

Therefore, with independently distributed error random variables, the variance of the difference, $d = \bar{s} - \bar{r}$, is simply the sum of the variances:

$$\sigma_{\bar{d}}^2 = (\sigma_\delta^2 + \sigma_\Delta^2) + \frac{\sigma_\epsilon^2 + \sigma_\eta^2}{n} \tag{8.34}$$

This is Eq. 8.28. From this point on, the statistical test is simply a test for the significance of the difference between two means with known variances.

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* For question 8 F it is not really necessary to assume that the sampled items represent the entire population If they do not Eqs 8 32 and 8.33 would each include a term of the form $c\sigma_x^2$, where c is the finite population correction factor, which is unity for infinite population size However, σ_d^2 will have the same variance as given in Eq 8 34 because the covariance between $\bar{s}$ and $\bar{r}$ is also $c\sigma_x^2$ in this instance. Since $\sigma_d^2 = \sigma_s^2 + \sigma_r^2 - 2\sigma_{sr}$, it is clear that $c\sigma_x^2$ cancels out Of course, this is the motivation behind the pairing—to remove the effect of the process variance In question 8 G, the assumption in question is required

The basis for the solution to question 8.G is as follows: There are two estimates of μ_x, namely, $\bar{s}$ and $\bar{r}$. A weighted average of these two quantities will provide the estimate of μ_x. Write this weighted average

$$\hat{\mu}_x = a\bar{s} + (1-a)\bar{r} \tag{8.35}$$

where a is chosen to minimize the variance of $\hat{\mu}_x$, which is

$$\sigma^2_{\hat{\mu}_x} = a^2\sigma^2_{\bar{s}} + (1-a)^2\sigma^2_{\bar{r}} \tag{8.36}$$

The minimization is accomplished by equating to zero the partial derivative of $\sigma^2_{\hat{\mu}_x}$ with respect to a and solving for a.

$$\frac{\partial \sigma^2_{\hat{\mu}_x}}{\partial a} = 2a\sigma^2_{\bar{s}} - 2(1-a)\sigma^2_{\bar{r}} = 0$$

This gives the solution

$$a = \frac{\sigma^2_{\bar{r}}}{\sigma^2_{\bar{s}} + \sigma^2_{\bar{r}}} = \frac{\sigma^2_\Delta + (\sigma^2_\eta/n)}{(\sigma^2_\delta + \sigma^2_\Delta) + [(\sigma^2_\epsilon + \sigma^2_\eta)/n]} \tag{8.37}$$

Then, letting

$$w_s = \left(\sigma^2_\delta + \frac{\sigma^2_\epsilon}{n}\right)^{-1} \tag{8.38}$$

and

$$w_r = \left(\sigma^2_\Delta + \frac{\sigma^2_\eta}{n}\right)^{-1} \tag{8.39}$$

we find that the value for a is

$$a = \frac{1/w_r}{(1/w_s) + (1/w_r)} = \frac{w_s}{w_s + w_r} \tag{8.40}$$

Also,

$$(1-a) = \frac{w_r}{w_s + w_r} \tag{8.41}$$

If we use these values for a and $1 - a$ in Eq. 8.35, the weighted average, $\hat{\mu}_x$, becomes

$$\hat{\mu}_x = \frac{w_s\bar{s} + w_r\bar{r}}{w_s + w_r} \tag{8.42}$$

where w_s and w_r are as defined in Eqs. 8.38 and 8.39. This is result 8.29. (It can be shown that this weighting is independent of σ_x^2, regardless of whether the sample represents only a part of the population or all of it.)

The variance of $\hat{\mu}_x$ comes directly from Eqs. 8.32, 8.33, 8.35, and 8.38 to 8.41.

$$\sigma^2_{\hat{\mu}_x} = \frac{w_s^2}{(w_s+w_r)^2}\left(\frac{1}{w_s}\right) + \frac{w_r^2}{(w_s+w_r)^2}\left(\frac{1}{w_r}\right) = \frac{1}{(w_s+w_r)} \qquad (8.43)$$

8.3 EVALUATION OF PAIRED DIFFERENCES OVER SEVERAL GROUPS OF DATA

8.3.1 Problem and Assumptions

Thus far we have assumed that δ and Δ, the measurement biases for the shipper and the receiver, remain constant. Although this is often a reasonable assumption for a given shipment (or, more generally, for a given set of paired data), when data from several shipments are analyzed collectively, we can expect that the measurement bias may have changed for one or both parties. At least, this possibility should be kept in mind when the analysis is performed.

In this section the problem of analyzing sets of data to make inferences about measurement variances is considered. The assumptions are as given in Sec. 8.1.1 except that δ and/or Δ may now depend on the data set. For a given measurement technique, it is assumed that σ_ε^2 and σ_η^2 are constants over the entire set of data.

8.3.2 Solution

Given the shipper–receiver data over a number of shipments (or given paired data over a number of data sets), the first step is to perform the analysis separately for each shipment. (Subsidiary information may suggest different breakdowns of the data. For example, it may be known that the N cans of PuO_2 powder in a shipment are based on k different percent plutonium factors, with each factor relating to several cans. The shipment would then be redefined to relate to all cans based on a given factor. In this case the random measurement variances are the weighing errors, and the different percent plutonium factors affect the size of the systematic-error variance. The interpretation of each set of results depends on the given situation even though the same mathematical treatment may cover a number of situations.) For each shipment inferences are made on the random-error variances

according to the methods of Sec. 8.1.2. Then the results over the entire data set are combined.

The method for combining the data over the entire set depends on the type inference being made. If the problem is one of testing some hypothesis, either H_{01}, H_{02}, or H_{04} specified in question 8.C, Sec. 8.1.1, then this should be tested over the entire set of data. [It is difficult to test H_{03} over the entire data set since the ways in which the hypothesis may not be true are so numerous. Test hypotheses for σ_ε^2 and σ_η^2 separately (H_{04}) or for their sum (H_{02})] The possibility exists that for any given shipment some hypothesis may not be rejected at a specified significance level but over all shipments sufficient evidence may have been accumulated to lead to its rejection. On the other hand, if the problem is one of estimation, some kind of averaging process should be made over the estimates for all shipments. Since these estimates will not have the same variances, a weighted average of some kind is indicated.

First, consider the hypothesis testing problem. The steps are indicated for H_{01}, H_{02}, and H_{04}. Assume that in each instance there are m shipments or data sets.

(a) *Hypothesis Testing*

Consider H_{01}: $\sigma_\varepsilon^2 \leqslant \sigma_\eta^2$ vs. the one-sided alternative, $\sigma_\varepsilon^2 > \sigma_\eta^2$.

Step a. For data set i, calculate t_i from Eq. 8.7.

Step b. Find p_i corresponding to t_i using Appendix C with $(n_i - 2)$ degrees of freedom. This process is illustrated in Table 8.11 by giving the relation between t_i and p_i for $n_i = 10$ or for 8 degrees of freedom. On the basis of this table, it should be apparent how Appendix C can be used for any given value of n_i. If t_i is negative for any i, use $(1 - p_i)$ rather than p_i.

TABLE 8.11 RELATION BETWEEN p_i AND t_i FOR 8 DEGREES OF FREEDOM

t_i	p_i	t_i	p_i	t_i	p_i
0	0.50	0 889	0.20	2.306	0.025
0.262	0 40	1.397	0 10	2.896	0.01
0 546	0.30	1.860	0 05	3.355	0.005

Step c. Calculate

$$P = -2 \sum_{i=1}^{m} \ln p_i$$

Step d. If H_{01} is true, P is distributed as the chi-square distribution with $2m$ degrees of freedom. Reject H_{01} if P is too large. The critical value for a given level of significance is read from Appendix B with $2m$ degrees of freedom.

Consider H_{02}: $(\sigma_\varepsilon^2 + \sigma_\eta^2) \leqslant \sigma_{m0}^2$ vs. the one-sided alternative, $(\sigma_\varepsilon^2 + \sigma_\eta^2) > \sigma_{m0}^2$.

Step a. From data set i, calculate R_i from Eq. 8.8.

Step b. Find the sum over the m data sets:

$$R = \sum_{i=1}^{m} R_i$$

Step c. If H_{02} is true, R is distributed as the chi-square distribution with $\sum_{i=1}^{m} (n_i - 1)$ degrees of freedom. Reject H_{02} if R is too large. If the alternative is in the other direction, H_{02} is rejected if R is too small. Again, the critical value may be read from Appendix B.

Consider H_{04}: $\sigma_\eta^2 \leqslant \sigma_{\eta 0}^2$ vs. the one-sided alternative, $\sigma_\eta^2 > \sigma_{\eta 0}^2$ (or $\sigma_\eta^2 < \sigma_{\eta 0}^2$). It is assumed that the data will tend to support one alternative or the other if H_{04} is not true. The λ_{4i} value is zero if H_{04} is true and increases in value as σ_η^2 differs from $\sigma_{\eta 0}^2$ in either direction.

Step a. For data set i, calculate λ_{4i} from Eq. 8.15.

Step b. Find the sum over the m data sets,

$$\lambda_4 = \sum_{i=1}^{m} \lambda_{4i}$$

Step c. If H_{04} is true, then λ_4 is distributed as the chi-square distribution with m degrees of freedom. [(Again, note that this result is based on large-sample-distribution theory, and no investigation has been made as to how large a sample size is required to permit valid application of this test.) Reject H_{04} *if* λ_4 is too large (read the critical value for a given level of significance from Appendix B).]

(b) *Estimation of Random-Error Variances*

The steps for solving the estimation problem are given here. Assume that for each shipment σ_ε^2 and σ_η^2 are estimated from Eqs. 8.16 and 8.17 (i.e., that no prior knowledge about these parameters is available and that they are not equal). For convenience the steps are detailed with reference to σ_ε^2; the corresponding steps for σ_η^2 are obvious.

Step a. For each shipment, find σ_ε^2 from Eq. 8.16. Call this $\sigma_{\varepsilon i}^2$ for shipment i.

Step b. For each shipment, calculate

$$V = \frac{2\sigma_\varepsilon^4}{m-1} + \frac{S_s^2 S_r^2 - S_{sr}^2}{m-1}$$

$$= \frac{S_s^2(2S_s^2 - 4S_{sr} + S_r^2) + S_{sr}^2}{m-1} \tag{8.44}$$

(The i subscript is omitted from this formula to avoid unnecessary complexity in the calculation.) For shipment i, call this quantity V_i.

Step c. Over the m shipments, the estimate of σ_ε^2 is

$$\bar{\sigma}_\epsilon^2 = \frac{\sum_{i=1}^{m} V_i^{-1}\sigma_{\epsilon i}^2}{\sum_{i=1}^{m} V_i^{-1}} \tag{8.45}$$

If this is negative, use $\sigma_\varepsilon^2 = 0$.

(c) *Estimation of Systematic-Error Variances*

Information about the systematic-error variances can also be found over a number of shipments, assuming that both parties are measuring the same quantities (i.e., that all the discrepancies that occur are due to measurement errors). This information is found by the following steps:

Step a. For each shipment, i, compute $d_i = \bar{s}_i - \bar{r}_i$

Step b. Calculate the variance of d_i. Under the problem assumption that the mean of d is zero, this is simply

$$s_d^2 = \sum_{i=1}^{m} \frac{d_i^2}{m} \tag{8.46}$$

Step c. With given values of σ_ε^2 and σ_η^2 (either known or estimated from the data), the estimate of $(\sigma_\delta^2 + \sigma_\Delta^2)$ is

$$\widehat{(\sigma_\delta^2 + \sigma_\Delta^2)} = s_d^2 - \frac{\sigma_\epsilon^2 + \sigma_\eta^2}{m} \sum_{i=1}^{m} \frac{1}{n_i} \tag{8.47}$$

which reduces to

$$s_d^2 - \frac{\sigma_\epsilon^2 + \sigma_\eta^2}{n} \qquad \text{(if all } n_i \text{ are equal)}$$

There is no way to obtain separate estimates of σ_δ^2 and σ_Δ^2 from the data unless, of course, either σ_δ^2 or σ_Δ^2 is given.

8.3.3. Examples

Example 8.J

Consider the data of example 8.A as tabulated in Table 8.5. The plot of these data in Fig. 8.1 indicated a relation between the relative bias between the two methods and the actual value for the plutonium concentration. This relation invalidated the analysis.

However, suppose the data are divided into two groups on the basis of the data plot, with all pairs of observations corresponding to $r_i \leq 12.63\%$ in one group and all other data in the second group. Then the same hypothesis is tested as before (namely, $\sigma_\varepsilon^2 = \sigma_\eta^2$). This is tested separately for each of the two groups, and then the results are combined by the methods of the previous section. The one-sided alternative hypothesis is given by $\sigma_\varepsilon^2 > \sigma_\eta^2$.

For group 1, with $r_i \leq 12.63\%$, the following results are found:

$$n = 9$$

$$S_s^2 = \frac{(10.48)^2 + \ldots + (11.88)^2 - [(10.48 + \ldots + 11.88)^2/9]}{8} = 0.615336$$

$$S_r^2 = \frac{(10.61)^2 + \ldots + (11.90)^2 - [(10.61 + \ldots + 11.90)^2/9]}{8} = 0.631500$$

$$S_{sr} = \{(10.48)(10.61) + \ldots + (11.88)(11.90) - [(10.48 + \ldots)(1061 + \ldots)/9]\} / 8 = 0.618508$$

Then, the steps of Question 8.A are followed:

Question 8.A

Step a. $S_u^2 = 0.615336 + 0.631500 + 2(0.618508) = 2.483852$

$S_v^2 = 0.615336 + 0.631500 - 2(0.618508) = 0.009820$

$S_{uv} = 0.615336 - 0.631500 = -0.016164$

Step b. $r = -\dfrac{0.016164}{\sqrt{(2.483852)(0.009820)}} = -0.103$

Step c. $t = -0.103\sqrt{7/0.9894} = -0.27$

This is the result called for in step a of Sec. 8.3.2 (a). Use it to calculate p_i in step b.

From Sec. 8.3.2(a)

Step b. From Appendix C with 7 degrees of freedom, find p_1 corresponding to $t_1 = -0.27$. The negative sign on t_1 is retained because this result is contrary to what the alternative hypothesis would specify. Thus it tends to support the null hypothesis rather than the alternative, and p_1 will exceed 0.50. Specifically from Appendix C, $p_1 \approx 1 - 0.40 = 0.60$.

The same calculations are now performed for the 11 remaining pairs of data comprising group 2.

$$n = 11$$

$$S_e^2 = \frac{(13.11)^2 + \ldots + (13.33)^2 - [(13.11 + \ldots + 13.33)^2/11]}{10} = 0.768660$$

$$S_r^2 = \frac{(13.00)^2 + \ldots + (13.30)^2 - [(13.00 + \ldots + 13.30)^2/11]}{10} = 0.702487$$

$$S_{er} = \{(13.11)(13.00) + \ldots + (13.33)(13.30) - [(13.11 + \ldots)(13.00 + \ldots)/11]\} / 10 = 0.729790$$

Question 8.A. From the steps of question 8.A, Sec. 8.1.2:

Step a.
$$S_u^2 = 0.768660 + 0.702487 + 2(0.729790) = 2.930727$$
$$S_v^2 = 0.768660 + 0.702487 - 2(0.729790) = 0.011567$$
$$S_{uv} = 0.768660 - 0.702487 = 0.066173$$

Step b. $$r = \frac{0.066173}{\sqrt{(2.930727)(0.011567)}} = 0.359$$

Step c. $$t_2 = 0.359\sqrt{9/0.8711} = 1.154$$

From Appendix C with 9 degrees of freedom, $p_2 \approx 0.15$. With $p_1 = 0.60$ and $p_2 = 0.15$, steps c and d of Sec. 8.3.2 (a) can now be followed:

From Sec. 8.3.2(a)

Step c. $P = -2[\ln (0.60) + \ln (0.15)] = 4.82$

Step d. At $\alpha = 0.05$, the critical value for P is found from Appendix B with $2m = 4$ degrees of freedom. This is 9.49. Since 4.82 is less than 9.49, the hypothesis $\sigma_\varepsilon^2 = \sigma_\eta^2$ is not rejected.

Recall that when the data were not grouped, the hypothesis was rejected, but, as was pointed out in example 8.A, that conclusion was not valid.

Example 8.K

(These data were extracted from D. E. Christensen, Application of Isotopic Correlation Safeguard Techniques to Verify the Plutonium Content of Humboldt Bay Spent Fuel, USAEC Report BNWL-SA-4274, Battelle Pacific Northwest Laboratory, Mar. 20, 1972.)

Chemical reprocessing plant dissolver batches were sampled, and duplicate samples were sent to two different laboratories for analysis. Among the analyses performed was a mass spectrometric analysis for percent ^{241}Pu. The data are given in Table 8.12.

TABLE 8.12 PERCENT ^{241}Pu ANALYSES BY TWO LABORATORIES (Example 8.K)

Batch No.	Lab. 1	Lab. 2	(Lab. 1 − Lab. 2)
12	4.937	4.899	0.038
13	4.729	4.688	0.041
14	4.526	4.505	0.021
15	4.632	4.623	0.009
16	4.215	4.200	0.015
17	3.743	3.759	−0.016
18	8.557	8.615	−0.058
19	8.274	8.260	0.014
20	7.892	7.910	−0.018
21	7.333	7.329	0.004
22	7.217	7.234	−0.017
23 *	6.229	6.285	−0.056
25	3.238	3.210	0.028
26	3.417	3.377	0.040
27	3.504	3.492	0.012
28	3.171	3.127	0.044
29	2.919	2.897	0.022

* Batch number 24 was a flush batch.

Before any hypotheses about σ_ε^2 and σ_η^2 are tested, the data of Table 8.12 are plotted to check for nonrandom behavior. If the data in the last column are plotted against the batch number, Fig. 8.2 is the result.

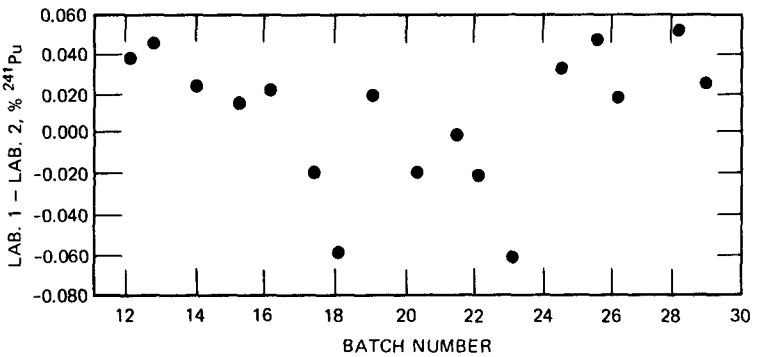


FIGURE 8.2 Analysis of % ^{241}Pu; data from Laboratory 1 minus data from Laboratory 2 vs. batch number.

The plot suggests that there may be some shifts in the relative bias between the laboratories. On this basis, divide the data into three groups as follows:

Group 1:	Batches 12 to 16	$(n_1=5)$
Group 2:	Batches 17 to 23	$(n_2=7)$
Group 3:	Batches 25 to 29	$(n_3=5)$

For the data as grouped, test the null hypothesis, $\sigma_\varepsilon^2 = \sigma_\eta^2$, vs. the alternative hypothesis, $\sigma_\varepsilon^2 > \sigma_\eta^2$, for $\alpha = 0.10$. First, the appropriate variances and covariances must be computed.

Group 1:	$S_s^2=0.071158$	$S_r^2=0.066314$	$S_{sr}=0.068636$
Group 2:	$S_s^2=2.699147$	$S_r^2=2.696713$	$S_{sr}=2.697555$
Group 3:	$S_s^2=0.052088$	$S_r^2=0.052927$	$S_{sr}=0.062422$

Question 8.A Then steps a to c of question 8.A, Sec. 8.1.2, are followed:

Step a. Group 1:

$$S_u^2=0.071158+0.066314+2(0.068636)=0.274744$$

$$S_v^2=0.071158+0.066314-2(0.068636)=0.000200$$

$$S_{uv}=0.071158-0.066314=0.004844$$

Group 2:

$S_u^2=10.790970$ $S_v^2=0.000750$ $S_{uv}=0.002434$

Group 3:

$S_u^2=0.209859$ $S_v^2=0.000171$ $S_{uv}=-0.000839$

Step b. Group 1: $r = \dfrac{0.004844}{\sqrt{(0.274744)(0.000200)}} = 0.653$

Group 2: $r = 0.027$

Group 3: $r = -0.140$

Step c. Group 1: $t_1 = 0.653\sqrt{3/0.5736} = 1.49$

Group 2: $t_2 = 0.06$

Group 3: $t_3 = -0.24$

From Sec. 8.3.2(a)

Step b. Group 1: $p_1 = 0.11$ (from Appendix C with 3 degrees of freedom)

Group 2: $p_2 = 0.49$

Group 3: $p_3 = 0.59$

Step c. $P = -2[\ln (0.11) + \ln (0.49) + \ln (0.59)] = 6.90$

Step d. At $\alpha = 0.10$ the critical value for P is found from Appendix B with 6 degrees of freedom. This is 10.64. Since 6.90 is less than 10.64, the hypothesis $\sigma_\varepsilon^2 = \sigma_\eta^2$ is not rejected.

(The reader can verify that, if the data are not grouped, $r = -0.632$ and $t = -3.16$, which would result in rejection of the hypothesis if the test were two sided. This result, of course, is not valid in view of the nonrandomness of the data.)

These data may now be used to estimate the systematic-error variance associated with a percent ^{241}Pu determination. Using Eqs. 8.46 and 8.47, we can calculate:

$$d_1 = \frac{0.038 + 0.041 + \ldots + 0.015}{5} = 0.0248$$

$$d_2 = \frac{-0.016 - 0.058 + \ldots - 0.056}{7} = -0.0210$$

$$d_3 = \frac{0.028 + 0.040 + \ldots + 0.022}{5} = 0.0292$$

From Eq. 8.46,

$$s_d^2 = \frac{(0.0248)^2 + (-0.0210)^2 + (0.0292)^2}{3} = 0.000636$$

From Eq. 8.47,

$$\widehat{(\sigma_\delta^2+\sigma_\Delta^2)}=0.000636-(\sigma_\epsilon^2+\sigma_\eta^2)\left(\frac{1}{5}+\frac{1}{7}+\frac{1}{5}\right)\left(\frac{1}{3}\right)$$

To evaluate this, we must assign a value to $(\sigma_\varepsilon^2 + \sigma_\eta^2)$. Since it has been accepted that $\sigma_\varepsilon^2 = \sigma_\eta^2$, then $(\sigma_\varepsilon^2 + \sigma_\eta^2)$ is estimated by S_v^2 for each group. (See Sec. 8.1.2, question 8.E, situation C.)

Group 1: $\sigma_\epsilon^2+\sigma_\eta^2=0.000200$

Group 2: $\sigma_\epsilon^2+\sigma_\eta^2=0.000750$

Group 3: $\sigma_\epsilon^2+\sigma_\eta^2=0.000171$

Use $(\sigma_\varepsilon^2 + \sigma_\eta^2)$ averaged over the three groups $[(\sigma_\varepsilon^2 + \sigma_\eta^2) = 0.000374]$. Inserting this value in Eq. 8.47 provides the estimate of the sum of the systematic-error variances for both mass spectrometers.

$$\widehat{(\sigma_\delta^2+\sigma_\Delta^2)}=0.000636-\frac{(0.000374)(0.5429)}{3}=0.000568$$

Example 8.L

Using the same data as in the previous example, at the $\alpha = 0.025$ level, test the hypothesis that $(\sigma_\varepsilon^2 + \sigma_\eta^2) = 0.0002$ against the alternative $(\sigma_\varepsilon^2 + \sigma_\eta^2) > 0.0002$. In the notation of Sec. 8.3.1, this is H_{02}.

First, refer to Sec. 8.1.2, question 8.B. Steps a to b are followed for each of the three groups defined in example 8.K.

Question 8.B

Step a. Group 1: $S_v^2 = 0.000200$

Group 2: $S_v^2 = 0.000750$

Group 3: $S_v^2 = 0.000171$

(These values were calculated in example 8.K, step a.)

Step b. Group 1: $R_1=\dfrac{(4)(0.000200)}{(0.0002)}=4.00$

Group 2: $R_2=\dfrac{(6)(0.000750)}{(0.0002)}=22.50$

Group 3: $R_3=\dfrac{(4)(0.000171)}{(0.0002)}=3.42$

In these calculations $\sigma_{m0}^2 = 0.0002$, the hypothesized value for $(\sigma_\varepsilon^2 + \sigma_\eta^2)$.

This comprises step a of Sec. 8.3.2 (a). Steps b and c of that section are now followed.

From Sec. 8.3.2(a)

Step b. $R = 4.00 + 22.50 + 3.42 = 29.92$

Step c. The critical value for R is read from Appendix B with $(4 + 6 + 4)$ or 14 degrees of freedom. For $\alpha = 0.025$ this critical value is 26.12. Since 29.92 exceeds 26.12, reject the hypothesis that $(\sigma_\varepsilon^2 + \sigma_\eta^2) = 0.0002$.

Example 8.M

Three separate shipments of PuO_2 powder each involved ten containers of powder. The PuO_2 was thoroughly characterized by both the shipper and the receiver, with a separate determination of percent plutonium made for each container. The data are given in Table 8.13.

TABLE 8.13 MEASUREMENTS OF PERCENT PLUTONIUM IN THREE SHIPMENTS OF PuO_2 POWDER
(Example 8.M)

Shipment 1		Shipment 2		Shipment 3	
s_i	r_i	s_i	r_i	s_i	r_i
87.039	87.071	86.935	86.973	87.004	86.913
87.088	87.103	86.837	86.848	87.074	86.049
87.107	87.080	87.054	87.019	87.053	87.220
87.330	87.367	87.023	86.970	87.158	87.183
87.023	87.100	87.064	86.977	87.079	87.068
86.988	87.083	86.935	86.889	86.984	86.995
87.003	87.050	86.895	86.872	86.845	86.854
86.910	86.835	86.828	86.770	87.002	86.925
87.123	87.087	86.868	86.769	87.016	86.999
87.111	87.144	86.979	87.018	87.068	87.011

These data are used to examine the following questions:

Question 8.H. At the $\alpha = 0.10$ level of significance, do the data support the hypothesis that σ_ε^2 and σ_η^2 are equal against the alternative that σ_ε^2 is less than σ_η^2?

Question 8.I. What is the estimate of σ_η^2?

Question 8.J. The hypothesized value for σ_η is 0.075. Do the data support this at the $\alpha = 0.01$ significance level against the one-sided alternative that $\sigma_\eta < 0.075$?

Question 8.K. What is the estimate of $(\sigma_\delta^2 + \sigma_\Delta^2)$, the combined systematic-error variances?

Question 8.H is a problem in hypothesis testing, with H_{01}: $\sigma_\varepsilon^2 = \sigma_\eta^2$ being the hypothesis. Following the steps of the solution, we must first calculate the sample averages, variances, and covariances. The results are:

Shipment 1	Shipment 2	Shipment 3
$\bar{s}=87.072$	$\bar{s}=86.942$	$\bar{s}=87.028$
$\bar{r}=87.092$	$\bar{r}=86.911$	$\bar{r}=87.022$
$S_s^2=0.012635$	$S_s^2=0.007462$	$S_s^2=0.006740$
$S_r^2=0.016335$	$S_r^2=0.008979$	$S_r^2=0.013207$
$S_{sr}=0.013119$	$S_{sr}=0.007071$	$S_{sr}=0.007375$
$n=10$	$n=10$	$n=10$

Then, the steps of question 8.A, Sec. 8.1.2, are followed:

Question 8.A

Steps a to c.

Shipment 1:

$S_u^2=0.055208$ (from Eq. 8.3)

$S_v^2=0.002732$ (from Eq. 8.4)

$S_{uv}=-0.003700$ (from Eq. 8.5)

$r_1=-0.301$ (from Eq. 8.6)

$t_1=-0.89$ (from Eq. 8.7)

Shipment 2:

$S_u^2=0.0030583$ $\quad r_2=-0.181$

$S_v^2=0.002299$ $\quad t_2=-0.52$

$S_{uv}=-0.001517$

Shipment 3:

$S_u^2=0.034697$ $\quad r_3=-0.482$

$S_v^2=0.005197$ $\quad t_3=-1.56$

$S_{uv}=-0.006467$

Then, the steps of H_{01} [Sec. 8.3.2 (a)] are followed:

From Sec. 8.3.2(a)

Step b. Since there are 8 degrees of freedom for each shipment, by interpolation in Table 8.11,

$p_1 = 0.20$ (for $t_1 = -0.89$)
$p_2 = 0.31$ (for $t_2 = -0.52$)
$p_3 = 0.077$ (graphical interpolation) (for $t_3 = -1.56$)

The one-sided alternative is $\sigma_\varepsilon^2 < \sigma_\eta^2$, whereas the table was constructed for $\sigma_\varepsilon^2 > \sigma_\eta^2$. Therefore, the sign of t_i is changed before determining the p_i value.

Step c. $P = -2(\ln 0.20 + \ln 0.31 + \ln 0.077)$
$= -2(-1.61 - 1.17 - 2.56) = 10.68$

Step d. At $\alpha = 0.10$, from Appendix B, with $2m = 6$ degrees of freedom, H_{01} is rejected if $P > 10.64$. Since $P = 10.68$, H_{01} is rejected, and it is concluded that σ_ε^2 is smaller than σ_η^2.

Question 8.I. What is the estimate of σ_η^2? Steps a to c of Sec. 8.3.2 (b) are followed.

From Sec. 8.3.2(b)

Step a. From Eq. 8.17,

$$\sigma_{\eta 1}^2 = 0.016335 - 0.013119 = 0.003216$$

$$\sigma_{\eta 2}^2 = 0.008979 - 0.007071 = 0.001908$$

$$\sigma_{\eta 3}^2 = 0.013207 - 0.007375 = 0.005832$$

Step b. In applying Eq. 8.44, note that the roles of S_s^2 and S_r^2 are reversed because the equation applies to estimation of σ_ε^2, but the problem under discussion is the estimation of σ_η^2.

$$V_1 = \frac{0.016335(0.032670 - 0.052476 + 0.012635) + 0.000172}{9}$$
$$= 0.00000610$$

$$V_2 = \frac{0.008979(0.017958 - 0.028284 + 0.007462) + 0.0000500}{9}$$
$$= 0.00000270$$

$$V_3 = \frac{0.013207(0.026414 - 0.029500 + 0.006740) + 0.0000544}{9}$$
$$= 0.0000114$$

Step c. $V_1^{-1} = 163{,}934 \qquad V_2^{-1} = 370{,}370 \qquad V_3^{-1} = 87{,}719$

$$\bar{\sigma}_\eta^2 = \frac{(163{,}934)(0.003216) + (370{,}370)(0.001908) + (87{,}719)(0.005832)}{163{,}934 + 370{,}370 + 87{,}719}$$
$$= 0.002806$$

[If we had determined that σ_ε^2 and σ_η^2 were not different, we could find the overall estimate of the random variance to apply to either the shipper or the receiver. According to Table 8.4, situation C, this is simply $S_r^2/2$ for each shipment:

Shipment 1: $\sigma_\varepsilon^2 = \sigma_\eta^2 = 0.002732/2 = 0.001366$

Shipment 2: $\sigma_\varepsilon^2 = \sigma_\eta^2 = 0.002299/2 = 0.001149$

Shipment 3: $\sigma_\varepsilon^2 = \sigma_\eta^2 = 0.005197/2 = 0.002598$

Averaged over all shipments, the straight average is a reasonable estimate since all are based on the same number of degrees of freedom, and the estimates are independent of σ_x^2, the process variance. In a more general situation, a weighted average would be calculated, with the weights being the degrees of freedom. Overall, the estimate of $\sigma_\varepsilon^2 = \sigma_\eta^2$ is 0.001704 for these data.]

Question 8.J. Test the hypothesis that $\sigma_\eta = 0.075$ against the alternative, $\sigma_\eta < 0.075$ [this is H_{04} of Sec. 8.3.2 (a)]. The first step involves calculating λ_{41}, λ_{42}, and λ_{43} from Eq. 8.15. To do this, we follow steps a to d of question 8.D, Sec. 8.1.2. The detailed calculations are shown only for Shipment 1.

Step a.

Shipment 1: Solve simultaneously Eqs. 8.13 and 8.14:

$$\hat{\sigma}_x^2 = \frac{0.0000003998 + 0.00014759\hat{\sigma}_\epsilon^2 + 0.016335\hat{\sigma}_\epsilon^4}{(\hat{\sigma}_\epsilon^2 + 0.005625)^2} - \frac{0.005625\hat{\sigma}_\epsilon^2}{\hat{\sigma}_\epsilon^2 + 0.005625}$$

$$\hat{\sigma}_\epsilon^2 = \frac{0.016335\hat{\sigma}_x^4 - 0.026238\hat{\sigma}_x^2(0.005625 + \hat{\sigma}_x^2) + 0.012635(0.005625 + \hat{\sigma}_x^2)^2}{(\hat{\sigma}_x^2 + 0.005625)^2} - \frac{0.005625\,\hat{\sigma}_x^2}{\hat{\sigma}_x^2 + 0.005625}$$

Using the iteration procedure (see example 8.B), we find the solutions to be

$$\hat{\sigma}_x^2 = 0.0160 \qquad \hat{\sigma}_\epsilon^2 = -0.00200$$

For Shipments 2 and 3 the solutions are

Shipment 2: $\hat{\sigma}_x^2 = 0.0101$ $\hat{\sigma}_\varepsilon^2 = -0.00153$

Shipment 3: $\hat{\sigma}_x^2 = 0.0073$ $\hat{\sigma}_\varepsilon^2 = -0.00056$

Step b.

Shipment 1: $\ln L(\hat{\Omega}) = -10 - 5 \ln (0.00020639 - 0.00017211)$
$= 41.405$

Shipment 2: $\ln L(\hat{\Omega}) = 44.911$

Shipment 3: $\ln L(\hat{\Omega}) = 41.355$

Step c.

Shipment 1: $\ln L(\hat{\omega}_4) = -5 \ln (0.00004675) - \dfrac{10\,(0.00008211)}{(0.00009350)}$
$= 41.072$

Shipment 2: $\ln L(\hat{\omega}_4) = 43.777$

Shipment 3: $\ln L(\hat{\omega}_4) = 41.351$

Step d.

Shipment 1: $\lambda_{41} = 2\,(41.405 - 41.072) = 0.67$

Shipment 2: $\lambda_{42} = 2.27$

Shipment 3: $\lambda_{43} = 0.01$

With these values for λ_{41}, λ_{42}, and λ_{43}, steps b and c of H_{04}, Sec. 8.3.2 (a), can now be followed.

From Sec. 8.3.2(a)

Step b. $\lambda_4 = 0.67 + 2.27 + 0.01 = 2.95$

Step c. The critical value for $\alpha = 0.01$ is found from Appendix B with $m = 3$ degrees of freedom. The hypothesis H_{04} is rejected if λ_4 exceeds the critical value, 11.34. Since $2.95 < 11.34$, do not reject the hypothesis. Conclude that $\sigma_\eta = 0.075$ is consistent with the data over the three shipments.

Question 8.K. Find the estimate of $(\sigma_\delta^2 + \sigma_\Delta^2)$. Follow the steps for estimating the systematic-error variance in Sec. 8.3.2 (c).

From Sec. 8.3.2(c)

Step a. $d_1 = 87.072 - 87.092 = -0.020$

$d_2 = 86.942 - 86.911 = 0.031$

$d_3 = 87.028 - 87.022 = 0.006$

Step b. $s_d^2 = \dfrac{(-0.020)^2 + (0.031)^2 + (0.006)^2}{3} = 0.000466$

Step c. With $\sigma_\varepsilon^2 = 0$ (which is the overall estimate of σ_ε^2 as would be determined by repeating question 8.I for σ_ε^2) and $\sigma_\eta^2 = 0.002806$, from Eq. 8.47,

$$\widehat{(\sigma_\delta^2+\sigma_\Delta^2)} = 0.000466 - \frac{(0.002806)}{3}\left(\frac{1}{10}+\frac{1}{10}+\frac{1}{10}\right) = 0.000185$$

This is the estimated sum of the systematic-error variances.

8.3.4 Basis

(a) *Hypothesis Testing*

For hypothesis H_{01} the solution is based on combining probabilities from different independent tests of the same hypothesis. Each p_i found in step a is the probability under the null hypothesis that the test statistic takes on a value of t_i or worse (worse in the sense that it offers even less support to the truth of the hypothesis). To combine the probabilities over the m sets of data, we use the fact that under the null hypothesis $-2\sum_{i=1}^{m} \ln p_i$ is distributed as chi-square with $2m$ degrees of freedom. Critical values for the test statistic are, therefore, read from a table of this distribution, Appendix B.

For hypothesis H_{02}, $(\sigma_\varepsilon^2 + \sigma_\eta^2)$ is estimated by the variance of the difference $(s - r)$ for each data set. Since the difference between the shipper and receiver value is a random variable assumed to be normally distributed, its sample variance multiplied by $(n_i - 1)$ and divided by the hypothesized variance $(\sigma_{\varepsilon o}^2 + \sigma_{\eta o}^2)$ is distributed as the chi-square distribution with $(n_i - 1)$ degrees of freedom for the ith data set. The sum of independently distributed chi-square random variables also is distributed as chi-square, with the degrees of freedom being the sum of the degrees of freedom for the individual chi-square variables. This is the basis for the test of significance for the R statistic given in step c, H_{02}, Sec. 8.3.2 (a).

For hypothesis H_{04} we use large-sample-distribution theory. Since λ_{41} in Eq. 8.15 is distributed as chi-square with 1 degree of freedom for each data set, i, it follows that the sum of the λ_{41} over all m data sets is also distributed as chi-square with $m \times 1$ or m degrees of freedom. This is the basis for the test of significance for the λ_4 statistic given in step c, H_{04}, Sec. 8.3.2 (a).

(b) *Estimation of Random-Error Variances*

It is assumed that for a given shipment σ_ε^2 is estimated from Eq. 8.16 and σ_η^2 from Eq. 8.17. The basis for the estimation procedure is established for σ_ε^2, with similar steps applying to σ_η^2.

For the i shipment, let V_i be the sampling variance of the estimate σ_ε^2. We will drop the i subscript for simplicity and calculate

$$V=\frac{2\sigma_\varepsilon^4+(\sigma_x^2\sigma_\varepsilon^2+\sigma_x^2\sigma_\eta^2+\sigma_\varepsilon^2\sigma_\eta^2)}{n-1} \tag{8.48}$$

This is a function of the two random-measurement variances, σ_ε^2 and σ_η^2; of the process variance, σ_x^2; and of number of paired observations, n. Since the variance parameters are not known, they are replaced by their estimates: S_{sr} is used for σ_x^2; $S_s^2 - S_{sr}$ is used for σ_ε^2; and $S_r^2 - S_{sr}$ is used for σ_η^2. Then, Eq. 8.48 reduces to

$$V=\frac{S_s^2(2S_s^2-4S_{sr}+S_r^2)+S_{rs}^2}{n-1} \tag{8.49}$$

This is Eq. 8.44.

Having found the variance of $\sigma_{\varepsilon_i}^2$ for the ith shipment, we find the overall estimate of σ_ε^2 by weighting the individual shipment estimates inversely as their variances. This is result 8.45. If it can be assumed that the process variance, σ_x^2, is constant over the data, Eq. 8.48 indicates that a simple weighted average, with the weights being the degrees of freedom, is suitable for finding the overall average of σ_ε^2. This is so because the numerator of V is then a constant.

We noted in example 8.M that we might wish to obtain an estimate of $\sigma_\varepsilon^2 = \sigma_\eta^2$ when there is no evidence to indicate that these two parameters are different. In this case, for a given shipment, the estimate is simply $S_{v_i}^2/2$. The sampling variance of this estimate does not depend on σ_x^2, and so a simple weighted average over the shipments, with the degrees of freedom providing the weights, is called for.

(c) Estimation of Systematic-Error Variances

The basis for the key estimation equation (8.47) is straightforward. The difference $d_i = \bar{s}_i - \bar{r}_i$ has variance $(\sigma_\delta^2 + \sigma_\Delta^2) + [(\sigma_\varepsilon^2 + \sigma_\eta^2)/n]$ from Eq. 8.34. Equation 8.47 then also follows immediately, the only complicating factor being that the different d_i can be based on different numbers of observations, n_i.

Chapter 9

INVENTORY VERIFICATION

OVERVIEW

The general situation treated is the inventory verification in which an audit team wishes to verify that the total physical inventory for a given facility, or for a given material balance area, is as represented by the operator of the facility. The term "audit team" is defined in general terms and would include a national agency such as the U.S. Atomic Energy Commission, an international agency such as the International Atomic Energy Agency, and a management audit team. Although the different groups have different motivations for verifying the physical inventory, the statistical problems are similar.

It is important to distinguish between *performing* a physical inventory and *verifying* an inventory. A facility operator performs a physical inventory of his nuclear material holdings with some given frequency. In general terms this involves physically accounting for all items whose special nuclear material (SNM) contents were measured when placed in inventory, reducing to measurable form the previously unmeasured items to the extent feasible, and obtaining measurements for such items. On the other hand, verification of a physical inventory is performed by an audit team and consists, again in general terms, in demonstrating that the items in the inventory are indeed locatable and, further, that they contain the amounts of SNM purported by the operator. As a matter of convenience, the operation and the audit team commonly carry on the two tasks simultaneously.

Chapter 9 is concerned with the latter task, that of inventory verification. In a sense the statistical problems associated with performing a physical inventory have been discussed in Chaps. 6 and 7, where it was shown how the measurement variance associated with the estimate of the total inventory affects the variance of material unaccounted for (MUF) to a degree that can be determined. The size of the inventory variance is affected by inventory practices, e.g., which analytical methods are used, to what extent common element and isotopic factors are applied, etc. Thus, in performing a physical inventory, the operator is guided in his

actions by the importance of the inventory variance as it affects the variance of MUF, the primary index of nuclear-materials-control performance.

What is the function of the inventory verification? In essence its role is to instill a degree of confidence in the integrity of the MUF value reported by the facility operator. There is no reduction in the measurement variance of MUF because of the activities of the audit team; in that sense the verification has accomplished nothing. If the audit team is a management team, however, this statement may not be strictly true, because measurements for audit purposes might also be used to obtain better estimates of the amount of SNM in inventory. But, unless intensive audit-inspection measurements are performed, the effect on the measurement variance of MUF will be negligible. Nevertheless, through verification we create some assurance that the inventory value used by the facility operator in the MUF calculation is valid. This degree of assurance can be calculated for certain verification activities, and audit inspection activities can be formulated to attain the specified degree of assurance. In general terms this is the statistical problem discussed in this chapter.

Of course, verification of an inventory is not equivalent to verification of the corresponding MUF, because MUF includes inputs and outputs in addition to inventories. In fact, in a facility that is not inventory dominated, verification of an inventory at some point in time might be of questionable importance. Although this limitation is recognized, it is common practice to verify inventories because it is feasible to do so and because it does serve as one checkpoint, while to verify inputs and outputs poses very real operational problems. Mathematically the results of this chapter on inventory verification can be extended to MUF verification by requiring that inputs and outputs also be audited. The problem is not mathematical but, rather, operational.

In broad terms two quite different verification activities are involved. On the one hand, the effort is directed at verifying that the frequency of gross discrepancies between the operator's stated values and the audit values is kept below a specified level. This can be called a step 1 activity and involves inspection on an attributes basis. For example, an item is weighed and a discrepancy is noted if the weight differs from the stated weight by more than a given amount.

Inspection on an attributes basis having been demonstrated with an acceptable degree of confidence, the next step is to draw a finer picture through variables inspection of the quality of the assigned inventory values that collectively comprise the entire inventory.

In an honest environment in which no diversion of SNM occurs, the step 1 verification activity is designed to detect operator mistakes (in the terminology of the Overview, Chap. 3); whereas the step 2 activity evaluates the validity of the stated measurement-error variances. On the other hand, in an audit situation in which the purported inventory may be

falsified to cover diversion of SNM, the two types of inspection activities, i.e., attributes and variables, will tend to react to different diversion strategies. For example, complete emptying of a few containers is combatted by attributes inspection, whereas partial emptying of a larger number of containers is more likely to be detected by the step 2 variables inspection. Whatever the diversion strategy, decisions on what actions to take should significant discrepancies be found by the audit team are complicated by the inability to distinguish, on the basis of the data alone, between honest mistakes and understated measurement-error variances on the one hand and diversions on the other hand. It is beyond the scope of this book to delve deeper into the problem of how to develop inspection strategies to counter diverter strategies. Rather, the emphasis is on determining the types of verification activities and the intensities that are needed to detect specified frequencies and kinds of discrepancies between inventory listings and actual inventories. Any given audit inspection strategy developed from this viewpoint can, of course, be evaluated against given diverter strategies.

The audit team must make a number of decisions as they design their verification effort and analyze the resulting data. One critical decision concerns specifying an unacceptable level of performance at step 1 and determining the probability that this unacceptable performance will be detected. If the audit indicates that actual performance at step 1 is worse than the specified tolerable level, whatever that level was decided to be, there may be little point in proceeding with the step 2 variables effort. Rather, the audit team may logically conclude that the frequency of discrepancies is such that the audit must be declared unsatisfactory regardless of the results of the variables inspection. In this sense the transition to step 2 occurs only when the step 1 performance is satisfactory. In mathematical terminology we might say that an acceptable step 1 audit is a necessary condition for an overall acceptable audit but not a sufficient condition.

In the verification activities in this chapter, the problem is structured to apply to facilities in which the inventory is kept in discrete containers that are accessible to the audit team. A container is defined in general terms to include a process vessel in a chemical reprocessing facility, for example, and in that sense the results of this chapter also apply to the production line in such a facility. In an audit inspection of certain types of containers there is a problem in that the audit team must in some instances rely on the sampling equipment of the operator and on the operator's bulk-determination equipment, although the team can still make its own independent analytical determination on the sample. In principle this chapter applies to all types of facilities, the only caution being that in some cases there is a question as to the degree of independence between measurement of the operator and that of the audit team.

To place the variables discussion in its proper framework, let me emphasize that here attention is focused on the total physical inventory as opposed to the inventory for a single class of items. If interest is restricted to a single class, the methods of Chap. 8, using paired comparisons, can be used for the variables data. Chapter 8 also gives some results on how information from several statistical tests can be combined to give an overall assessment of the validity of some hypothesis. This approach is not used here to combine information from the various strata, because the strata differ in their importance to the total inventory. Instead, for the variables data a single hypothesis test on the total inventory is performed. Material is classified into strata primarily to help define the verification effort.

Further, for the variables data a known error structure for both the plant and the inspector is assumed in this chapter. This assumption is essential in designing the inventory and is also used in the analysis unless the data indicate that some of the error variances estimated from the actual data differ significantly from the variances assumed. The validity of this assumption can be investigated for random-error variances by the methods of Chap. 8 within each class or stratum prior to the analysis indicated in Sec. 9.3.

There are compelling reasons for recommending that we assume known error variances. Often systematic-error variances dominate, and information about such errors cannot be derived from the inspection data unless we are willing to assume that the observed average differences are wholly explained by systematic errors. This clearly defeats the whole purpose of an audit, where the intent of the variables inspection is to detect measurement biases or small diversions against a backdrop of known systematic-error variances. Also, the use of known error variances counteracts the diverter strategy, which consists in intentionally inflating the random-error variances by removing differing amounts from a large number of containers. If the difference between the operator and audit measurement varies by a considerable amount over the data because of this strategy and if we must depend on the variation of this difference variable to estimate the random errors, the ability to detect real discrepancies is clearly reduced. Finally, as industrial experience continues to accumulate, the error variances will become better and better characterized. In this environment it is a waste of information to reestimate the error variances with each new set of data and to disregard previous experience.

In Secs. 9.1 and 9.2, the step 1 verification effort involving attributes inspection is treated first for a single class and then for all classes combined. Section 9.3 deals with the analysis of step 2 variables data on a paired comparison basis in which the audit measurement for a given item is compared with the corresponding facility result. Finally, Sec. 9.4 is concerned with the design of the variables verification from the viewpoint of optimal allocation of resources.

9.1 STEP 1 VERIFICATION ON AN ATTRIBUTES BASIS, SINGLE CLASS

9.1.1 Problem and Assumptions

For a given type of step 1 audit, N items in the total class or population are to be verified. A random sample of n of these items is selected by the audit team. Each item sampled is classified either as a defect or as being acceptable, the classification depending upon the size and nature of the discrepancy between the result of the operator and that of the audit team. The criteria for making this judgment are predetermined. In the population of N items, some unknown number, D, are truly defects. It is assumed that the audit team will not make errors of classification. That is, if the item in question is truly acceptable, the audit team will always reach this decision; if it is a defect, the team will always detect it.

The problem is to determine the sample size, n, and the critical value d_0 such that, if the number of defects in the sample equals or exceeds d_0, the audit result is considered to be unacceptable.

9.1.2 Solution

In solving this problem, we assign values to some input parameters. The value of N, of course, is known. Values must be chosen for D_0, D_1, α, and β, where these quantities are defined as follows:

1. If D_0 defects occur in the population of N items, conclude that the sample results are unsatisfactory with probability α.
2. If D_1 defects occur in the population of N items, conclude that the sample results are satisfactory with probability β or are unsatisfactory with probability $(1-\beta)$.

In the terminology of statistical hypothesis testing (Sec. 2.8), the null hypothesis is H_0: $D=D_0$, and the alternative hypothesis is H_1: $D=D_1$, with $D_1>D_0$. The value of α is the significance level or the probability of committing a type I error, and β is that of committing a type II error. For readers familiar with the terminology of acceptance sampling, D_0 can be regarded as an acceptable quality level (AQL) and D_1 as a rejectable quality level (RQL). In this context α is generally fixed at 0.05. In the special case of $\beta=0.10$, the RQL and the lot tolerance percent defective (LTPD) are identical.

Having specified N, D_0, D_1, α, and β, we can then determine the sample size n, the n items can be inspected, and the number of defects in the sample, d, can be counted. If $d \geq d_0$, H_0 is rejected, i.e., the audit result is considered unacceptable. [The quantity (d_0-1) is commonly called the acceptance number.]

The parameters n and d are the solutions to the following two equations.

The reader will recognize that these equations are based on the hypergeometric probability density function (see Sec. 2.4.2 and Eq. 2.90).

$$\sum_{d=d_0}^{D_0} \frac{\binom{D_0}{d}\binom{N-D_0}{n-d}}{\binom{N}{n}} = \alpha \tag{9.1}$$

$$\sum_{d=0}^{d_0-1} \frac{\binom{D_1}{d}\binom{N-D_1}{n-d}}{\binom{N}{n}} = \beta \tag{9.2}$$

These equations are difficult to solve. In practice, n and d_0 can be chosen by using published tables or approximate formulas. However, because of the many parameters involved, tabulation sufficiently extensive to meet all requirements is a physical impossibility. Tables designed specifically to meet the requirements of nuclear materials control applications have been published (Theodore S. Sherr, Attribute Sampling Inspection Procedure Based on the Hypergeometric Distribution, USAEC Report WASH-1210, Division of Nuclear Materials Security, May 1972). These tables provide solutions for 16 different combinations of α, β, AQL, and RQL.

If tables are not available or do not cover a particular case of interest, an approximation can be used. For large samples an approximate solution that may be useful follows. (This approximation was supplied by K. B. Stewart.) Define

$$p_0 = D_0/N \qquad \text{and} \qquad p_1 = D_1/N$$

Then n and d_0 have approximate solutions:

$$n \approx \frac{NG}{(N-1)(p_1-p_0)^2+G} \tag{9.3}$$

and

$$d_0 \approx np_0 + z_{1-\alpha}\sqrt{np_0(1-p_0)\left(1-\frac{n-1}{N-1}\right)} + 0.5 \tag{9.4}$$

where

$$G = \left[z_{1-\alpha}\sqrt{p_0(1-p_0)} + z_{1-\beta}\sqrt{p_1(1-p_1)}\right]^2 \tag{9.5}$$

and where z_p is defined by Appendix A for $p = (1-\alpha)$ and $p = (1-\beta)$.

The solutions for n and d will not be integers, but integral solutions are required in application, of course. Stewart suggests that, when d_0 is rounded down to d_{01} or up to d_{02}, then n can also be rounded down or up according to $d_{01}n/d_0$ or $d_{02}n/d_0$. A reasonable approach then is to round d_0 in both directions and determine the corresponding exact values of α and β from Eqs. 9.1 and 9.2. This not only provides information about the effect of rounding d_0 up or down but also indicates how well the approximation applies in the particular case being treated.

A different approximation is preferred in the common situation in which the audit team requires an acceptance number of zero defects and wishes to determine the sample size necessary to provide a specified value of β for a given D_1. Then the sample size n is given by

$$n=0.5(1-\beta^{1/D_1})(2N-D_1+1) \tag{9.6}$$

For this sample size and an acceptance number of 0, the α probability corresponding to a given D_0 can then be found from

$$1-\alpha=\left(1-\frac{2n}{2N-D_0+1}\right)^{D_0} \tag{9.7}$$

Note that when $D_0=0$, $\alpha=0$. Clearly there is zero probability of finding any defects in the sample when there are none in the population.

If the α probability is judged to be too large in a given application, the audit team may choose to use an acceptance number of 1, i.e., to conclude that the results are unsatisfactory if 2 or more defects are found in the sample. Then n can be found by solving Eq. 9.8 by trial and error:

$$\beta=\left(1-\frac{2n}{2N-D_1+1}\right)^{D_1}\left(1+\frac{nD_1}{N-D_1-n+1}\right) \tag{9.8}$$

This equation is solved rather easily. The α probability corresponding to a given D_0 is then calculated from Eq. 9.8 with $(1-\alpha)$ replacing β and D_0 replacing D_1.

In summary, the solution to choosing the appropriate attributes inspection procedure for a given population of N items is as follows:

Step 1. Select values for α, β, D_0, and D_1.

Step 2. Use a table such as in USAEC Report WASH-1210 to determine the sample size and the acceptance number.

Step 3. If a table is not available or does not cover the situation of interest and if an acceptance number of 0 is desired, find n from Eq. 9.6. The α probability corresponding to a given D_0 then is found by Eq. 9.7.

Step 4. If an acceptance number of 1 is desired, find n from Eq. 9.8. The value of α for given D_0 is then found by Eq. 9.8 with $(1-\alpha)$ replacing β and D_0 replacing D_1.

Step 5. If an acceptance number of 2 or more is desired, find n and d_0 from Eqs. 9.3 to 9.5. Round d_0 to integers d_{01} and d_{02} in both directions, and adjust n accordingly by $d_{01}n/d_0$ or $d_{02}n/d_0$, respectively. Evaluate the quality of the approximation and the effect of rounding d_0 up or down by calculating α and β from Eqs. 9.1 and 9.2.

9.1.3 Examples

Example 9.A

An inventory of cans containing UO_2 powder lists 400 items. A sample of n of these items is to be selected at random and weighed. If the weight disagrees by more than 100 g from that on the listing, this is called a defect. Four or fewer such defects in the listing are considered to be an acceptable performance, and the probability of reaching the opposite conclusion in this situation is set at 0.025. If there are 20 or more such defects, the probability of failing to detect the performance as unacceptable is set at 0.05. Determine n and the rejection number d_0 such that if the number of defects is greater than or equal to d_0 the performance is labeled unacceptable.

The parameters are

$$\begin{aligned} N &= 400 & \alpha &= 0.025 \\ D_0 &= 4 & \beta &= 0.05 \\ D_1 &= 20 \end{aligned}$$

This particular combination of parameter values is not contained in USAEC Report WASH-1210. (Since the audit team is free to select the parameter values, they can often choose values such that the tables in USAEC Report WASH-1210 will apply. The document also contains examples of how to apply the tables.) Since the acceptance number of 0 or 1 is not specified, step 5 is followed.

Step 5. First find p_0, p_1, $z_{1-\alpha}$, and $z_{1-\beta}$.

$$\begin{aligned} p_0 &= D_0/N = 0.01 \\ p_1 &= D_1/N = 0.05 \\ z_{1-\alpha} &= z_{0.975} = 1.960 \quad \text{(from Appendix A)} \\ z_{1-\beta} &= z_{0.95} = 1.645 \quad \text{(from Appendix A)} \end{aligned}$$

Then, from Eq. 9.5,

$$G = \left[1.960\sqrt{(0.01)(0.99)} + 1.645\sqrt{(0.05)(0.95)}\right]^2 = 0.3064$$

From Eq. 9.3,

$$n=\frac{(400)(0.3064)}{(399)(0.04)^2+(0.3064)}=129.7$$

From Eq. 9.4,

$$d_0=(129.7)(0.01)+1.960\sqrt{(129.7)(0.01)(0.99)\left(1-\frac{128.7}{399}\right)}+0.5$$
$$=3.63$$

Then evaluate α and β for the two decision rules:

Rule 1. Choose $n=[(3)(129.7)/3.63]=108$ and label the performance unacceptable if there are ≥ 3 defects in the sample. (Acceptance number = 2.)

Rule 2. Choose $n=[(4)(129.7)/3.63]=143$, with a reject criterion of ≥ 4 defects.

For rule 1, with $d_{01}=3$ and $n=125$, find α from Eq. 9.1 and β from Eq. 9.2. In the evaluation of α by Eq. 9.1, if D_0 is considerably larger than d_0, i.e., if d_0 is small relative to (D_0-d_0), it will be simpler to evaluate $(1-\alpha)$ as the summation from $d_0=0$ to d_0-1.

$$\alpha=\frac{\binom{4}{3}\binom{396}{105}}{\binom{400}{108}}+\frac{\binom{4}{4}\binom{396}{104}}{\binom{400}{108}}$$
$$=\frac{4!\,396!\,108!\,292!}{3!\,1!\,105!\,291!\,400!}+\frac{396!\,108!\,292!}{104!\,292!\,400!}$$
$$=0.0567+0.0051=0.0618$$
$$\beta=\frac{\binom{20}{0}\binom{380}{108}}{\binom{400}{108}}+\frac{\binom{20}{1}\binom{380}{107}}{\binom{400}{108}}+\frac{\binom{20}{2}\binom{380}{106}}{\binom{400}{108}}$$
$$=0.0015+0.0122+0.0452=0.0589$$

A table of logarithms of factorials is helpful in this calculation.

For rule 2, $d_{02}=4$ and $n=143$. Then

$$\alpha=\frac{\binom{4}{4}\binom{396}{139}}{\binom{400}{143}}=0.0159$$

$$\beta = \frac{\binom{20}{0}\binom{380}{143}}{\binom{400}{143}} + \cdots + \frac{\binom{20}{3}\binom{380}{140}}{\binom{400}{143}}$$

$$= 0.0001 + 0.0013 + 0.0074 + 0.0261 = 0.0349$$

Thus, to summarize with rule 1:

$$\alpha = 0.0618 \qquad \beta = 0.0589$$

and to summarize with rule 2:

$$\alpha = 0.0159 \qquad \beta = 0.0349$$

These values are compared with the design value for α and β of 0.025 and 0.05, respectively, and the choice is then made as to which rule to use, depending on the emphasis placed on the importance of attaining the design values, or better, for α and β. It is impossible to select a plan that will produce exactly the design values for α and β.

Example 9.B

An inventory of bottles of plutonium nitrate lists 300 items in various locations. A sample of n of these is to be selected at random and an attempt made to locate them. If even one item in the sample cannot be located, the performance will be declared unacceptable. If, in fact, as many as 2 items on the list cannot be found, the audit team wishes to detect this condition with a probability of 0.90. How many items should be checked?

In this example, since the acceptance number is set at 0, step 3 applies, and the sample size n is given by Eq. 9.6. The parameter values are $N = 300$, $D_1 = 2$, and $\beta = 1 - 0.90 = 0.10$. Then

Step 3. $n = 0.5[1 - (0.10)^{0.5}](600 - 2 + 1) = 204.8 = 205$

To evaluate the α probability at $D_0 = 1$, apply Eq. 9.7:

$$1 - \alpha = \left(1 - \frac{410}{600 - 1 + 1}\right)^1 = 0.317 \qquad \alpha = 0.683$$

Example 9.C

Using the information in example 9.B, assume that the β error probability is set at 0.10 when there are 4 defects rather than 2 defects in the population of size 300. Then, from Eq. 9.6, the sample size n is

$$n = 0.5[1 - (0.10)^{0.25}](600 - 4 + 1) = 130.6 = 131$$

Evaluate α at $D_0=2$ defects. By the application of Eq. 9.7,

$$1-\alpha=\left(1-\frac{262}{599}\right)^2=0.317 \qquad \alpha=0.683$$

Suppose this error probability is larger than desired. It can be reduced by increasing the sample size and changing the acceptance number from 0 to 1 to retain the same β probability. For an acceptance number of 1, the sample size n is calculated from Eq. 9.8.

$$0.10=\left(1-\frac{2n}{597}\right)^4\left(1+\frac{4n}{297-n}\right)$$

By trial and error, n is easily found as follows:

At n equal to	The expression is
180	0.178
200	0.110
210	0.082
205	0.095
204	0.098←——Value for n to give $\beta=0.10$

The corresponding α error probability for $D_0=2$ is given by Eq. 9.8, with $(1-\alpha)$ replacing β and D_0 replacing D_1,

$$1-\alpha=\left(1-\frac{408}{599}\right)^2\left(1+\frac{408}{95}\right)$$

$$=0.538 \qquad \alpha=0.462$$

In this example, since d_0 is so small relative to D_0 and in fact they are equal, it would be simpler to calculate α directly by Eq. 9.1 than to use the approximation (Eq. 9.8). To three decimals, the results are equivalent.

9.1.4 Basis

Equations 9.1 and 9.2 are based on the hypergeometric probability distribution discussed in Sec. 2.4.2. The left-hand side of Eq. 9.1 is the probability of finding d_0 or more defects in a sample of size n selected from a population of size N when there are D_0 defects in the population. This occurrence of d_0 or more effects results in rejection of the hypothesis $D=D_0$ when in fact the hypothesis is true and is to occur with probability α. The left-hand side of Eq. 9.2 is the probability of finding less than d_0 defects in this sample when there are D_1 defects in the population. This is a type II error and is to occur with probability β.

Equations 9.3 to 9.5 provide approximate solutions to Eqs. 9.1 and 9.2. Use is made of the normal approximation to the hypergeometric distribution. If X is the random variable that is the number of defects in a sample of size n, we know that the random variable has a mean and variance given by

$$E(x)=np$$

$$\sigma_x^2=np(1-p)\left(1-\frac{n-1}{N-1}\right)$$

where $p=d/N$ and d is the true number of defects in the population. (See Eqs. 2.37 and 2.39.) Then α and β are given by

$$\alpha=\Pr\,(x\geq d_0\,|p_0) \qquad \text{and} \qquad \beta=\Pr\,(x<d_0\,|p_1)$$

where the null hypothesis is

$$H_0:\ p=p_0$$

and the alternative is

$$H_1:\ p=p_1$$

Assume that x is approximately normally distributed, and make a correction for continuity; i.e., replace Pr $(x\geq d_0)$ with Pr $(x>d_0-0.5)$, and replace Pr $(x<d_0)$ with Pr $(x<d_0-0.5)$. Then the equations for α and β reduce to Eqs. 9.9 and 9.10 after standardization of the variables by subtracting the means and dividing by the standard deviations.

$$\frac{d_0-0.5-np_0}{\sqrt{np_0(1-p_0)[1-(n-1)/(N-1)]}}=z_{1-\alpha} \tag{9.9}$$

and

$$\frac{d_0-0.5-np_1}{\sqrt{np_1(1-p_1)[1-(n-1)/(N-1)]}}=-z_{1-\beta} \tag{9.10}$$

where

$$\int_z^\infty f(x)\,dx=1-p$$

defines α and β, where $f(x)\,dx$ is the standardized normal density function.

Then Eq. 9.4 is found by solving Eq. 9.9 for d_0. Also, Eq. 9.3 is found by using this value for d_0 in Eq. 9.10 and solving for n. For simplicity in notation, G is defined as in Eq. 9.5 in writing the solution for n.

Finally, consider the basis for Eqs. 9.6 to 9.8. With an acceptance number of 0, β in Eq. 9.2 is evaluated at $d_0=1$. This is

$$\beta=\frac{\binom{D_1}{0}\binom{\mathcal{N}-D_1}{n}}{\binom{\mathcal{N}}{n}}=\frac{(\mathcal{N}-D_1)!\,n!\,(\mathcal{N}-n)!}{n!\,(\mathcal{N}-D_1-n)!\,\mathcal{N}!}$$

$$=\frac{(\mathcal{N}-n)(\mathcal{N}-n-1)(\mathcal{N}-n-2)\ldots(\mathcal{N}-n-D_1+1)}{\mathcal{N}(\mathcal{N}-1)(\mathcal{N}-2)\ldots(\mathcal{N}-D_1+1)}$$

$$=\left(1-\frac{n}{\mathcal{N}}\right)\left(1-\frac{n}{\mathcal{N}-1}\right)\left(1-\frac{n}{\mathcal{N}-2}\right)\ldots\left(1-\frac{n}{\mathcal{N}-D_1+1}\right)$$

There are D_1 factors in this expression. The "middle" factor is

$$\left(1-\frac{2n}{2\mathcal{N}-D_1+1}\right)$$

Therefore β can be written approximately

$$\beta\approx\left(1-\frac{2n}{2\mathcal{N}-D_1+1}\right)^{D_1} \tag{9.11}$$

That is, all the D_1 factors are assumed to have the same value as the middle factor; therefore the product is this middle factor raised to the D_1 power.

Solving this for n gives

$$n=0.5(1-\beta^{1/D_1})(2\mathcal{N}-D_1+1) \tag{9.12}$$

which is the result, Eq. 9.6. Equation 9.7 is derived by the same reasoning and is, in fact, Eq. 9.11 with β replaced by $(1-\alpha)$ and D_1 replaced by D_0.

To derive Eq. 9.8, we find the probability of obtaining zero or one defect and equate this to β. The probability of obtaining zero defects is given by Eq. 9.11. The probability of obtaining one defect is

$$\frac{\binom{D_1}{1}\binom{\mathcal{N}-D_1}{n-1}}{\binom{\mathcal{N}}{n}}=\frac{D_1(\mathcal{N}-D_1)!\,n!\,(\mathcal{N}-n)!}{(n-1)!\,(\mathcal{N}-D_1-n+1)!\,\mathcal{N}!}$$

This expression is exactly $[nD_1/(\mathcal{N}-D_1-n+1)]$ times the corresponding probability for zero defects.

Therefore for an acceptance number of 1, β can be written

$$\beta \approx \left(1-\frac{2n}{2N-D_1+1}\right)^{D_1}+\frac{nD_1}{(N-D_1-n+1)}\left(1-\frac{2n}{2N-D_1+1}\right)^{D_1}$$

$$\approx \left(1-\frac{2n}{2N-D_1+1}\right)^{D_1}\left(1+\frac{nD_1}{N-D_1-n+1}\right) \tag{9.13}$$

which is Eq. 9.8.

9.2 STEP 1 VERIFICATION ON AN ATTRIBUTES BASIS, SEVERAL CLASSES

9.2.1 Problem and Assumptions

In Sec. 9.1, only a single population or class of N items was considered. In an actual audit several classes normally are involved, and a decision is made as to the acceptability of each class on the basis of attributes data. When this is done and when it is required that *all* the classes produce acceptable results before the step 1 verification is accepted as satisfactory, the overall significance level is smaller than the significance level of any one of the individual tests. Since a very small significance level implies that the operator has little chance of successfully meeting the audit requirements, it is important to take into account the multiplicity of individual significance tests made during the course of the audit.

Specifically, suppose the step 1 attributes inspection consists of m separate classes, with a decision made as to acceptability of the results for each class. Further, suppose that each class must produce a satisfactory result (i.e., no hypotheses can be rejected) for the overall step 1 audit results to be satisfactory. The problem is to choose the α_i $(i=1, 2, \ldots, m)$ to produce a given value for α for the entire attributes inspection. Here, α_i is the significance level for the ith class or for the ith test of hypothesis, whereas α is the probability of declaring that the overall step 1 audit results are unsatisfactory when, in fact, they do meet the requirements for satisfactory performance.

9.2.2 Solution

In application some attributes analyses may be much more important than others, the importance depending on the material involved and/or the nature of the defect. This section is concerned only with the control of the α value, and, except for the possibility that different α values can apply to the different tests of significance, all tests are comparable in the sense that each must produce a satisfactory result before the entire attributes

verification audit is judged satisfactory. The relative importance of the various analyses can be taken into account by controlling the size of the β probability for a given D_1 value, rather than by controlling the size of α.

Select a value for α for the overall step 1 audit. Also select $\alpha'_1, \alpha'_2, \ldots, \alpha'_m$ values for each significance test, initially disregarding the fact that m such tests will be performed. Then the values of $\alpha_1, \alpha_2, \ldots, \alpha_m$ to use in application are given by solving Eq. 9.15 for c and using the relation

$$\alpha_i = c\alpha_i' \tag{9.14}$$

$$\prod_{i=1}^{m} (1 - c\alpha_i') = 1 - \alpha \tag{9.15}$$

In the event all the α_i' are equal, the solution for $\alpha_i = c\alpha_i'$ becomes

$$\alpha_i = c\alpha_i' = [1 - (1-\alpha)^{1/m}] \tag{9.16}$$

When this situation does not obtain, since the α's are normally small quantities, an approximate solution for c in Eq. 9.15 is

$$c \approx \frac{\alpha}{\alpha_1' + \alpha_2' + \ldots + \alpha_m'} \tag{9.17}$$

9.2.3 Examples

Example 9.D

In a step 1 verification activity, five different attributes tests are to be made, and all tests must produce satisfactory results before the step 1 verification audit is deemed satisfactory. The overall α value selected is 0.05. Other significance tests being disregarded, the α value for each analysis would be the same, 0.10. (The solution is independent of this value and depends only on the requirement that all α_i values be the same.) What values of α_i should be used for each analysis, i, to achieve the overall α value of 0.05? The solution is Eq. 9.16 with $\alpha = 0.05$ and $m = 5$.

$$\alpha_i = 1 - (0.95)^{1/5} = 0.0102$$

Thus an α value of 0.0102 should be used in each analysis.

Example 9.E

In example 9.D suppose the a priori α values for the five analyses are set at

$$\alpha_1' = \alpha_2' = 0.025 \qquad \alpha_4' = \alpha_5' = 0.10$$
$$\alpha_3' = 0.05$$

Then, by Eq. 9.17,

$$c \approx \frac{0.05}{(0.025+0.025+0.05+0.10+0.10)} = 0.167$$

By Eq. 9.14, the values assigned to the α_i are then

$$\alpha_1 = \alpha_2 = (0.167)(0.025) = 0.0042$$
$$\alpha_3 = (0.167)(0.05) = 0.0084$$
$$\alpha_4 = \alpha_5 = (0.167)(0.10) = 0.0167$$

As a check on this approximation, the true α corresponding to these values of the α_i is given by Eq. 9.15.

$$\alpha = 1 - (0.9958)(0.9958)(0.9916)(0.9833)(0.9833) = 0.0493$$

which is a satisfactory approximation.

9.2.4 Basis

The situation is as follows: For test of significance i, the null hypothesis is designated by H_{0i}: number of defects $\leq D_{0i}$. Assign α_i' such that

$$\alpha_i' = \Pr\,(H_{0i} \text{ is rejected} \mid H_{0i} \text{ is true}) \tag{9.18}$$

Here, α_i' is chosen without regard to the number of attributes tests that will be made. When there are m such tests, with an overall α corresponding to the probability that H_{0i} is rejected for one or more i when in fact H_{0i} is true for all i, it is reasonable to multiply each α_i' value by some constant, c, to attain this value of α. The fundamental relation is

$$\alpha = 1 - (1-\alpha_1)(1-\alpha_2) \ldots (1-\alpha_m) = 1 - \prod_{i=1}^{m} (1-c\alpha_i')$$

or

$$\prod_{i=1}^{m} (1-c\alpha_i') = 1-\alpha$$

which is Eq. 9.15.

If all the α_i' are equal, Eq. 9.15 becomes

$$(1-c\alpha_i')^m = (1-\alpha)$$

or

$$c\alpha_i' = 1-(1-\alpha)^{1/m}$$

which is Eq. 9.16.

If the α_i' values differ, Eq. 9.15 becomes

$$\ln (1-c\alpha_1') + \ln (1-c\alpha_2') + \ldots + \ln (1-c\alpha_m') = \ln (1-\alpha) \quad (9.19)$$

For small values of the α's, which usually obtain, these logarithms are approximated by the relation

$$\ln (1-x) \approx -x$$

so that Eq. 9.19 becomes

$$-c(\alpha_1' + \alpha_2' + \ldots + \alpha_m') \approx -\alpha$$

or

$$c \approx \frac{\alpha}{\alpha_1' + \alpha_2' + \ldots + \alpha_m'}$$

which is Eq. 9.17.

9.3 VERIFICATION ON A VARIABLES BASIS, PAIRED COMPARISONS

9.3.1 Problem and Assumptions

Having verified that the frequency of gross discrepancies is below a tolerable level on the basis of the step 1 attributes inspection, the inspection team moves to step 2 for a closer investigation of the quality of the facility's assigned values. This involves verifying that the total inventory is as stated by the facility within known errors of measurement.

Although the attributes inspection has demonstrated that the frequency of gross discrepancies is below a tolerable level, it is conceivable that during the step 2 variables inspection one or more instances of a gross discrepancy between the facility and the audit team value may be noted. Although it is not reasonable to simply ignore such a result, it is less reasonable to include it in the variables data analysis, which is aimed at evaluating the general quality of the facility data exclusive of the gross discrepancies. We assume in this section that any such discrepancy noted during the step 2 inspection effort is not included in the variables analysis.

In this section the verification is assumed to be with respect to the amount of element (uranium or plutonium). But, if interest is centered on the amount of isotope, the results can easily be extended to accomplish this.

We further assume that the entire inventory can be divided into strata such that within each stratum the items are comparable with respect to their nuclear material accountability characteristics; i.e., within a given stratum the items are of similar material form and have about the same weight and element concentration. Although there may be a certain degree of arbitrariness in defining the strata in a given situation, this does not pose any serious problem in application. This assumption of similarity within a given stratum makes it natural to compare operator results with audit team results within a given stratum by the method of paired differences, discussed in Chap. 8. In this section the emphasis is on total inventory, whereas in Chap. 8 it is on a single stratum. If the analysis discloses a significant discrepancy between the facility and audit team total inventory values, then an analysis on a per stratum basis would help isolate the cause or causes for the discrepancy. Also note that the methods of Chap. 8 can be applied to verify that the random-error variances are as stated by the operator. With the method of paired differences, measurement-error standard deviations can more conveniently be expressed on an absolute basis than on a relative basis. This is possible because of the uniformity of items within a given stratum such that a relative error of 0.3%, for example, associated with a given measurement can readily be expressed in absolute terms by taking 0.3% of an average value within the stratum for the measurement in question.

The data are as follows: Each item in inventory is assigned a value of total element weight by the operator. For the items within a given stratum, this can be accomplished in one of three ways:

Method 1. The element weight is determined uniquely for each item in the stratum by bulk determination plus sampling and analysis for the element factor. The element factor is the ratio of the amount of the element (uranium or plutonium) to the total amount of material comprising the net weight (or volume) for the item in question.

Method 2. The element weight is determined uniquely for each item in the stratum by nondestructive assay (NDA).

Method 3. The material net weight (or volume) is determined uniquely for each item, but an average element factor is used to apply to all items in the stratum in determining the element weight.

Measurements between the various strata may not be statistically independent of one another. For example, a given scale may be used in more than one stratum, or the same analytical technique may be used in different strata, or, possibly, the same NDA instrument may be used. This information can be supplied by filling out a table such as Table 9.1.

TABLE 9.1 MEASUREMENT METHODS FOR VARIOUS STRATA

Stratum	Method*	Scale†	Analytical technique	NDA equipment
1	1	2	1	
2	1	1	1	
3	3	2	3	
4	2			1
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.

* Method 1, 2, or 3 as defined in text.

† In the case of volume determinations, the scale would be replaced by the equipment used to determine the volume.

The final information required from the operator is his stated error standard deviations, both random and systematic. (No short-term systematic-error variances are defined; if such are identified, they are included in the long-term component.) These standard deviations are identified as

σ_{Ω_k} Systematic-error standard deviation due to weighing on scale k

σ_{ξ_k} Random-error standard deviation due to weighing on scale k

σ_{Γ_p} Systematic-error standard deviation due to determining element factor with technique p; includes the effects of errors introduced by sampling the materials

σ_{τ_p} Random-error standard deviation due to determining element factor with technique p; includes the effects of errors introduced by sampling the materials

σ_{Λ_t} Systematic-error standard deviation due to making NDA measurement with equipment t

τ_{ζ_t} Random-error standard deviation due to making NDA measurement with equipment t

In the verification activity, the audit team uses the same method as the operator in each stratum. (The term "method" refers to methods 1, 2, and 3, previously defined in this section. This does not mean that the operator and facility necessarily use the same analytical technique.) This assumption is not as restrictive or unreasonable as may appear at first glance. Verification on a variables basis is under discussion, and any wide-scale use of relatively crude NDA instruments, for example, by the audit team would likely be on an attributes basis, i.e., in the step 1 inspection

effort. With variables measurements the audit team would be inclined to make fewer measurements but use the best means available for analysis.

As a further assumption the measurements made by the audit team are independent of those made by the operator. This independence is achieved (1) by the use of different scales (or at least a different set of standard weights to use with the operator's scales) and NDA instruments and (2) by submitting samples to a different laboratory for analysis (see Example 9.H to indicate the effect of a failure in this assumption). The audit team also prepares a table similar to Table 9.1 identifying the method, scale, and analytical technique, or NDA equipment, used in each stratum and associating the appropriate error standard deviations with each type of measurement. There is no overlap between the operator's identification and that of the audit team. Even if the same analytical technique is used in a given stratum for both parties, this is done in two different laboratories and hence is identified as separate techniques.

Given this background information and data consisting of the operator's inventory listing plus the results of measurements by the audit team, the problem is to determine whether or not the total inventory is as stated by the operator within the stated measurement errors.

9.3.2 Solution

The total inventory to be verified is divided into q strata. For each stratum the available information is given as in Table 9.1 for the operator, with a similar table for the audit team. In addition, the following values are given:

N_i = the number of items in stratum i

Methods 1 and 2. n_i = the number of items *measured* by the audit team.

Method 3. n_i = number of items *weighed* by the audit team.
M_i = number of samples used (assume one analysis per sample) to determine the element factor for the operator.
m_i = number of samples used (assume one analysis per sample) to determine the element factor for the audit team.

The sample sizes n_i and m_i are assumed given in this section (see Sec. 9.4 for their optimal selection in designing the audit).

In addition to the preceding information, the error standard deviations are supplied by the operator for his measurements, and the audit team has similar information about its error standard deviations.

The following notation is used:

Method 1. Y_{ij} = operator element weight, stratum i, item j.
y_{ij} = audit team element weight, stratum i, item j.

Method 2. $\mathcal{Z}_{ij}$, z_{ij} similarly defined for NDA measurements.

Method 3. W_{ij}, w_{ij} similarly defined for net *item* weight, as opposed to *element* weight.

$\overline{U}_i$ = operator average element factor, stratum i.

$\bar{u}_i$ = audit team average element factor, stratum i.

Then the estimated total discrepancy, or difference, between the audit team's estimate of the total inventory and that of the operator is found as follows:

Step 1. For each stratum using method 1, sum the differences $(y_{ij}-\mathcal{Y}_{ij})$ from $j=1$ to n_i. In this step and in all subsequent discussions in this chapter, it is convenient to index the items in each stratum such that the items sampled by the inspector are the first n_i of the N_i total items.

Step 2. Multiply each sum of step 1 by N_i/n_i.

Step 3. Sum these quantities over all strata using method 1. Call this sum D_1.

Step 4. For each stratum using method 2, sum the differences $(z_{ij}-\mathcal{Z}_{ij})$ from $j=1$ to n_i.

Step 5. Multiply each sum by N_i/n_i.

Step 6. Sum these quantities over all strata using method 2. Call this sum D_2.

Step 7. For each stratum using method 3, sum the differences $(w_{ij}-W_{ij})$ from $j=1$ to n_i.

Step 8. Multiply each sum by N_i/n_i.

Step 9. Sum the W_{ij} from $j=1$ to N_i.

Step 10. Add the quantities of steps 8 and 9, and multiply by $\bar{u}_i$.

Step 11. Multiply each sum in step 9 by $\overline{U}_i$.

Step 12. Subtract each quantity in step 11 from the quantity in step 10 for each stratum.

Step 13. Sum the results of step 12 over all strata using method 3. Call this sum D_3.

Step 14. Find $D=D_1+D_2+D_3$. This is the estimated total difference between the audit team's estimate of the total inventory and that of the operator. A positive value of D indicates the audit team's estimate is higher.

The statistical significance of D is judged by knowing its variance, denoted by $V(D)$. There are six types of error variances: $\sigma^2_{\Omega_k}$, $\sigma^2_{\xi_k}$, $\sigma^2_{\Gamma_p}$, $\sigma^2_{\tau_p}$, $\sigma^2_{\Lambda_t}$, and $\sigma^2_{\zeta_t}$. The $V(D)$ is given by the formula

$$V(D) = \sum_{k=1}^{K} A_{1k}\sigma^2_{\Omega_k} + \sum_{k=1}^{K} A_{2k}\sigma^2_{\xi_k} + \sum_{p=1}^{P} A_{3p}\sigma^2_{\Gamma_p} + \sum_{p=1}^{P} A_{4p}\sigma^2_{\tau_p} + \sum_{t=1}^{T} A_{5t}\sigma^2_{\Lambda_t} + \sum_{t=1}^{T} A_{6t}\sigma^2_{\zeta_t} \tag{9.20}$$

where K is the total number of scales for both the operator and the audit team and P and T are similarly defined for analytical techniques and NDA instruments, respectively.

Table 9.2 gives the rules for calculating the A coefficients in Eq. 9.20.

Once D and $V(D)$ are calculated, D can be tested for statistical significance. The hypothesis is $D=0$ against the two-sided alternative,

TABLE 9.2 RULES FOR CALCULATING THE COEFFICIENTS IN EQ 9.20

Rule	Description	Calculation steps*
A	Systematic-error variance, scale k†	(1) Multiply N by average element factor (2) Sum over the strata (3) Square the sum; this is A_{1k}
B	Random-error variance, scale k	(1) Multiply N by average element factor (2) Square this quantity (3) Divide by n (4) Sum over the strata; this is A_{2k}
C	Systematic-error variance, analytical technique p	(1) Multiply N by average item net weight (2) Sum over the strata (3) Square the sum; this is A_{3p}
D	Random-error variance, analytical technique p	(1) Multiply N by average item net weight (2) Square this quantity (3) Divide by n if a method 1 stratum Divide by M if a method 3 stratum, operator measurement Divide by m if a method 3 stratum, audit team measurement (4) Sum over the strata; this is A_{4p}
E	Systematic-error variance, NDA instrument t	(1) Sum the N values over the strata (2) Square the sum; this is A_{5t}
F	Random-error variance, NDA instrument t	(1) Square N (2) Divide by n (3) Sum over the strata; this is A_{6t}

* In each case the calculation is performed for all strata using scale k, analytical technique p, or NDA instrument t. This is done for both the operator and the audit team.

† This development is in terms of bulk determination by weight rather than by volume. The same type of rules would apply to volume determinations.

$D \neq 0$, since both understatements and overstatements of inventory by the operator are to be detected. The test consists in forming the statistic

$$D^* = \frac{D}{\sqrt{V(D)}} \tag{9.21}$$

and concluding that the difference is not zero if D^* exceeds the critical value, D_α, in absolute value. The value D_α depends on the significance level of the test, and values of particular interest are extracted from Appendix A and appear in Table 9.3.

TABLE 9.3 CRITICAL VALUES OF D_α

α	D_α
0.10	1.645
0.05	1.960
0.025	2.242
0.01	2.576

9.3.3 Examples

Example 9.F

An inventory in a fuel fabrication facility is verified by using variables data. The definition of the strata and other appropriate information are given in Table 9.4. The pertinent data are as follows:

Stratum 1 (UO_2 Powder)

$$\sum_{j=1}^{40} (w_{1j} - W_{1j}) = -0.062 \quad \text{kg}$$

$$\sum_{j=1}^{300} W_{1j} = 6030.60 \quad \text{kg}$$

Average net item weight $= 6030.60/300 = 20.102$ kg
Operator uranium factor $= 0.8760 = \bar{U}_1$
Audit team uranium factor $= 0.8754 = \bar{u}_1$

Stratum 2 (Sintered UO_2 Pellets)

$$\sum_{j=1}^{26} (w_{2j} - W_{2j}) = -0.29 \quad \text{kg}$$

$$\sum_{j=1}^{180} W_{2j} = 1102.320 \quad \text{kg}$$

Average net item weight = 1102.320/180 = 6.124 kg
Operator uranium factor = 0.8810 = $\bar{U}_2$
Audit team uranium factor = 0.8807 = $\bar{u}_2$

Stratum 3 (ADU Scrap)

$$\sum_{j=1}^{6} (y_{3j} - Y_{3j}) = -2.136 \quad \text{kg}$$

Average net item weight = 18.214 kg
Average uranium factor = 0.527

Stratum 4 (Grinder Sludge)

$$\sum_{j=1}^{4} (y_{4j} - Y_{4j}) = +0.413 \quad \text{kg}$$

Average net item weight = 5.907 kg
Average uranium factor = 0.664

Stratum 5 (Solid Waste)

$$\sum_{j=1}^{12} (z_{5j} - Z_{5j}) = -0.048 \quad \text{kg}$$

The error standard deviations supplied by the operator and the audit team are shown in Table 9.5.

TABLE 9.4 INVENTORY VERIFICATION DATA
(Example 9.F)

Stratum	Material	N_i	Method	n_i	m_i	M_i	Operator			Audit team		
							Scale	Anal.	NDA	Scale	Anal.	NDA
1	UO_2 powder	300	3	40	5	22	1	1		4	4	
2	Sintered UO_2 pellets	180	3	26	8	30	2	1		4	4	
3	ADU scrap	15	1	6			3	2		4	5	
4	Grinder sludge	30	1	4			3	3		4	5	
5	Solid waste	75	2	12					1			2

TABLE 9.5 MEASUREMENT-ERROR STANDARD DEVIATIONS
(Example 9.F)

	Scale (k)	Systematic (σ_{δ_k})	Random (σ_{ξ_k})
Operator	1	0.0010	0.0015
	2	0.0006	0.0010
	3	0.005	0.010
Audit team	4	0.002	0.005
	Analytical technique (p)	**Systematic (σ_{Γ_p})**	**Random (σ_{τ_p})**
Operator	1	0.0003	0.0005
	2	0.020	0.028
	3	0.006	0.022
Audit team	4	0.0004	0.0007
	5	0.015	0.020
	NDA instrument (t)	**Systematic (σ_{Δ_t})**	**Random (σ_{Γ_t})**
Operator	1	0.002	0.009
Audit team	2	0.003	0.010

This is all the information required to evaluate the audit results. First, D, the difference in the estimates of the total inventory, is found from the 14 steps of Sec. 9.3.2.

From Sec. 9.3.2:

Step 1

Stratum 3: $\sum_{j=1}^{6} (y_{3j} - Y_{3j}) = -2.136$ kg of U

Stratum 4: $\sum_{j=1}^{4} (y_{4j} - Y_{4j}) = +0.413$ kg of U

Step 2

Stratum 3: $(15/6)(-2.136) = -5.340$ kg of U

Stratum 4: $(30/4)(0.413) = +3.098$ kg of U

Step 3

$D_1 = -5.340 + 3.098 = -2.242$ kg of U

Step 4

Stratum 5: $\sum_{j=1}^{12} (z_{5j} - \bar{z}_{5j}) = -0.048$ kg of U

Step 5

Stratum 5: $(75/12)(-0.048) = -0.300$ kg of U

Step 6

$D_2 = -0.300$ kg of U

Step 7

Stratum 1: $\sum_{j=1}^{40} (w_{1j} - W_{1j}) = -0.062$ kg of UO_2

Stratum 2: $\sum_{j=1}^{26} (w_{2j} - W_{2j}) = -0.029$ kg of UO_2

Step 8

Stratum 1: $(300/40)(-0.062) = -0.465$ kg of UO_2

Stratum 2: $(180/26)(-0.029) = -0.201$ kg of UO_2

Step 9

Stratum 1: $\sum_{j=1}^{300} W_{1j} = 6030.60$ kg of UO_2

Stratum 2: $\sum_{j=1}^{180} W_{2j} = 1102.320$ kg of UO_2

Step 10

Stratum 1: $(-0.465 + 6030.60)(0.8754) = 5278.780$ kg of U

Stratum 2: $(-0.201 + 1102.320)(0.8807) = 970.636$ kg of U

Step 11

Stratum 1: $(6030.60)(0.8760) = 5282.806$ kg of U

Stratum 2: $(1102.320)(0.8810) = 971.144$ kg of U

Step 12

Stratum 1: $5278.780 - 5282.806 = -4.026$ kg of U

Stratum 2: $970.636 - 971.144 = -0.508$ kg of U

Step 13

$D_3 = -4.026 - 0.508 = -4.534$ kg of U

Step 14

$$D = -2.242 - 0.300 - 4.534 = -7.076 \quad \text{kg of U}$$

The audit team's estimate of the inventory is 7.076 kg of uranium less than the operator's value.

To find $V(D)$, the variance of D, apply the appropriate rules of Table 9.2.

From Table 9.2:

Rule A

Scale 1: (1) $N_1\overline{U}_1 = (300)(0.8760) = 262.80$

(It is convenient to use $\overline{U}_1$ rather than an average of $\overline{U}_1$ and $\overline{u}_1$, and this makes no essential difference in the results.)

(2) $N_1\overline{U}_1 = 262.80$

(Scales 1 and 2 are each used in only one stratum; so the sum of step 2 is only over the one term.)

(3) $(262.80)^2 = 69064 = A_{11}$

Scale 2: (1) $N_2\overline{U}_2 = (180)(0.8810) = 158.58$

(2) $N_2\overline{U}_2 = 158.58$

(Scales 1 and 2 are each used in only one stratum; so the sum of step 2 is only over the one term.)

(3) $(158.58)^2 = 25148 = A_{12}$

Scale 3: (1) $(N_3\overline{U}_3) = (15)(0.527) = 7.905$

$(N_4\overline{U}_4) = (30)(0.644) = 19.920$

(2) $7.905 + 19.920 = 27.825$

(3) $(27.825)^2 = 774 = A_{13}$

Scale 4: (1) $N_1\overline{U}_1 = 262.80 \qquad N_2\overline{U}_2 = 158.58$

$N_3\overline{U}_3 = 7.905 \qquad N_4\overline{U}_4 = 19.920$

(2) $262.80 + 158.58 + 7.905 + 19.920 = 449.205$

(3) $(449.205)^2 = 201785 = A_{14}$

Rule B

Scale 1: (1) $N_1\overline{U}_1 = 262.80$

(2) $(262.80)^2 = 69063.84$

(3) $69063.84/40 = 1726.60$

(4) $1727 = A_{21}$

Scale 2: (1) $N_2\overline{U}_2 = 158.58$

(2) $(158.58)^2 = 25147.62$

(3) $25147.62/26 = 967.22$

(4) $967 = A_{22}$

Scale 3: (1) $N_3\overline{U}_3 = 7.905$ $N_4\overline{U}_4 = 19.920$

(2) $(7.905)^2 = 62.49$ $(19.920)^2 = 396.81$

(3) $62.49/6 = 10.42$ $396.81/4 = 99.20$

(4) $10.42 + 99.20 = 110 = A_{23}$

Scale 4: (1) $N_1\overline{U}_1 = 262.80$ $N_2\overline{U}_2 = 158.58$

$N_3\overline{U}_3 = 7.905$ $N_4\overline{U}_4 = 19.920$

(2) $(262.80)^2 = 69063.84$
$(158.58)^2 = 25147.62$

$(7.905)^2 = 62.49$
$(19.920)^2 = 396.81$

(3) $69063.84/40 = 1726.60$
$25147.62/26 = 967.22$

$62.49/6 = 10.42$
$396.81/4 = 99.20$

(4) $1726.60 + 967.22 + 10.42 + 99.20 = 2803 = A_{24}$

Rule C

Technique 1: (1) $N_1\overline{W}_1 = (300)(20.102) = 6030.600$

$N_2\overline{W}_2 = (180)(6.124) = 1102.320$

(2) $6030.600 + 1102.320 = 7132.920$

(3) $(7132.920)^2 = 50878548 = A_{31}$

Technique 2: (1) $N_3\overline{W}_3 = (15)(18.214) = 273.21$

(2) 273.21

(3) $(273.21)^2 = 74644 = A_{32}$

Technique 3: (1) $N_4\overline{W}_4 = (30)(5.907) = 177.21$

(2) 177.21

(3) $(177.21)^2 = 31403 = A_{33}$

Technique 4: (1) $N_1\overline{W}_1 = 6030.600$

$N_2\overline{W}_2 = 1102.320$

(2) $6030.600 + 1102.320 = 7132.920$

(3) $(7132.920)^2 = 50878548 = A_{34}$

Technique 5: (1) $N_3\overline{W}_3 = 273.21$

$N_4\overline{W}_4 = 177.21$

(2) $273.21 + 177.21 = 450.42$

(3) $(450.42)^2 = 202878 = A_{35}$

Rule D

Technique 1: (1) $N_1\overline{W}_1 = 6030.600$

$N_2\overline{W}_2 = 1102.320$

(2) $(6030.600)^2 = 36368136$
$(1102.320)^2 = 1215109$

(3) $36368136/22 = 1653097$
$1215109/30 = 40504$

(4) $1653097 + 40504 = 1693601 = A_{41}$

Technique 2: (1) $N_3\overline{W}_3 = 273.21$

(2) $(273.21)^2 = 74643.70$

(3) $74643.70/6 = 12441$

(4) $12441 = A_{42}$

Technique 3: (1) $N_4\overline{W}_4 = 177.21$

(2) $(177.21)^2 = 31403.38$

(3) $31403.38/4 = 7851$

(4) $7851 = A_{43}$

Technique 4: (1) $\mathcal{N}_1\overline{W}_1 = 6030.600$

$\mathcal{N}_2\overline{W}_2 = 1102.320$

(2) $(6030.600)^2 = 36368136$
$(1102.320)^2 = 1215109$

(3) $36368136/5 = 7273627$
$1215109/8 = 151889$

(4) $7273637 + 151889 = 7425516 = A_{44}$

Technique 5: (1) $\mathcal{N}_3\overline{W}_3 = 273.21$

$\mathcal{N}_4\overline{W}_4 = 177.21$

(2) $(273.21)^2 = 74643.70$
$(177.21)^2 = 31403.38$

(3) $74643.70/6 = 12441$
$31403.38/4 = 7851$

(4) $12441 + 7851 = 20292 = A_{45}$

Rule E

Instrument 1: (1) 75

(2) $(75)^2 = 5625 = A_{51}$

Instrument 2: (1) 75

(2) $(75)^2 = 5625 = A_{52}$

Rule F

Instrument 1: (1) $(75)^2 = 5625$

(2) $5625/12 = 468.75$

(3) $468.75 = A_{61}$

Instrument 2: (1) $(75)^2 = 5625$

(2) $5625/12 = 468.75$

(3) $468.75 = A_{62}$

The variance of D, $V(D)$, is now given by Eq. 9.20, the data in Table 9.5, and the coefficients just calculated from the rules of Table 9.2.

$V(D) =$	$69064(0.0010)^2 =$	0.069	Systematic–scale–operator
$+$	$25148(0.0006)^2 =$	0.009	
$+$	$774(0.005)^2 =$	0.019	

+	$201785(0.002)^2$ =	0.807	Systematic–scale–audit
+	$1727(0.0015)^2$ =	0.004	Random–scale–operator
+	$967(0.0010)^2$ =	0.001	
+	$110(0.010)^2$ =	0.011	
+	$2803(0.005)^2$ =	0.070	Random–scale–audit
+	$50878548(0.0003)^2$ =	4.579	Systematic–analytical–operator
+	$74644(0.020)^2$ =	29.858	
+	$31403(0.006)^2$ =	1.131	
+	$50878548(0.0004)^2$ =	8.141	Systematic–analytical–audit
+	$202878(0.015)^2$ =	45.648	
+	$1693601(0.0005)^2$ =	0.423	Random–analytical–operator
+	$12441(0.028)^2$ =	9.754	
+	$7851(0.022)^2$ =	3.800	
+	$7425516(0.0007)^2$ =	3.639	Random–analytical–audit
+	$20292(0.020)^2$ =	8.117	
+	$5625(0.002)^2$ =	0.023	Systematic–NDA–operator
+	$5625(0.003)^2$ =	0.051	Systematic–NDA–audit
+	$469(0.009)^2$ =	0.038	Random–NDA–operator
+	$469(0.010)^2$ =	0.047	Random–NDA–audit
		$V(D) = 116.239$	

If, recalling that $D = -7.076$ kg of U, we apply Eq. 9.21, the test statistic D^* is

$$D^* = -7.076/\sqrt{116.239} = -0.66$$

Let $\alpha = 0.05$, so $D_\alpha = 1.960$ from Table 9.3. Since $0.66 < 1.960$, we conclude that the discrepancy between the operator's and the audit team's estimates of the inventory is not statistically significant. Thus we consider the operator's inventory to be verified.

9.3.4 Basis

The determination by the operator of the element weight for items within a given stratum is made by one of three methods described in Sec. 9.3.1. During the step 2 variables audit, it is assumed that the audit team uses the same method as the operator in each stratum.

Consider the model for each of the three methods. An additive error model is assumed to apply. This is reasonable in this application, even

though error standard deviations are commonly expressed on a relative basis, because the classification of the inventory into strata tends to make the items within each stratum similar with respect to weights and element factors. This permits making comparisons between the operator results and those of the audit team by paired differences. With a relative error structure, this comparison would more logically be done by paired ratios than by differences. For a method 1 type of measurement, the following quantities are defined. In this notation the letters in parentheses indicate that the net weight was determined on scale k by analytical technique p. Primes are used on p and k for the audit team measurements to emphasize that the scales and analytical techniques are not the same as those used by the operator. In this chapter analytical technique includes the effects both of sampling and of analysis.

$Y_{ij(kp)}$ = operator's element weight for item j in stratum i; $j = 1, 2, \ldots, N_i$

$y_{ij(k'p')}$ = audit team's element weight for item j in stratum i; $j = 1, 2, \ldots, n_i$ (For convenience in notation assume that the items are the first n_i of the total N_i items in that stratum)

μ_{ij} = true item weight for item j in stratum i; $j = 1, 2, \ldots, N_i$

Υ_{ij} = true element factor for item j in stratum i; $j = 1, 2, \ldots, N_i$

Ω_k = systematic-error deviation due to use of scale k

$\xi_{ij(k)}$ = random-error deviation for jth weighing on kth scale in stratum i

Γ_p = systematic-error deviation due to use of analytical technique p

$\tau_{ij(p)}$ = random-error deviation for jth analytical determination in stratum i with analytical technique p

The model for the operator then becomes

$$\begin{aligned} Y_{ij(kp)} &= [\mu_{ij}+\Omega_k+\xi_{ij(k)}][\Upsilon_{ij}+\Gamma_p+\tau_{ij(p)}] \\ &\approx \mu_{ij}\Upsilon_{ij}+\mu_{ij}[\Gamma_p+\tau_{ij(p)}]+\Upsilon_{ij}[\Omega_k+\xi_{ij(k)}] \end{aligned} \tag{9.22}$$

A similar model holds for the audit team measurements:

$$y_{ij(k'p')} \approx \mu_{ij}\Upsilon_{ij}+\mu_{ij}[\Gamma_{p'}+\tau_{ij(p')}]+\Upsilon_{ij}[\Omega_{k'}+\xi_{ij(k')}] \tag{9.23}$$

The quantity of interest is the difference between the audit team's estimate of the total element inventory in this stratum and that of the operator. This is the average difference times the number of items in the stratum.

$$D_{1i} = N_i \sum_{j=1}^{n_i} \frac{y_{ij(k'p')} - Y_{ij(kp)}}{n_i} \tag{9.24}$$

Assume that the strata are defined in such a manner that μ_{ij} is reasonably constant over the j items and can be replaced by μ_i for all j. Similarly, replace Υ_{ij} by Υ_i for all j. Upon application of Eqs. 9.22 and 9.23, Eq. 9.24 becomes

$$D_{1i} \approx N_i\mu_i\left[(\Gamma_{p'}-\Gamma_p)+\sum_{j=1}^{n_i}\frac{\tau_{ij(p')}-\tau_{ij(p)}}{n_i}\right] + N_i\Upsilon_i\left[(\Omega_{k'}-\Omega_k)+\sum_{j=1}^{n_i}\frac{\xi_{ij(k')}-\xi_{ij(k)}}{n_i}\right] \tag{9.25}$$

A similar result is found for a stratum with method 2 measurements. Let

$Z_{ij(t)}$ = operator's element weight for item j in stratum i, based on NDA instrument t

$z_{ij(t')}$ = audit team's element weight for item j in stratum i, based on NDA instrument t'

Λ_t = systematic-error deviation due to use of NDA instrument t

$\zeta_{ij(t)}$ = random-error deviation for jth item in stratum i due to use of NDA instrument t

Then the difference between the estimate of the audit team and that of the operator for the inventory in a method 2 stratum is

$$D_{2i} = N_i\sum_{j=1}^{n_i}\frac{z_{ij(t')}-Z_{ij(t)}}{n_i} = N_i\left[(\Lambda_{t'}-\Lambda_t)+\sum_{j=1}^{n_i}\frac{\zeta_{ij(t')}-\zeta_{ij(t)}}{n_i}\right] \tag{9.26}$$

Finally, for method 3, let

$W_{ij(k)}$ = operator's item weight for jth item in stratum i, with scale k

$w_{ij(k')}$ = audit team's item weight for jth item in stratum i, with scale k'

$\bar{U}_{i(p)}$ = operator's average element factor for stratum i, based on M_i determinations using analytical technique p

$\bar{u}_{i(p')}$ = audit team's element factor for stratum i, based on m_i determinations using analytical technique p'

The difference in inventory estimates can be written

$$D_{3i} = \sum_{j=1}^{N_i} W_{ij(k)}[\bar{u}_{i(p')}-\bar{U}_{i(p)}]+N_i\bar{u}_i\sum_{j=1}^{n_i}\frac{w_{ij(k')}-W_{ij(k)}}{n_i} \tag{9.27}$$

where, for a method 3 stratum, n_i refers to the number of items weighed by the audit team.

To write D_{3i} in terms of its basic error structure, first rewrite Eq. 9.27 as follows, by collecting terms in $\bar{u}_{i(p')}$:

$$D_{3i}=\bar{u}_{i(p')}\left[N_i\sum_{j=1}^{n_i}\frac{w_{ij(k')}}{n_i}+\left(1-\frac{N_i}{n_i}\right)\sum_{j=1}^{n_i}W_{ij(k)}+\sum_{j=n_i+1}^{N_i}W_{ij(k)}\right]$$
$$-\bar{U}_{i(p)}\sum_{j=1}^{N_i}W_{ij(k)} \tag{9.28}$$

Then, if we write

$$\bar{u}_{i(p')}=\sum_{j=1}^{m_i}\frac{\Upsilon_{ij}+\Gamma_{p'}+\tau_{ij(p')}}{m_i} \tag{9.29}$$

define $\bar{U}_{i(p)}$ in a similar way, and assume that Υ_{ij} can be replaced by Υ_i for all j, Eq. 9.28 becomes approximately

$$D_{3i}\approx N_i\Upsilon_i\left[(\Omega_{k'}-\Omega_k)+\sum_{j=1}^{n_i}\frac{\xi_{ij(k')}-\xi_{ij(k)}}{n_i}\right]$$
$$+N_i\mu_i\left[(\Gamma_{p'}-\Gamma_p)+\sum_{j=1}^{m_i}\frac{\tau_{ij(p')}}{m_i}-\sum_{j=1}^{M_i}\frac{\tau_{ij(p)}}{M_i}\right] \tag{9.30}$$

Equations 9.25, 9.26, and 9.30 are now used to find the variance of D.

$$D=\sum D_{1i}+\sum D_{2i}+\sum D_{3i} \tag{9.31}$$

where the first summation is over all strata employing method 1, the second is over all strata using method 2, and the third is over all strata based on method 3.

Equation 4.6 is used to find the variance of D. This variance is of the form

$$V(D)=\sum_{k=1}^{K}A_{1k}\sigma^2_{\Omega_k}+\sum_{k=1}^{K}A_{2k}\sigma^2_{\xi_k}+\sum_{p=1}^{P}A_{3p}\sigma^2_{\Gamma_p}+\sum_{p=1}^{P}A_{4p}\sigma^2_{\tau_p}$$
$$+\sum_{t=1}^{T}A_{5t}\sigma^2_{\Lambda_t}+\sum_{t=1}^{T}A_{6t}\sigma^2_{\zeta_t} \tag{9.32}$$

where K is the total number of scales for both the operator and the audit team, P is the total number of analytical techniques, and T is the total number of NDA instruments. In this summation, the terms in k', p', and t' are included in the various sums. The primes are used only to differentiate between the results for the operator and those for the audit team.

From Eq. 4.6, A_{1k} is the squared partial derivative of D with respect to Ω_k, evaluated at the means of all the variables (all the error-random variables have zero means in the additive model); A_{2k} is the squared partial derivative of D with respect to ξ_k, etc In particular, from Eqs. 9.25 and 9.30,

$$\frac{\partial D}{\partial \Omega_k} = -N_i \Upsilon_i \qquad \text{(for the strata in which scale } k \text{ is used)}$$

$$\frac{\partial D}{\partial \Omega_{k'}} = N_i \Upsilon_i \qquad \text{(for the strata in which scale } k' \text{ is used)}$$

Since scales k and k' are not used in the same stratum (the operator and audit team use different scales), since the partial derivative is negative for all operator scales and positive for all audit team scales, and since the square of the negative number is positive, it follows that

$$A_{1k} = \left(\sum_i N_i \Upsilon_i\right)^2 \tag{9.33}$$

where the summation is over all strata in which scale k is used. This result is the basis for the calculational rule A in Table 9.2.

Similarly,

$$\frac{\partial D}{\partial \xi_{ij(k)}} = -\frac{N_i \Upsilon_i}{n_i}$$

for the jth error in a stratum in which scale k is used.

This partial derivative is the same for all $\xi_{ij(k)}$. In stratum i, there are n_i such derivatives. Each is squared to give $N_i^2 \Upsilon_i^2 / n_i^2$. Since there are n_i such factors multiplying $\sigma_{\xi_k}^2$ in the ith stratum, the coefficient of $\sigma_{\xi_k}^2$ in that stratum is $(N_i \Upsilon_i)^2 / n_i$. This is then summed over all strata using scale k to give

$$A_{2k} = \sum_i \frac{(N_i \Upsilon_i)^2}{n_i} \tag{9.34}$$

The same result is found for scale k', and so Eq. 9.34 is the basis for calculational rule B in Table 9.2.

A similar development leads to the values for A_{3p}, A_{4p}, A_{5i}, and A_{6i}.

$$A_{3p} = \left(\sum_i N_i \mu_i\right)^2 \tag{9.35}$$

where the summation is over all strata in which analytical technique p is used. This is the basis for rule C of Table 9.2.

$$A_{4p} = \sum_{i} \frac{(N_i \mu_i)^2}{l_i} \tag{9.36}$$

where $l_i = n_i$ in a method 1 stratum
$l_i = m_i$ in a method 3 stratum involving an audit team measurement
$l_i = M_i$ in a method 3 stratum involving an operator measurement

and where the summation is over all strata in which analytical technique p is used. Equation 9.36 is the basis for rule D of Table 9.2.

$$A_{5t} = (\sum N_i)^2 \tag{9.37}$$

where the summation is over all strata in which NDA instrument t is used. This is the basis for rule E of Table 9.2.

Finally,

$$A_{6t} = \sum_{i} \frac{N_i^2}{n_i} \tag{9.38}$$

where the summation is over all strata in which NDA instrument t is used. This is the basis for rule F of Table 9.2.

With D and $V(D)$ given, the test of significance is the usual one applied to test the hypothesis $\mu_D = 0$, where μ_D is the expected value of D. The test is based on an assumed known error structure, with the random variable, D, normally distributed. A two-sided test of significance is used since the hypothesis of a zero difference may logically be violated in either direction.

9.4 OPTIMIZATION OF STEP 2 VARIABLES INSPECTION EFFORT

9.4.1 Problem and Assumptions

Let me emphasize that the optimization of inspection effort considered in this section is only with respect to the variables inspection. The problem of how to allocate total effort between the step 1 attributes inspection and the step 2 variables inspection is another matter and one that is not easily solved in a quantitative fashion.

In the preceding section the analysis of variables inspection data was considered. In that analysis the sample sizes used by the audit team in the ith stratum were given. In application, the audit team must first decide how many measurements of each kind to make. This section discusses the basis for making that decision.

The goal of the audit team is to perform the inspection in such a way as to maximize the probability of detecting a given discrepancy between the two estimates of the total inventory. This is equivalent to minimizing $V(D)$, the variance of the overall difference statistic, D. In practice, the audit team has limited resources, and there are constraints placed upon the team members in the sense that they must limit the effort devoted to this phase of the audit. Thus the problem is to minimize $V(D)$ subject to specified constraints.

This problem can be approached from a different viewpoint, which involves determining the variables inspection effort required to detect a given discrepancy with a specified probability. That is, a maximum value for $V(D)$ is established, and the amount of effort required to attain a value of $V(D)$ that small or smaller is determined. The problem is in essence no different from that of the previous paragraph. It is a question of emphasis. On the one hand, the emphasis is on maximizing test sensitivity for a given amount of resources; on the other hand, the emphasis is on determining what resources are needed to achieve a given test sensitivity.

Whichever emphasis is preferred, in application the audit team will wish to examine the relation between test sensitivity related to $V(D)$ and total cost, or effort. It is convenient to examine this by fixing total effort at different levels and calculating $V(D)$ for the corresponding optimum allocation of effort.

The audit team might wish to include other criteria in addition to cost of inspection for optimization in a given situation. For example, the value of the material, measured by enrichment (^{235}U enrichment or plutonium), might well be a factor, with greater attention to the materials with higher enrichment. Further, depending on the nature of the inspection, the audit team might wish to take into account the accessibility of material to a potential diverter and/or the form of the material. A method of factoring these and other criteria into the optimization scheme is also considered.

The models and assumptions are the same in this section as in Sec. 9.3.

9.4.2 Solution

Define a *cell* as a stratum for methods 1 and 2 (the methods are defined in Sec. 9.3.1). For method 3, a cell is either a stratum in which a bulk measurement is made or a stratum in which an analytical determination is made, i.e., there are two cells defined for each stratum. Thus, if v_i strata employ method i ($i=1, 2, 3$), then the total number of cells is $(v_1+v_2+2v_3)=s$.

For each cell j, define r_j to be the number of measurements in cell j. (For a method 1 cell, a measurement consists of both a bulk and an analytical determination; for a method 2 cell, it consists of an NDA measure-

ment; for a method 3 cell, it consists of either a bulk or an analytical determination.) Then r_j is selected as follows:

1. In cell j, choose the sample size, r_j, proportional to

$$\sigma_j/\sqrt{c_j h_j d_j \ldots} = \phi_j \tag{9.39}$$

2. For a given total effort, measured by $\Sigma\, c_j r_j = \phi$, compute $V(D)$ from the methods of Sec. 9.3.2. The r_j must, of course, be integers in application. Each r_j must equal at least 1.

3. Examine the relation between $V(D)$ and ϕ, and select the sample sizes either by fixing ϕ or by fixing $V(D)$ and choosing ϕ to achieve this value of $V(D)$.

The quantities in Eq. 9.39 are defined as follows: The quantity σ_j^2 is the random-error variance of a given difference in cell j and is defined in one of four ways, the definition depending on the type of cell in question.

Definition 1. If cell j is a stratum based on method 1, then

$$\sigma_j^2 = N_i^2 \Upsilon_i^2 (\sigma_{\xi_k}^2 + \sigma_{\xi_{k'}}^2) + N_i^2 \mu_i^2 (\sigma_{\tau_p}^2 + \sigma_{\tau_{p'}}^2) \tag{9.40}$$

where cell j corresponds to stratum i, N_i is the number of items in stratum i, Υ_i is the average element concentration factor for stratum i, and μ_i is the average item net weight for stratum i. In this stratum the operator uses scale k and analytical technique p, whereas the inspector uses scale k' and analytical technique p'.

Definition 2. If cell j is a stratum based on method 2, then

$$\sigma_j^2 = N_i^2 (\sigma_{\xi_t}^2 + \sigma_{\xi_{t'}}^2) \tag{9.41}$$

where cell j corresponds to stratum i. In this stratum the operator uses NDA instrument t, and the inspector uses NDA instrument t'.

Definition 3. If cell j relates to the bulk measurement in a stratum based on method 3, then,

$$\sigma_j^2 = N_i^2 \Upsilon_i^2 (\sigma_{\xi_k}^2 + \sigma_{\xi_{k'}}^2) \tag{9.42}$$

with the quantities defined following Eq. 9.40.

Definition 4. If cell j relates to an analytical determination in a stratum based on method 3, then,

$$\sigma_j^2 = N_i^2 \mu_i^2 \sigma_{\tau_{p'}}^2 \tag{9.43}$$

with the quantities defined following Eq. 9.40.

Let us define the other quantities in Eq. 9.39. The c_j is the cost of making a measurement in cell j. This can be expressed on some arbitrary scale to measure cost, or effort, on a relative basis. Actual dollar costs are not required.

Finally, the quantities $h_j d_j \ldots$ represent other factors that the audit team might introduce into the optimization process. These factors are scaled in such a way that the higher the value assigned a given factor, the fewer the measurements. This is to be consistent with the c_j factor since the higher the cost of a given measurement, the fewer the measurements of that type.

For example, h_j might be the factor that takes the value of the material into account, defined by

$$h_j = 1/(^{235}\text{U enrichment})^2 \qquad \text{for uranium-bearing items}$$

$$= 1 \qquad \text{for plutonium-bearing items}$$

where ^{235}U enrichment is measured on the scale from 0 to 1, e.g., $h_j = 1/(0.05)^2 = 400$ for 5% enriched material.

The factor d_j might be used to describe the potential for diversion within a given cell, taking into account such factors as the form of the material, the accessibility to diversion, etc. In essence, d_j might be a measure of the relative emphasis the audit team would like to give to certain segments of the inventory because discrepancies are more or less likely to occur in that cell in their judgment. As with c_j and h_j, the scale chosen to describe this potential for diversion might be arbitrary.

Other factors might be introduced. Alternatively, the audit team might choose to disregard such factors as h_j and d_j. As a minimum, however, the cost factor, c_j, should be retained.

9.4.3 Examples

Example 9.G

Example 9.F is reconsidered with a different viewpoint. Here the problem is to select the n_i and m_i in an optimal way.

With reference to Table 9.4, there are five strata, two based on method 1, one on method 2, and two on method 3. Thus $v_1 = 2$, $v_2 = 1$, $v_3 = 2$, and the total number of cells, s, is $(v_1 + v_2 + 2v_3)$, or 7. These 7 cells are identified in Table 9.6.

TABLE 9.6 DEFINITION OF CELLS
(Example 9.G)

Cell	Stratum	Method	Measurement
1	1	3	Bulk: scale 1 for operator; scale 4 for audit team
2	1	3	Analysis: technique 4 for audit team*
3	2	3	Bulk: scale 2 for operator; scale 4 for audit team
4	2	3	Analysis: technique 4 for audit team*
5	3	1	Bulk–analysis: scales 3 and 4; techniques 2 and 5
6	4	1	Bulk–analysis: scales 3 and 4; techniques 3 and 5
7	5	2	NDA: instruments 1 and 2

* The technique used by the operator does not enter into the optimization procedure with method 1. The average element factor, $\overline{U}_i$, has already been estimated based on the M_i determinations.

The σ_j values are calculated by Eqs. 9.40 to 9.43, the equation used depending upon the type of cell. The values for the error parameters are in Table 9.5. The values for the N_i, Υ_i, and μ_i needed to compute σ_j, given in Table 9.4 and the following text, are repeated here.

$$N_1 = 300 \qquad \Upsilon_1 = 0.8760 \qquad \mu_1 = 20.102$$
$$N_2 = 180 \qquad \Upsilon_2 = 0.8810 \qquad \mu_2 = 6.124$$
$$N_3 = 15 \qquad \Upsilon_3 = 0.527 \qquad \mu_3 = 18.214$$
$$N_4 = 30 \qquad \Upsilon_4 = 0.664 \qquad \mu_4 = 5.907$$
$$N_5 = 75$$

The values for σ_j are found as follows:

Cell 1. From Eq. 9.42,
$$\sigma_1^2 = (300)^2(0.8760)^2[(0.0015)^2 + (0.005)^2] = 1.8820$$
$$\sigma_1 = 1.37$$

Cell 2. From Eq. 9.43,
$$\sigma_2^2 = (300)^2(20.102)^2(0.0007)^2 = 17.8204$$
$$\sigma_2 = 4.22$$

Cell 3. From Eq. 9.42,
$$\sigma_3^2 = (180)^2(0.8810)^2[(0.0010)^2 + (0.005)^2] = 0.6538$$
$$\sigma_3 = 0.81$$

Cell 4. From Eq. 9.43,
$$\sigma_4^2 = (180)^2(6.124)^2(0.0007)^2 = 0.5954$$
$$\sigma_4 = 0.77$$

Cell 5. From Eq. 9.40,

$$\sigma_5^2 = (15)^2(0.527)^2[(0.010)^2+(0.005)^2] + (15)^2(18.214)^2[(0.028)^2+(0.020)^2] = 88.3860$$

$$\sigma_5 = 9.40$$

Cell 6. From Eq. 9.40,

$$\sigma_6^2 = (30)^2(0.664)^2[(0.010)^2+(0.005)^2] + (30)^2(5.907)^2[(0.022)^2+(0.020)^2] = 27.8102$$

$$\sigma_6 = 5.27$$

Cell 7. From Eq. 9.41,

$$\sigma_7^2 = (75)^2[(0.009)^2+(0.010)^2] = 1.0181$$

$$\sigma_7 = 1.01$$

Finally, assume that the enrichment is the same for all the materials so that h_j, which measures material value, is constant and does not enter into the optimization. Assume further that c_j, the cost of a measurement, and d_j, the measure of the potential for diversion, are given as follows on arbitrary scales. (The values for c_j and d_j are for illustration only; the user should not infer any validity beyond this.)

$c_1 = 2$	$c_5 = 15$	$d_1 = 2$	$d_5 = 3$
$c_2 = 10$	$c_6 = 15$	$d_2 = 8$	$d_6 = 2$
$c_3 = 1$	$c_7 = 20$	$d_3 = 1$	$d_7 = 5$
$c_4 = 10$		$d_4 = 10$	

With values for σ_j, c_j, and d_j now given, ϕ_j can be calculated by Eq. 9.39.

$$\phi_1 = 1.37/\sqrt{(2)(2)} = 0.69 \qquad \phi_5 = 9.40/\sqrt{(15)(3)} = 1.40$$

$$\phi_2 = 4.22/\sqrt{(10)(8)} = 0.47 \qquad \phi_6 = 5.27/\sqrt{(15)(2)} = 0.96$$

$$\phi_3 = 0.81/\sqrt{(1)(1)} = 0.81 \qquad \phi_7 = 1.01/\sqrt{(20)(5)} = 0.10$$

$$\phi_4 = 0.77/\sqrt{(10)(10)} = 0.08$$

The r_j should then be selected proportional to these ϕ_j values. This does not indicate how many total measurements should be made. To determine this, consider three inspection levels in which r_j are chosen proportional to the ϕ_j, and compute $V(D)$ for each inspection level by the methods of Sec. 9.3.3. The three inspection levels are indicated in Table 9.7.

TABLE 9.7 NUMBERS OF MEASUREMENTS FOR DIFFERENT INSPECTION LEVELS

Cell	Level 1	Level 2	Level 3
1 $r_1=n_1=$	3	5	7
2 $r_2=m_1=$	2	3	5
3 $r_3=n_2=$	3	6	8
4 $r_4=m_2=$	1	1	1
5 $r_5=n_3=$	6	10	14
6 $r_6=n_4=$	4	7	10
7 $r_7=n_5=$	1	1	1
Total number of weighings * =	16	28	39
Total number of analyses † =	13	21	30
Total number of NDA measurements =	1	1	1
Total "cost" ‡	209	331	462

* Total number of weighings $= (n_1+n_2+n_3+n_4)$.

† Total number of analyses $= (m_1+m_2+n_3+n_4)$.

‡ Total cost $= \sum_{j=1}^{7} c_j r_j$.

In finding $V(D)$ for the three levels of inspection, we can use some of the results of example 9.F. In particular, the systematic-error variances are not affected by the inspection level, nor is the random-error variance due to analysis for technique 1, that used by the operator in the method 3 strata. These results are given in Table 9.8.

TABLE 9.8 VARIANCES FOR ERROR SOURCES NOT AFFECTED BY INSPECTION INTENSITY

Source	Variance, kg^2 of U
Scales–systematic	0.904
Analytical techniques–systematic	89.357
NDA–systematic	0.074
Analytical technique 1–random	0.423
	90.758

To calculate the variances due to the other sources, follow the pertinent steps of example 9.F. (The "data" in this example are such as would appear on an a priori inventory listing rather than from the actual inventory.) Only the steps affected by the particular n_i, m_i are shown in the following calculations (refer to the calculations in example 9.F). The rules are those of Table 9.2. The levels refer to the inspection levels of Table 9.7.

Rule B

Scale 1:

(3) Level 1: $69063.84/3=23021.28$
Level 2: $69063.84/5=13812.77$
Level 3: $69063.84/7=9866.26$

(4) Level 1: $23021 = A_{21}$
Level 2: $13813 = A_{21}$
Level 3: $9866 = A_{21}$

Scale 2:

(3) Level 1: $25147.62/3=8382.54$
Level 2: $25147.62/6=4191.27$
Level 3: $25147.62/8=3143.45$

(4) Level 1: $8383 = A_{22}$
Level 2: $4191 = A_{22}$
Level 3: $3143 = A_{22}$

Scale 3:

(3) Level 1: $62.49/6=10.42$
$396.81/4=99.20$
Level 2: $62.49/10=6.25$
$396.81/7=56.69$
Level 3: $62.49/14=4.46$
$396.81/10=39.68$

(4) Level 1: $10.42+99.20=109.62=A_{23}$
Level 2: $6.25+56.69=62.94=A_{23}$
Level 3: $4.46+39.68=44.14=A_{23}$

Scale 4:

(3) Level 1: $69063.84/3=23021.28$
$25147.62/3=8382.54$
$62.49/6=10.42$
$396.81/4=99.20$
Level 2: $69063.84/5=13812.77$
$25147.62/6=4191.27$
$62.49/10=6.25$
$396.81/7=56.69$
Level 3: $69063.84/7=9866.26$
$25147.62/8=3143.45$
$62.49/14=4.46$
$396.81/10=39.68$

(4) Level 1: $23021+8383+10+99=31513=A_{24}$
Level 2: $13813+4191+6+57=18067=A_{24}$
Level 3: $9866+3143+4+40=13053=A_{24}$

Rule D

Technique 2:

(3),(4) Level 1: $74643.70/6 = 12441 = A_{42}$
Level 2: $74643.70/10 = 7464 = A_{42}$
Level 3: $74643.70/14 = 5332 = A_{42}$

Technique 3:

(3),(4) Level 1: $31403.38/4 = 7851 = A_{43}$
Level 2: $31403.38/7 = 4486 = A_{43}$
Level 3: $31403.38/10 = 3140 = A_{43}$

Technique 4:

(3) Level 1: $36368136/2 = 18184068$
$1215109/1 = 1215109$
Level 2: $36368136/3 = 12122712$
$1215109/1 = 1215109$
Level 3: $36368136/5 = 7273627$
$1215109/1 = 1215109$

(4) Level 1: $18184068 + 1215109 = 19399177 = A_{44}$
Level 2: $12122712 + 1215109 = 13337821 = A_{44}$
Level 3: $7273627 + 1215109 = 8488736 = A_{44}$

Technique 5:

(3) (See results of techniques 2 and 3)
(4) From techniques 2 and 3,
Level 1: $12441 + 7851 = 20292 = A_{45}$
Level 2: $7464 + 4486 = 11950 = A_{45}$
Level 3: $5332 + 3140 = 8472 = A_{45}$

Rule F. (Level 1 ≡ level 2 ≡ level 3)

Instrument 1:

(3) $468.75/1 = 468.75 = A_{61}$

Instrument 2:

(3) $468.75/1 = 468.75 = A_{62}$

The $V(D)$ is then calculated for the three inspection levels. The calculations are shown in Table 9.9.

The limiting value of $\sqrt{V(D)}$ is $\sqrt{90.758} = 9.53$ kg of U. It is doubtful on this basis whether inspection intensity beyond level 1 is necessary in this instance.

Example 9.H

In a scrap recovery plant, the plutonium inventory in a certain material balance area is to be verified. The inventory is contained in 26

TABLE 9.9 CALCULATION OF $V(D)$ FOR THREE INSPECTION LEVELS

	Variance, kg² of U		
	Level 1	Level 2	Level 3
Fixed variance*	90.758	90.758	90.758
Scales:			
$A_{21}\sigma^2_{\xi 1}$	0.052	0.031	0.022
$A_{22}\sigma^2_{\xi 2}$	0.008	0.004	0.003
$A_{23}\sigma^2_{\xi 3}$	0.011	0.006	0.004
$A_{24}\sigma^2_{\xi 4}$	0.788	0.452	0.326
Analyses:			
$A_{42}\sigma^2_{\tau 2}$	6.155	5.852	4.180
$A_{43}\sigma^2_{\tau 3}$	3.800	2.171	1.520
$A_{44}\sigma^2_{\tau 4}$	9.506	6.536	4.159
$A_{45}\sigma^2_{\tau 5}$	8.117	4.780	3.389
NDA:			
$A_{61}\sigma^2_{\zeta 1}$	0.038	0.038	0.038
$A_{62}\sigma^2_{\zeta 2}$	0.047	0.047	0.047
$V(D)=$	119.280	110.675	104.446
$\sqrt{V(D)}$, kg of U =	10.92	10.52	10.22
Cost† =	209	331	462

* From Table 9.8.

† From Table 9.7.

process vessels that can be classified into four strata on the basis of the plutonium concentration and the ability to sample and analyze the contents. Verification method 1 is to be used in each stratum. That is, the plutonium content is to be determined uniquely for each vessel by determining the volume of the vessel contents and the plutonium factor for those contents.

The data required to design the inventory verification procedure are given in Table 9.10. The problem is to determine the optimum allocation of verification effort. Since method 1 applies to all strata, the number of cells equals the number of strata.

The cost of sampling and analysis is assumed to be similar for all process vessels. Further, h_j, measuring material value, is assumed constant in all strata. It is considered important to verify with greater intensity the contents of the tanks containing the more concentrated plutonium. This is accomplished by including the variable d_j, where d_j measures potential for diversion. Assume the following specific values are assigned.

$$d_1=4 \qquad d_3=1$$
$$d_2=10 \qquad d_4=4$$

TABLE 9.10 PARAMETER VALUES
(Example 9.H)

N_i*	Υ_i†	μ_i‡	σ_{ξ_k}§	σ_{τ_p}	$\sigma_{\xi_{k'}}$	$\sigma_{\tau_{p'}}$
6	5	20	0.20	0.12	0.20	0.16
9	0.01	1000	15	0.0015	15	0.002
4	50	20	0.10	0.25	0.10	0.20
7	6	50	1.5	0.22	1.5	0.24

* Number of process vessels in each stratum.

† Average plutonium factor for each stratum (g of Pu/liter).

‡ Average volume of process vessel in each stratum (liters).

§ In this example, σ_{ξ_k} relates to the volume measurement rather than to a weight measurement.

It is important to remember that all the factors used in the optimization procedure are to be inversely proportional to the intensity of the measurement effort; i.e., a high value for d_j implies fewer measurements.

The values for ϕ_j can now be calculated from Eq. 9.39. First, σ_j must be calculated. Since all strata are based on a method 1 measurement, Eq. 9.40 is used to calculate σ_j.

Cell 1: $\sigma_1^2 = (6)^2(5)^2[(0.20)^2+(0.20)^2]+(6)^2(20)^2[(0.12)^2+(0.16)^2] = 648$
$\sigma_1 = 26$

Cell 2: $\sigma_2^2 = (9)^2(0.01)^2[(15)^2+(15)^2]+(9)^2(1000)^2[(0.0015)^2+(0.002)^2]$
$= 510$
$\sigma_2 = 23$

Cell 3: $\sigma_3^2 = (4)^2(50)^2[(0.10)^2+(0.10)^2]+(4)^2(20)^2[(0.25)^2+(0.20)^2] = 1456$
$\sigma_3 = 38$

Cell 4: $\sigma_4^2 = (7)^2(6)^2[(1.5)^2+(1.5)^2]+(7)^2(50)^2[(0.22)^2+(0.24)^2] = 20923$
$\sigma_4 = 145$

Then, from Eq. 9.39,

$$\phi_1 = 26/\sqrt{4} = 14 \qquad \phi_3 = 38/\sqrt{1} = 38$$
$$\phi_2 = 23/\sqrt{10} = 7 \qquad \phi_4 = 145/\sqrt{4} = 72$$

The number of tanks whose contents should be verified in each stratum is then proportional to ϕ_j. Two possible inspection levels are

$n_1 = 1$	$n_1 = 2$
$n_2 = 1$	$n_2 = 1$
$n_3 = 2$	$n_3 = 4$
$n_4 = 4$	$n_4 = 7$

The total amount of inspection is chosen to attain the desired value for $V(D)$, the variance of the difference in inventory estimates between

the audit team and the operator. The solution in Sec. 9.3.2 is generally applicable. Note one caution, however. Since both the operator and audit team use the same equipment for measuring the volume of the vessel contents, the systematic-error variance due to bulk determination is zero. Thus rule A in Table 9.2 does not apply; i.e., $A_{1k}=0$ for all k. Also, if the systematic-error variance due to the analysis for plutonium concentration is dominated by sampling errors, as opposed to analytical errors, A_{3p} will also tend to be 0, since the same sampling equipment is used by both parties.

9.4.4 Basis

From the results of Sec. 9.3.4, the variance of the difference statistic, $V(D)$, is expressible as a sum of the form

$$V(D)=\sum_{k=1}^{K} A_{1k}\sigma_{\Omega_k}^2+\sum_{k=1}^{K} A_{2k}\sigma_{\xi_k}^2+\sum_{p=1}^{P} A_{3p}\sigma_{\Gamma_p}^2+\sum_{p=1}^{P} A_{4p}\sigma_{\tau_p}^2 + \sum_{t=1}^{T} A_{5t}\sigma_{\Lambda_t}^2+\sum_{t=1}^{T} A_{6t}\sigma_{\Gamma_t}^2 \tag{9.44}$$

where K is the total number of scales (operator+inspector), P is the total number of analytical techniques, and T is the total number of NDA instruments. The A coefficients are themselves summations of quantities, *where the summations are over the strata in which the given scale, analytical technique, or NDA instrument applies.* In particular, the A's are defined in Eqs. 9.29 to 9.34.

In choosing the n_i and m_i (M_i is already determined) to minimize $V(D)$, we see that A_{1k}, A_{3p}, and A_{5t} are independent of the n_i and m_i. The reason for this is that they relate to the systematic-error variances, which are not reduced as a result of additional measurements. Thus the problem reduces to minimizing $V'(D)$,

$$V'(D)=\sum_{k=1}^{K} A_{2k}\sigma_{\xi_k}^2+\sum_{p=1}^{P} A_{4p}\sigma_{\tau_p}^2+\sum_{t=1}^{T} A_{6t}\sigma_{\Gamma_t}^2 \tag{9.45}$$

From Eqs. 9.30, 9.32, and 9.34, we see that $V'(D)$ is of the form

$$V'(D)=\sum \frac{\sigma_j^2}{r_j} \tag{9.46}$$

where r_j is the number of measurements, n_i or m_i, depending on the method used in the stratum in question. To determine the range on j, assume there are v_1 strata employing method 1, v_2 employing method 2, and v_3 employing

method 3. Then the total number of sample sizes that must be selected is $(v_1+v_2+2v_3)$, and this is the number of terms in Eq. 9.46.

Each term in Eq. 9.46 is related to a cell such that there are $(v_1+v_2+2v_3)$ cells. The σ_j must be determined for each cell. For a cell based on method 1 (this involves terms of the form $A_{2k}\sigma^2_{\xi_k}$ and $A_{4p}\sigma^2_{\tau_p}$ involving the operator plus corresponding terms for the audit team),

$$\sigma_j^2=N_i^2\Upsilon_i^2(\sigma^2_{\xi_k}+\sigma^2_{\xi_{k'}})+N_i^2\mu_i^2(\sigma^2_{\tau_p}+\sigma^2_{\tau_{p'}}) \tag{9.47}$$

where the cell in question consists of measurements made on stratum i with scales k and k' (operator and audit team) and analytical techniques p and p' (operator and audit team). There are v_1 values of σ_j^2 of the form Eq. 9.47.

For a cell based on method 2,

$$\sigma_j^2=N_i^2(\sigma^2_{\xi_t}+\sigma^2_{\xi_{t'}}) \tag{9.48}$$

where the jth cell consists of measurements made on stratum i with NDA instruments t and t' (operator and audit team). There are v_2 values of σ_j^2 of the form Eq. 9.48.

For a cell based on method 3, bulk measurement,

$$\sigma_j^2=N_i^2\Upsilon_i^2(\sigma^2_{\xi_k}+\sigma^2_{\xi_{k'}}) \tag{9.49}$$

where the jth cell consists of bulk measurements made on stratum i with scales k and k' (operator and audit team). There are v_3 values of σ_j^2 of the form Eq. 9.49.

For a cell based on method 3, analytical determination,

$$\sigma_j^2=N_i^2\mu_i^2\sigma^2_{\tau_{p'}} \tag{9.50}$$

where the jth cell consists of analytical measurements made by the audit team on stratum i with analytical technique p'. There are v_3 values of σ_j^2 of the form Eq. 9.50.

The problem is to minimize $V'(D)$ in Eq. 9.46, subject to some constraint. Initially assume that this constraint is the very simple one in which $\sum r_j=r$ is fixed. (This case is treated only for mathematical reasons at this point. The constraint is unreasonable in that we would hardly equate a simple weighing with a sampling and analysis with respect to either cost or information.) This minimization is a simple procedure if the method of Lagrange multipliers is used. On the assumption that this technique is beyond the ken of many readers of this book, a more familiar approach is used. This approach consists in equating the partial derivatives of $V'(D)$ with respect to r_j to zero and solving the system of equations for the r_j.

The constraint is taken into account by writing $r_s = r - \sum_{j=1}^{s-1} r_j$, where $s = (v_1 + v_2 + 2v_3)$. Then $V'(D)$ is written

$$V'(D) = \frac{\sum_{j=1}^{s-1} \sigma_j^2}{r_j} + \frac{\sigma_s^2}{r - \sum_{j=1}^{s-1} r_j} \tag{9.51}$$

Consider $\partial V'(D)/\partial r_j$ for $j = 1, 2, \ldots, (s-1)$.

$$\frac{\partial V'(D)}{\partial r_j} = -\frac{\sigma_j^2}{r_j^2} + \frac{\sigma_s^2}{\left(r - \sum_{j=1}^{s-1} r_j\right)^2} = 0$$

which gives

$$r_j = \frac{\left(r - \sum_{j=1}^{s-1} r_j\right)\sigma_j}{\sigma_s} \tag{9.52}$$

Then, for any j, $k \neq s$,

$$\frac{r_j}{r_k} = \frac{\sigma_j}{\sigma_k}$$

which indicates that $\sum_{j=1}^{s-1} r_j$ in Eq. 9.52 can be replaced by $[(r_j \sum_{k=1}^{s-1} \sigma_k)/\sigma_j]$ to give

$$r_j = \frac{r\sigma_j - r_j \sum_{k=1}^{s-1} \sigma_k}{\sigma_s}$$

Solving this for r_j gives

$$r_j = \frac{r\sigma_j}{\sum_{k=1}^{s} \sigma_k} \tag{9.53}$$

Thus optimal sampling and measurement in the sense that $V'(D)$ is minimized for fixed r consists in choosing r_j proportional to σ_j.

Now suppose, as is likely, that additional constraints are imposed on the system. One rather obvious constraint is the cost of making a given type of measurement. Denote this by c_j, and, if this were the only constraint, r_j would simply be replaced by $r_j c_j$. The problem would then be to minimize $V'(D)$ subject to a fixed total cost rather than a fixed total number of measurements.

Other factors might be introduced. For example, we might wish to sample more heavily the strata in which the material has higher value. Value can be expressed in terms of (enrichment)^2, ranging from 0 to 1 (for plutonium). On this scale an item containing 5% ^{235}U has a value of $(0.05)^2=0.0025$, whereas the value of an item containing 90% ^{225}U is $(0.90)^2=0.81$. Of course, other value scales can be used. For convenience insert the value factor into the analysis by defining $h^{-1}=(\text{enrichment})^2$ such that the higher the enrichment, the lower the value of h. Then r_jc_j in the previous paragraph is replaced by $r_jc_jh_j$.

The audit team might also wish to take into account the diversion potential of the material in a given stratum in a certain application. This is a measure of the likelihood that diversion of a given type would occur, with consideration given to such factors as the form of the material, its accessibility, the static nature of the material, etc. A divertibility index using an arbitrary scale can be introduced. Let this value be d_j such that a low value of d_j corresponds to a high potential for diversion. (This refers to the diversion strategy of making small changes in a large number of containers. Diversion strategies in which large changes are made for few items are countered by the step 1 attributes inspection.) Then $r_jc_jh_j$ of the preceding paragraph can be replaced by $r_jc_jh_jd_j$.

It is clear that, depending on the application, many or few factors can be introduced into the optimization. By proper definition, the factors become simple multipliers of r_j, the number of measurements. Thus the additional factors introduce no complexity in the optimization process. The r_j can simply be replaced by

$$t_j=r_jc_jh_jd_j \ldots \tag{9.54}$$

and the analysis proceeds as before. Then $V'(D)$ in Eq. 9.46 can be written

$$V'(D)=\sum_{j=1}^{s}\frac{\sigma_j^2c_jh_jd_j \ldots}{t_j} \tag{9.55}$$

which is of the form

$$V'(D)=\sum_{j=1}^{s}\frac{g_j^2}{t_j} \tag{9.56}$$

where

$$g_j^2=\sigma_j^2c_jh_jd_j \ldots \tag{9.57}$$

Then, with the constraint being $\sum_{j=1}^{s} t_j=t$ fixed, t_j is simply, by Eq. 9.55,

$$t_j=\frac{tg_j}{\sum_{k=1}^{s} g_k} \tag{9.58}$$

In turn then, by Eqs. 9.54 and 9.57,

$$r_j = \frac{t\sigma_j}{\sqrt{c_j h_j d_j \ldots} \sum_{k=1}^{s} g_k} \tag{9.59}$$

Thus the optimal strategy calls for choosing r_j proportional to $\sigma_j / \sqrt{c_j h_j d_j \ldots} = \phi_j$.

In practice, ϕ_j is calculated for several cases of total inspection effort by choosing the r_j proportional to the ϕ_j. The $V(D)$ in Eq. 9.44 is then computed for each case, and the total inspection effort is selected which corresponds to an acceptable value for $V(D)$, i.e., to an acceptable test sensitivity. Alternatively, the total inspection effort can be fixed, in which case only the single set of calculations corresponding to this fixed effort need be made.

Chapter 10

INTEGRATED APPLICATIONS

OVERVIEW

Most of the statistical methods presented in this book can be applied to several types of nuclear facilities. For this reason it is logical to organize the book by type of application rather than by type of facility to minimize needless repetition.

Nevertheless, it is also helpful to organize the material by type of nuclear facility so that the reader who prefers to concentrate on examples of greatest personal interest can avoid making the transition from one type of facility to another. This is the principal purpose of this chapter.

In all types of facilities, the statistical contents of the problems of nuclear materials control are similar in kind, if not in degree of importance. Thus, in all facilities there are the problems of estimating measurement-error variances, analyzing shipper–receiver data, verifying an inventory, calculating the variance of the special nuclear material (SNM) content of an individual item or of the algebraic sum of SNM for groups of items, and analyzing accumulated material unaccounted for (MUF) data. Therefore, the material in this chapter is organized along topical lines, and within each section examples are identified which illustrate the application of a given statistical method to a particular type of facility.

The five topics treated in this chapter include estimation of measurement-error variances, analysis of shipper–receiver data, verification of inventories, calculation of variances [which can then be expressed as limits of error (LE)] of SNM contents (single item or algebraic sum), and analysis of MUF data. Within each topic each example presented in the previous chapters is listed under the type of facility on which it is based. (Since Chapter 2 is introductory in nature, examples presented there are not included). Some examples are identified as general in nature and apply equally well to several types of facilities. This is not to say that examples of problems associated with fuel fabrication facilities, say, are not general in nature either. Thus,

even though the reader may wish to concentrate his attention on examples identified as being appropriate to his type of facility, he should not exclude entirely those categorized under other types. (It is rather evident in what follows that the greatest attention has been given to conversion and fabrication plants. This is a natural result of the author's greater amount of experience in that type of facility. This emphasis should not seriously lessen the utility of the book in applications to problems of other types of facilities since such problems are similar in statistical content.)

The chapter is structured as follows: For each of the five statistical topics identified, each example presented in the earlier chapters is listed in a table under the type of facility on which the example is based. If the example itself is general in nature, it is so designated. The examples listed in each table are described briefly. Included in this description is an indication of the degree of generality of application of the statistical methods illustrated by the example in question.

10.1 ESTIMATION OF MEASUREMENT-ERROR VARIANCES

Table 10.1 gives the examples of methods that can be used to estimate measurement-error variances, and each example is described briefly.

TABLE 10.1 EXAMPLES OF MEASUREMENT-ERROR-VARIANCE ESTIMATION LISTED BY FACILITY TYPE

Conversion and fabrication		Chemical reprocessing		Scrap recovery		General	
Example	Section	Example	Section	Example	Section	Example	Section
3.G	3.3.4	3.D	3.3.2	8.A	8.1.3	3.B	3.3.2
3.H	3.3.4	3.L	3.3.6	8.J	8.3.3	3.C	3.3.2
3.I	3.3.4	3.M	3.3.7			3.E	3.3.3
3.J	3.3.4	3.P	3.3.9			3.F	3.3.4
3.K	3.3.5	8.K	8.3.3			3.N	3.3.8
4.A	4.1.3	8.L	8.3.3			3.O	3.3.8
4.H	4.3.3					3.Q	3.3.10
4.I	4.3.3					8.F	8.1.3
4.J	4.3.3						
8.B	8.1.3						
8.C	8.1.3						
8.G	8.2.3						

10.1.1 Conversion and Fabrication

Example 3.G. This is an analysis-of-variance example illustrating how the random-error variances of sampling and analysis can be estimated separately. The example pertains to the percent uranium in scrap ammonium diuranate (ADU), but it is applicable to any type of facility for situations in which samples are drawn and analyzed for percent element and/or percent isotope.

Example 3.H. This example shows how the random-error variance due to sampling can be estimated. It pertains to the percent uranium in dry waste that has been burned, with the ash stored in drums awaiting chemical leaching and recovery. The method of estimation is applicable to any situation in which samples are drawn and analyzed for percent element and/or percent isotope. The resulting estimate measures the combined random effects of sampling and analysis, but for this particular example the sampling variance is dominant.

Example 3.I. This analysis-of-variance example is similar in statistical content to example 3.G and deals with obtaining separate estimates of the random-error variances due to sampling and analysis for percent plutonium in fuel pellets. Like example 3.G, this one is also of general interest.

Example 3.J. This example shows how the random-error variance for the combined effects of sampling and analysis and the short-term systematic-error variance can be estimated. It pertains to replicate samples of UO_2 powder drawn from production lots, with each group of samples corresponding to a given lot analyzed for percent uranium under the same analytical laboratory conditions. The statistical method is applicable whenever groups of samples are analyzed individually, with the samples comprising each group being analyzed under similar conditions.

Example 3.K. This example illustrates Bartlett's test of the hypothesis that several variances are equal, where these variances are separately estimated. This particular example deals with the random errors due to sampling ADU scrap for percent uranium, but the test is applicable in any situation in which several estimates of population variances are available and the question is whether or not these population variances are equal. This problem is of special interest because error parameters are constantly being re-estimated on the basis of recent data, and it is important to know whether the more recent data are indicative of real changes in the corresponding true error variances.

Example 4.A. This example shows how the variance in the weight

of a fuel rod is affected by the variances in the weights of the components of the assembled rod. This illustrates any situation in which the variance of a sum is to be found. Emphasis is given to classifying the components in the sum with respect to their effect on the overall variance, thus indicating where improvements in the sense of tighter specifications might be required.

Example 4.H. This example is similar to example 4.A, except that the variances of the component parts are now regarded as estimates rather than known quantities. It illustrates how to calculate the degrees of freedom for a variance that is a linear function of estimated variances and is applicable to any situation of this kind.

Example 4.I. This is another example of how to calculate the degrees of freedom for a variance that is a function of estimated variances. This example involves finding the variance associated with the amount of ^{235}U in a container, when the amount is calculated by measuring the net weight, the percent uranium, and the percent ^{235}U. The example illustrates situations encountered in any type of facility.

Example 4.J. The problem situation is identical to that of example 3.J. In this instance, however, the problem is to calculate the degrees of freedom for the various estimated error variances. This is of general interest and especially is directly applicable to situations in which the estimates are derived from an analysis-of-variance table.

Example 8.B. Samples of UO_2 powder are measured for total ^{235}U content by two methods. The twofold problem specifically treated involves testing the hypothesis that the random analytical-error variance for one method is as stated and then obtaining separate estimates of this variance for each method. The method is applicable to any situation in which paired measurements are made.

Example 8.C. This is a continuation of example 8.B. The level of significance is changed to demonstrate the effect on the estimates.

Example 8.G. This is a continuation of example 8.C. The question now is to determine whether or not there is a significant bias between the two measurement methods.

10.1.2 Chemical Reprocessing

Example 3.D. This example involves measurements made on a known standard. The problem deals with uranium nitrate hexahydrate (UNH) transfer measurements in which bias is controlled by running a known standard each time a process sample is analyzed. The statistical analysis produces an estimate of the bias and of the systematic- and

random-error variances due to analysis. It is applicable to any situation in which measurements are made on known standards.

Example 3.L. This example involves an experiment designed to estimate the systematic-error variance due to sampling the contents of an input accountability tank using an air-lift sampler. The air-lift samples are compared with companion dip samples. An estimate of the random-error variance due to the combined effects of sampling and analysis is also found. The problem is generally applicable in any situation in which the systematic-error variance due to sampling is to be estimated.

Example 3.M. Total uranium in a process tank is determined by measuring the volume of the tank and then measuring the concentration from a tank sample. The problem is to estimate the systematic-error variance associated with determining the uranium concentration. This example illustrates the synthetic approach to estimating error variances and is applicable in principle to any measurement situation.

Example 3.P. A process vessel is to be calibrated. This example shows how the calibration data can be analyzed using a cumulative-error model to estimate the random- and systematic-error variances associated with the weight of the contained liquid. This example is restricted in materials control applications to the calibration of process vessels.

Example 8.K. Paired samples from dissolver plant batches are analyzed for percent ^{241}Pu by different mass spectrometers. The problem is to test the hypothesis that both mass spectrometers have the same analytical random-error variance. Because of nonrandom behavior over the batches, an estimate of the analytical systematic-error variance is also derived from the data. The statistical techniques illustrated are applicable whenever there are paired data involving measurements made on the same samples by two instruments, laboratories, operators, etc.

Example 8.L. The problem situation is the same as in example 8.K, but now the hypothesis is that the sum of the random-error variances equals some given value. Again, this has general application.

10.1.3 Scrap Recovery

Example 8.A. Samples of nitrate solution are drawn from each container being loaded into a recovery plant for purification and are analyzed for percent plutonium using two different analytical techniques. The problem is to test the hypothesis that the analytical

random-error variances are the same for both methods. The analysis is complicated by the fact that the relative bias between the two methods depends on the plutonium concentration, which invalidates the analysis. Whenever paired data are available, the statistical techniques illustrated here are applicable.

Example 8.J. This is the same problem situation as in example 8.A, but the statistical analysis is altered to account for the nonrandom relative bias between the two methods. The method of allowing for this nonrandomness is generally applicable whenever the two measurement methods exhibit a relative bias that is nonrandom over the data set.

10.1.4 General

Example 3.B. This example deals with mass spectrometer measurements of percent ^{235}U on known standards. The data permit estimation of the bias and of the systematic- and random-error variances due to analysis. Although based on mass spectrometer data, the statistical methods are applicable whenever measurements of some kind are made on known standards.

Example 3.C. In this example percent plutonium measurements on a known standard are made by two analysts. As in example 3.B, the bias and the analytical systematic- and random-error variances can be estimated for the analytical method. In addition, the two analysts' results are compared to determine if there is a bias between them and to see if one produces more variable results than the other. The applition is very general in nature.

Example 3.E. This example also deals with measurements made on a known standard. In this case the measurements consist of weights, with the standard being a standard weight. There are two unique aspects to this problem. For one thing, the effects on the error variances due to rounding must often be included when weight measurements are made. Also, net weights are determined by subtraction of a tare weight from a gross weight; the errors introduced by both weighing operations must be factored into the analysis. For these two reasons this particular example is generally restricted in application to net weight measurements.

Example 3.F. This is an example of an analysis of variance in which the data consist of percent ^{235}U measurements on known standard samples. The example is similar to example 3.B except that now the data are collected over an extended time interval, thus permitting estimation of the short-term systematic error due to analysis.

Example 3.N. This example involves linear calibration. In particular, it concerns the calibration of a nondestructive assay (NDA) instrument used to measure solid waste. The method of calibration is discussed, and techniques are presented to estimate the random- and systematic-error variances for a single measurement and for the sum of a number of measurements. The methods are applicable in any linear calibration case except when the error model is cumulative, as may be the case in process vessel calibration work (see example 3.P).

Example 3.O. This is a second example involving linear calibration. The same situation obtains as in example 3.N, except that the total amount of ^{235}U in five containers is determined, along with the corresponding systematic- and random-error variances.

Example 3.Q. The situation is identical to that of examples 3.N and 3.O, except that the calibration relation is curvilinear. The same comments apply.

Example 8.F. Two mass spectrometers are used to measure samples of uranium for percent ^{235}U. The data are paired. The problem is to obtain estimates of the random-error variance due to analysis for each mass spectrometer. In this particular example this variance is a function of the percent ^{235}U, which must be taken into account in the analysis. The methods are applicable whenever paired measurement data are given.

10.2 ANALYSIS OF SHIPPER–RECEIVER DATA

Shipper–receiver data, as a by-product, contain useful information about errors of measurement. Because of this, the five examples cited in this section should also be referred to when the problem is to estimate measurement-error variances.

All the examples are based on data relating to shipments to a conversion and fabrication facility. Receipts at a reactor are based on item counts and verification of rod identifications. At a chemical reprocessing facility, shipments from a reactor have no direct shipper measurements but rather only predictions based on reactor experience. Likewise, the receipt measurement is made at the input accountability tank. Shipper–receiver problems at a scrap recovery plant are similar in statistical content to those at a conversion and fabrication facility, and the methods of statistical analysis discussed in these examples are applicable there also.

Table 10.2 lists the examples dealing with the analysis of shipper–receiver data.

TABLE 10.2 EXAMPLES OF SHIPPER–RECEIVER DATA ANALYSIS FOR A CONVERSION AND FABRICATION FACILITY

Example	Section
6.A	6.1.3
8.D	8.1.3
8.E	8.1.3
8.H	8.2.3
8.I	8.2.3
8.M	8.3.3

10.2.1 Conversion and Fabrication

Example 6.A. This example involves a shipment of PuO_2 powder in which the problem is to find the standard deviation of the difference in the measured amounts of plutonium for the shipper and the receiver. Each party provides information about his pertinent measurement-error variances and the manner in which the plutonium content is calculated for each container. The variances provided by the shipper and receiver are accepted as being valid.

Example 8.D. This example involves a shipment of UF_6 cylinders in which the net weight of uranium per cylinder is the statistic. The random-error variances for the shipper and receiver are tested for equality, and estimates of these variances are found depending on the result of the significance test.

Example 8.E. The situation is the same as in example 8.D. In this instance the shipper and receiver both assign values to their error variances, and these are tested for validity by using the shipper–receiver data. The test is made jointly and then individually. Values that should be assigned to the error variance for each party are determined based on the results of the statistical tests of significance.

Example 8.H. For the data of example 8.D, the problem is to find the best estimate of the total uranium in the shipment, where this estimate is best in the sense of having minimum variance among all unbiased estimates.

Example 8.I. This is a continuation of example 8.H. The question of whether or not there is a significant difference between the shipper and receiver value for total uranium is considered.

Example 8.M. This example consists of shipper and receiver measurements of percent plutonium in three shipments of PuO_2 powder. The problems of how to make the various tests of significance

for the combined data from the three shipments are considered. Further, the data are used to estimate the combined systematic-error variances for the two parties, assuming that both parties are, in fact, measuring the same quantities.

10.3 VERIFICATION OF INVENTORIES

Table 10.3 lists examples of methods that can be used in verifying inventory holdings, and the examples are briefly described.

TABLE 10.3 EXAMPLES OF INVENTORY VERIFICATION BY TYPE OF FACILITY

Conversion and fabrication		Chemical reprocessing		Scrap recovery		General	
Example	Section	Example	Section	Example	Section	Example	Section
9.A	9.1.3	9.B	9.1.3	9.H	9.4.3	9.D	9.2.3
9.F	9.3.3	9.C	9.1.3			9.E	9.2.3
9.G	9.4.3						

10.3.1 Conversion and Fabrication

Example 9.A. This example is concerned with verifying the operator's gross weights assigned to 400 containers of UO_2 powder. The audit is on an attributes basis, with each container being either accepted or rejected on the basis of the size of the discrepancy between weight measurement of the operator and the audit team. The situation is perfectly general, the techniques being applicable to any attributes inspection situation involving a single population.

Example 9.F. This problem involves verification of the entire inventory of uranium in a material balance area (MBA) on the basis of variables measurements. The inventory is divided into strata, and different methods of measuring the uranium contents are used depending on the stratum. Although the example is presented for a fuel fabrication facility, the statistical methods have broader applicability and can be used in other types of nuclear facilities as well.

Example 9.G. The situation is the same as in example 9.F. Now, however, the emphasis is on designing the verification effort by selecting the various sample sizes, rather than on analyzing the data that result from the verification measurements.

10.3.2 Chemical Reprocessing

Example 9.B. This is an example of attributes inspection involving bottles of plutonium nitrate, where failure to locate a particular bottle appearing on the inventory listing constitutes a defect. The problem is to determine the sample size. The situation is perfectly general and is applicable to any attributes inspection for a single population.

Example 9.C. This is a continuation of example 9.B with the parameter values changed. In this example, one defect is permitted in the sample of n bottles, whereas in the previous example, as soon as one defect is located, the inventory must be 100% verified. Again the problem is to determine the sample size.

10.3.3 Scrap Recovery

Example 9.H. The problem involves designing the inspection effort to verify the plutonium inventory in a scrap recovery facility MBA through variables inspection. The inventory is contained in process vessels, and strata are formed on the basis of vessel size and concentration of the contents. The statistical methods are not limited to this type of facility.

10.3.4 General

Example 9.D. This example illustrates an attributes inspection involving several classes, and the problem is to control the significance level for the entire audit. This shows test procedures that can be applied in any type of facility in which attributes inspection is performed.

Example 9.E. This is a continuation of example 9.D. In this case the significance levels of the individual tests are presumed to differ depending on the class of items and the relative importance of detecting defects.

10.4 CALCULATION OF VARIANCES OF SNM CONTENTS

Table 10.4 lists examples that illustrate how to calculate the variance of the measured SNM content either for an individual item or for the algebraic sum for groups of items. The algebraic sum is perfectly general and can represent such quantities as total amounts in a part or all of an inventory, a shipper–receiver difference, or MUF for some MBA. Since MUF is an especially important index of nuclear

materials control, it receives most attention in the examples. The examples listed in Table 10.4 are described briefly.

TABLE 10.4 EXAMPLES OF CALCULATING SNM VARIANCES BY TYPE OF FACILITY

Conversion and fabrication		Chemical reprocessing		Scrap recovery		General	
Example	Section	Example	Section	Example	Section	Example	Section
5.B	5.1.3	5.A	5.1.3	6.G	6.1.3	6.B	6.1.3
5.D	5.2.3	5.C	5.2.3			6.C	6.1.3
5.E	5.2.3	6.F	6.1.3			6.D	6.1.3
6.E	6.1.3						
6.H	6.1.3						
6.I	6.1.3						

10.4.1 Conversion and Fabrication

Example 5.B. The problem is to find the standard deviation on the total amount of uranium and of ^{235}U in a can of UO_2 powder. This example is of general interest in other types of facilities.

Example 5.D. This is a companion example to example 5.B. The difference is that now the error standard deviations are expressed on a relative basis as opposed to an absolute basis as in example 5.B.

Example 5.E. This is another illustration of how to find the standard deviation for the SNM content of an individual item. In this case the item is a fuel rod containing PuO_2–UO_2 pellets and the SNM is fissile plutonium. This example is also of general applicability.

Example 6.E. In this example the standard deviation of the ^{235}U MUF for a small-scale fuel fabrication facility is computed. This example is one of the more important ones in the book and is representative of calculations to be performed in any such facility.

Example 6.H. This is a continuation of example 6.E, the difference being that now a part of the inventory is measured by nondestructive assay methods.

Example 6.I. This is a detailed example of a material balance analysis for a PuO_2–UO_2 fabrication facility. The analysis is performed before the start of a campaign and is motivated by the need to anticipate measurement-control problems in advance so that corrective action can be taken. Incremental and cumulative MUF's are considered.

10.4.2 Chemical Reprocessing

Example 5.A. The standard deviation is calculated for the total amount of plutonium in a dissolver batch. The statistical methods illustrated in the example are applicable in a wide variety of situations.

Example 5.C. This is a companion example to example 5.A. The difference is that now the error standard deviations are expressed on a relative basis rather than absolutely.

Example 6.F. In this example the standard deviation of the plutonium MUF over a single campaign is computed. This has the same importance to a chemical reprocessing facility as example 6.E has to a fabrication facility.

10.4.3 Scrap Recovery

Example 6.G. The month-end inventory holding of plutonium is determined and its variance is found. In this case the algebraic sum represents the total amount of plutonium in inventory. Interest in this problem is not limited to scrap recovery facilities.

10.4.4 General

Example 6.B. At a given point in time, an unidentified type of facility has on inventory seven batches of uranium-bearing materials. The problem is to find the variance of the total amount of uranium in inventory. The statistical methods used are applicable to any type of facility.

Example 6.C. This example is artificially contrived but is included because it applies all the rules for finding the variance of an algebraic sum of SNM in their more complex forms. It is a good example to refer to if the application of certain computational rules is not clear in other examples.

Example 6.D. This is a continuation of example 6.C. It illustrates how more than one short-term systematic-error variance due to analysis can be included.

10.5 ANALYSIS OF MUF DATA

Table 10.5 lists the examples how MUF data can be analyzed. Some examples relate to interpreting a single, individual MUF, and others illustrate how information can be extracted from a series of MUF's.

Since MUF is common to all types of facilities, no effort was made to present examples specific to each type. The examples are described briefly.

TABLE 10.5 EXAMPLES OF HOW TO ANALYZE MUF DATA BY TYPE OF FACILITY

Conversion and fabrication		General	
Example	Section	Example	Section
7.E	7.1.3	4.C	4.1.3
7.F	7.2.3	7.A	7.1.3
7.K	7.4.3	7.B	7.1.3
		7.C	7.1.3
		7.D	7.1.3
		7.G	7.2.3
		7.H	7.3.3
		7.I	7.3.3
		7.J	7.3.3

10.5.1 Conversion and Fabrication

Example 7.E. When the error variances are regarded as known constants, the test of significance and/or the construction of confidence intervals for MUF are based on the normal density function. If this assumption of known variance is poor, then Student's t distribution must be used. This example illustrates this for the MUF in a fabrication facility when the sampling-error variances for ADU scrap are poorly estimated (the data are otherwise the same as in example 6.E). The method is applicable to other similar situations.

Example 7.F. Monthly ^{235}U MUF's are given for a fuel fabrication facility. These data are analyzed to obtain estimates of the variance of an inventory and of a given difference between inputs and outputs. It is assumed that the true MUF is constant from month to month. The statistical analysis is applicable to any situation in which sequences of MUF's are given if the underlying assumptions are valid.

Example 7.K. This example illustrates how material balance closings can be made at intervals of time even though complete physical inventories are not taken. This can be done for any facility in which the major portion of the inventory has been measured when placed in inventory, i.e., in which the unmeasured or hidden inventory is small relative to the measured inventory.

10.5.2 General

Example 4.C. This example shows how successive MUF's are correlated by virtue of the fact that the beginning inventory for one time period is identically the ending inventory for the prior period.

Example 7.A. This is a test of significance for a given observed MUF. The hypothesis is that MUF is zero units. The standard deviation of MUF is assumed to be known.

Example 7.B. With the data of example 7.A, this example illustrates how confidence limits are found for the true MUF, given an observed MUF and its known standard deviation.

Example 7.C. This is identical with example 7.A except that the hypothesis is now that the true MUF is some given positive value.

Example 7.D. A hypothesized value and a larger alternative value are established for MUF. With given probabilities of rejecting the hypothesis when true, on one hand, and of accepting it when the alternative hypothesis is true, on the other hand, the value is found for the standard deviation of MUF required to meet these criteria. This can then be related to measurement effort needed to result in this value of the standard deviation.

Example 7.G. This example is based on monthly MUF data for 12 years of operation of a diffusion plant. These data are used to estimate the variance of the true MUF and the covariance between any two successive true MUF's. The measurement-error variances are assumed known. Also, a control chart is constructed to provide a visual picture of the state of control. The methods are applicable whenever sequences of MUF's are given.

Example 7.H. The so-called minimum-variance MUF differs from the standard MUF in that the beginning inventory is a weighted average of prior inventories plus the sum of the differences between inputs and outputs. This is calculated for data over ten time periods and compared with the standard MUF. The degree to which the minimum-variance MUF concept can be applied in practice, and under what circumstances, is not known.

Example 7.I. This is another example of the minimum-variance MUF for an arbitrary facility.

Example 7.J. The diffusion plant data of example 7.G are analyzed by the minimum-variance MUF technique, and a control chart is constructed.

Appendix A

CUMULATIVE NORMAL DISTRIBUTION—VALUES OF P

Values of P corresponding to z_P for the normal curve. z is the standard normal variable. The value of P for $-z_P$ equals one minus the value of P for $+z_P$, e.g., the P for -1.62 equals $1 - .9474 = .0526$.

z_P	.00	.01	.02	.03	.04	.05	.06	.07	.08	.09
.0	5000	5040	5080	5120	5160	5199	5239	5279	5319	5359
.1	5398	5438	5478	5517	5557	5596	5636	5675	5714	5753
.2	5793	5832	5871	5910	5948	5987	6026	6064	6103	6141
.3	6179	6217	6255	6293	6331	6368	6406	6443	6480	6517
.4	6554	6591	6628	6664	6700	6736	6772	6808	6844	6879
.5	6915	6950	6985	7019	7054	7088	7123	7157	7190	7224
.6	7257	7291	7324	7357	7389	7422	7454	7486	7517	7549
.7	7580	7611	7642	7673	7704	7734	7764	7794	7823	7852
.8	7881	7910	7939	7967	7995	8023	8051	8078	8106	8133
.9	8159	8186	8212	8238	8264	8289	8315	8340	8365	8389
1.0	8413	8438	8461	8485	8508	8531	8554	8577	8599	8621
1.1	8643	8665	8686	8708	8729	8749	8770	8790	8810	8830
1.2	8849	8869	8888	8907	8925	8944	8962	8980	8997	9015
1.3	9032	9049	9066	9082	9099	9115	9131	9147	9162	9177
1.4	9192	9207	9222	9236	9251	9265	9279	9292	9306	9319
1.5	9332	9345	9357	9370	9382	9394	9406	9418	9429	9441
1.6	9452	9463	9474	9484	9495	9505	9515	9525	9535	9545
1.7	9554	9564	9573	9582	9591	9599	9608	9616	9625	9633
1.8	9641	9649	9656	9664	9671	9678	9686	9693	9699	9706
1.9	9713	9719	9726	9732	9738	9744	9750	9756	9761	9767
2.0	9772	9778	9783	9788	9793	9798	9803	9808	9812	9817
2.1	9821	9826	9830	9834	9838	9842	9846	9850	9854	9857
2.2	9861	9864	9868	9871	9875	9878	9881	9884	9887	9890
2 3	9893	9896	9898	9901	9904	9906	9909	9911	9913	9916
2.4	9918	9920	9922	9925	9927	9929	9931	9932	9934	9936
2.5	9938	9940	9941	9943	9945	9946	9948	9949	9951	9952
2.6	9953	9955	9956	9957	9959	9960	9961	9962	9963	9964
2.7	9965	9966	9967	9968	9969	9970	9971	9972	9973	9974
2 8	9974	9975	9976	9977	9977	9978	9979	9979	9980	9981
2.9	9981	9982	9982	9983	9984	9984	9985	9985	9986	9986
3.0	9987	9987	9987	9988	9988	9989	9989	9989	9990	9990
3.1	9990	9991	9991	9991	9992	9992	9992	9992	9993	9993
3.2	9993	9993	9994	9994	9994	9994	9994	9995	9995	9995
3.3	9995	9995	9995	9996	9996	9996	9996	9996	9996	9997
3 4	9997	9997	9997	9997	9997	9997	9997	9997	9997	9998

From *Experimental Statistics,* NBS Handbook 91, Report ORDP-20-114, p. T-2, Government Printing Office, Washington, D. C., 1963.

Appendix B

PERCENTILES OF THE χ^2 DISTRIBUTION

Values of χ^2_P corresponding to P

df	$\chi^2_{.005}$	$\chi^2_{.01}$	$\chi^2_{.025}$	$\chi^2_{.05}$	$\chi^2_{.10}$	$\chi^2_{.90}$	$\chi^2_{.95}$	$\chi^2_{.975}$	$\chi^2_{.99}$	$\chi^2_{.995}$
1	000039	00016	00098	0039	0158	2 71	3 84	5 02	6 63	7 88
2	0100	0201	0506	1026	2107	4 61	5 99	7 38	9 21	10 60
3	0717	115	216	352	584	6 25	7 81	9 35	11 34	12 84
4	207	297	484	711	1 064	7 78	9 49	11 14	13 28	14 86
5	412	554	831	1 15	1 61	9 24	11 07	12 83	15 09	16 75
6	676	872	1 24	1 64	2 20	10 64	12 59	14 45	16 81	18 55
7	989	1 24	1 69	2 17	2 83	12 02	14 07	16 01	18 48	20 28
8	1 34	1 65	2 18	2 73	3 49	13 36	15 51	17 53	20 09	21 96
9	1 73	2 09	2 70	3 33	4 17	14 68	16 92	19 02	21 67	23 59
10	2 16	2 56	3 25	3 94	4 87	15 99	18 31	20 48	23 21	25 19
11	2 60	3 05	3 82	4 57	5 58	17 28	19 68	21 92	24 73	26 76
12	3 07	3 57	4 40	5 23	6 30	18 55	21 03	23 34	26 22	28 30
13	3 57	4 11	5 01	5 89	7 04	19 81	22 36	24 74	27 69	29 82
14	4 07	4 66	5 63	6 57	7 79	21 06	23 68	26 12	29 14	31 32
15	4 60	5 23	6 26	7 26	8 55	22 31	25 00	27 49	30 58	32 80
16	5 14	5 81	6 91	7 96	9 31	23 54	26 30	28 85	32 00	34 27
18	6 26	7 01	8 23	9 39	10 86	25 99	28 87	31 53	34 81	37 16
20	7 43	8 26	9 59	10 85	12 44	28 41	31 41	34 17	37 57	40 00
24	9 89	10 86	12 40	13 85	15 66	33 20	36 42	39 36	42 98	45 56
30	13 79	14 95	16 79	18 49	20 60	40 26	43 77	46 98	50 89	53 67
40	20 71	22 16	24 43	26 51	29 05	51 81	55 76	59 34	63 69	66 77
60	35 53	37 48	40 48	43 19	46 46	74 40	79 08	83 30	88 38	91 95
120	83 85	86 92	91 58	95 70	100 62	140 23	146 57	152 21	158 95	163 64

Adapted with permission from W. J. Dixon and F. J. Massey, Jr., *Introduction to Statistical Analysis* (2nd ed.), McGraw-Hill Book Company, Inc., New York, 1957.

Appendix C

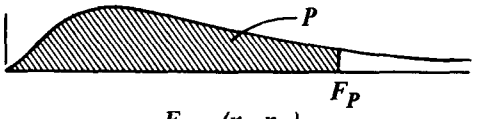
PERCENTILES OF THE t DISTRIBUTION

df	$t_{.60}$	$t_{.70}$	$t_{.80}$	$t_{.90}$	$t_{.95}$	$t_{.975}$	$t_{.99}$	$t_{.995}$
1	325	727	1 376	3 078	6 314	12 706	31 821	63 657
2	289	617	1 061	1 886	2 920	4 303	6 965	9 925
3	277	584	978	1 638	2 353	3 182	4 541	5 841
4	271	569	941	1 533	2 132	2 776	3 747	4 604
5	267	559	920	1 476	2 015	2 571	3 365	4 032
6	265	553	906	1 440	1 943	2 447	3 143	3 707
7	263	549	896	1 415	1 895	2 365	2 998	3 499
8	262	546	889	1 397	1 860	2 306	2 896	3 355
9	261	543	883	1 383	1 833	2 262	2 821	3 250
10	260	542	879	1 372	1 812	2 228	2 764	3 169
11	260	540	876	1 363	1 796	2 201	2 718	3 106
12	259	539	873	1 356	1 782	2 179	2 681	3 055
13	259	538	870	1 350	1 771	2 160	2 650	3 012
14	258	537	868	1 345	1 761	2 145	2 624	2 977
15	258	536	866	1 341	1 753	2 131	2 602	2 947
16	258	535	865	1 337	1 746	2 120	2 583	2 921
17	257	534	863	1 333	1 740	2 110	2 567	2 898
18	257	534	862	1 330	1 734	2 101	2 552	2 878
19	257	533	861	1 328	1 729	2 093	2 539	2 861
20	257	533	860	1 325	1 725	2 086	2 528	2 845
21	257	532	859	1 323	1 721	2 080	2 518	2 831
22	256	532	858	1 321	1 717	2 074	2 508	2 819
23	256	532	858	1 319	1 714	2 069	2 500	2 807
24	256	531	857	1 318	1 711	2 064	2 492	2 797
25	256	531	856	1 316	1 708	2 060	2 485	2 787
26	256	531	856	1 315	1 706	2 056	2 479	2 779
27	256	531	855	1 314	1 703	2 052	2 473	2 771
28	256	530	855	1 313	1 701	2 048	2 467	2 763
29	256	530	854	1 311	1 699	2 045	2 462	2 756
30	256	530	854	1 310	1 697	2 042	2 457	2 750
40	255	529	851	1 303	1 684	2 021	2 423	2 704
60	254	527	848	1 296	1 671	2 000	2 390	2 660
120	254	526	845	1 289	1 658	1 980	2 358	2 617
∞	253	524	842	1 282	1 645	1 960	2 326	2 576

Adapted by permission from W. J. Dixon and F. J. Massey, Jr, *Introduction to Statistical Analysis* (2nd ed.), McGraw-Hill Book Company, Inc., New York, 1957 Originally from R. A. Fisher and F. Yates, *Statistical Tables,* Oliver and Boyd, Ltd, London, 1938.

Appendix D

PERCENTILES OF THE F DISTRIBUTION



$F_{.90}(n_1, n_2)$

n_1 = degrees of freedom for numerator

n_2 = degrees of freedom for denominator

n_2 \ n_1	1	2	3	4	5	6	7	8
1	39 86	49 50	53 59	55 83	57 24	58 20	58 91	59 44
2	8 53	9 00	9 16	9 24	9 29	9 33	9 35	9 37
3	5 54	5 46	5 39	5 34	5 31	5 28	5 27	5 25
4	4 54	4 32	4 19	4 11	4 05	4 01	3 98	3 95
5	4 06	3 78	3 62	3 52	3 45	3 40	3 37	3 34
6	3 78	3 46	3 29	3 18	3 11	3 05	3 01	2 98
7	3 59	3 26	3 07	2 96	2 88	2 83	2 78	2 75
8	3 46	3 11	2 92	2 81	2 73	2 67	2 62	2 59
9	3 36	3 01	2 81	2 69	2 61	2 55	2 51	2 47
10	3 29	2 92	2 73	2 61	2 52	2 46	2 41	2 38
11	3 23	2 86	2 66	2 54	2 45	2 39	2 34	2 30
12	3 18	2 81	2 61	2 48	2 39	2 33	2 28	2 24
13	3 14	2 76	2 56	2 43	2 35	2 28	2 23	2 20
14	3 10	2 73	2 52	2 39	2 31	2 24	2 19	2 15
15	3 07	2 70	2 49	2 36	2 27	2 21	2 16	2 12
16	3 05	2 67	2 46	2 33	2 24	2 18	2 13	2 09
17	3 03	2 64	2 44	2 31	2 22	2 15	2 10	2 06
18	3 01	2 62	2 42	2 29	2 20	2 13	2 08	2 04
19	2 99	2 61	2 40	2 27	2 18	2 11	2 06	2 02
20	2 97	2 59	2 38	2 25	2 16	2 09	2 04	2 00
21	2 96	2 57	2 36	2 23	2 14	2 08	2 02	1 98
22	2 95	2 56	2 35	2 22	2 13	2 06	2 01	1 97
23	2 94	2 55	2 34	2 21	2 11	2 05	1 99	1 95
24	2 93	2 54	2 33	2 19	2 10	2 04	1 98	1 94
25	2 92	2 53	2 32	2 18	2 09	2 02	1 97	1 93
26	2 91	2 52	2 31	2 17	2 08	2 01	1 96	1 92
27	2 90	2 51	2 30	2 17	2 07	2 00	1 95	1 91
28	2 89	2 50	2 29	2 16	2 06	2 00	1 94	1 90
29	2 89	2 50	2 28	2 15	2 06	1 99	1 93	1 89
30	2 88	2 49	2 28	2 14	2 05	1 98	1 93	1 88
40	2 84	2 44	2 23	2 09	2 00	1 93	1 87	1 83
60	2 79	2 39	2 18	2 04	1 95	1 87	1 82	1 77
120	2 75	2 35	2 13	1 99	1 90	1 82	1 77	1 72
∞	2 71	2 30	2 08	1 94	1 85	1 77	1 72	1 67

Adapted with permission from E. S. Pearson and H. O. Hartley (Eds.), *Biometrika Tables for Statisticians*, Vol. I (2nd ed.), Cambridge University Press, New York, 1958.

9	10	12	15	20	24	30	40	60	120	∞
59.86	60.19	60.71	61.22	61.74	62.00	62.26	62.53	62.79	63.06	63.33
9.38	9.39	9.41	9.42	9.44	9.45	9.46	9.47	9.47	9.48	9.49
5.24	5.23	5.22	5.20	5.18	5.18	5.17	5.16	5.15	5.14	5.13
3.94	3.92	3.90	3.87	3.84	3.83	3.82	3.80	3.79	3.78	3.76
3.32	3.30	3.27	3.24	3.21	3.19	3.17	3.16	3.14	3.12	3.10
2.96	2.94	2.90	2.87	2.84	2.82	2.80	2.78	2.76	2.74	2.72
2.72	2.70	2.67	2.63	2.59	2.58	2.56	2.54	2.51	2.49	2.47
2.56	2.50	2.50	2.46	2.42	2.40	2.38	2.36	2.34	2.32	2.29
2.44	2.42	2.38	2.34	2.30	2.28	2.25	2.23	2.21	2.18	2.16
2.35	2.32	2.28	2.24	2.20	2.18	2.16	2.13	2.11	2.08	2.06
2.27	2.25	2.21	2.17	2.12	2.10	2.08	2.05	2.03	2.00	1.97
2.21	2.19	2.15	2.10	2.06	2.04	2.01	1.99	1.96	1.93	1.90
2.16	2.14	2.10	2.05	2.01	1.98	1.96	1.93	1.90	1.88	1.85
2.12	2.10	2.05	2.01	1.96	1.94	1.91	1.89	1.86	1.83	1.80
2.09	2.06	2.02	1.97	1.92	1.90	1.87	1.85	1.82	1.79	1.76
2.06	2.03	1.99	1.94	1.89	1.87	1.84	1.81	1.78	1.75	1.72
2.03	2.00	1.96	1.91	1.86	1.84	1.81	1.78	1.75	1.72	1.69
2.00	1.98	1.93	1.89	1.84	1.81	1.78	1.75	1.72	1.69	1.66
1.98	1.96	1.91	1.86	1.81	1.79	1.76	1.73	1.70	1.67	1.63
1.96	1.94	1.89	1.84	1.79	1.77	1.74	1.71	1.68	1.64	1.61
1.95	1.92	1.87	1.83	1.78	1.75	1.72	1.69	1.66	1.62	1.59
1.93	1.90	1.86	1.81	1.76	1.73	1.70	1.67	1.64	1.60	1.57
1.92	1.89	1.84	1.80	1.74	1.72	1.69	1.66	1.62	1.59	1.55
1.91	1.88	1.83	1.78	1.73	1.70	1.67	1.64	1.61	1.57	1.53
1.89	1.87	1.82	1.77	1.72	1.69	1.66	1.63	1.59	1.56	1.52
1.88	1.86	1.81	1.76	1.71	1.68	1.65	1.61	1.58	1.54	1.50
1.87	1.85	1.80	1.75	1.70	1.67	1.64	1.60	1.57	1.53	1.49
1.87	1.84	1.79	1.74	1.69	1.66	1.63	1.59	1.56	1.52	1.48
1.86	1.83	1.78	1.73	1.68	1.65	1.62	1.58	1.55	1.51	1.47
1.85	1.82	1.77	1.72	1.67	1.64	1.61	1.57	1.54	1.50	1.46
1.79	1.76	1.71	1.66	1.61	1.57	1.54	1.51	1.47	1.42	1.38
1.74	1.71	1.66	1.60	1.54	1.51	1.48	1.44	1.40	1.35	1.29
1.68	1.65	1.60	1.55	1.48	1.45	1.41	1.37	1.32	1.26	1.19
1.63	1.60	1.55	1.49	1.42	1.38	1.34	1.30	1.24	1.17	1.00

(Appendix D continues on next page)

Appendix D (Continued)

PERCENTILES OF THE F DISTRIBUTION

$$F_{.95}(n_1,n_2)$$

n_1 = degrees of freedom for numerator

n_2 = degrees of freedom for denominator

n_2 \ n_1	1	2	3	4	5	6	7	8
1	161.4	199.5	215.7	224.6	230.2	234.0	236.8	238.9
2	18.51	19.00	19.16	19.25	19.30	19.33	19.35	19.37
3	10.13	9.55	9.28	9.12	9.01	8.94	8.89	8.85
4	7.71	6.94	6.59	6.39	6.26	6.16	6.09	6.04
5	6.61	5.79	5.41	5.19	5.05	4.95	4.88	4.82
6	5.99	5.14	4.76	4.53	4.39	4.28	4.21	4.15
7	5.59	4.74	4.35	4.12	3.97	3.87	3.79	3.73
8	5.32	4.46	4.07	3.84	3.69	3.58	3.50	3.44
9	5.12	4.26	3.86	3.63	3.48	3.37	3.29	3.23
10	4.96	4.10	3.71	3.48	3.33	3.22	3.14	3.07
11	4.84	3.98	3.59	3.36	3.20	3.09	3.01	2.95
12	4.75	3.89	3.49	3.26	3.11	3.00	2.91	2.85
13	4.67	3.81	3.41	3.18	3.03	2.92	2.83	2.77
14	4.60	3.74	3.34	3.11	2.96	2.85	2.76	2.70
15	4.54	3.68	3.29	3.06	2.90	2.79	2.71	2.64
16	4.49	3.63	3.24	3.01	2.85	2.74	2.66	2.59
17	4.45	3.59	3.20	2.96	2.81	2.70	2.61	2.55
18	4.41	3.55	3.16	2.93	2.77	2.66	2.58	2.51
19	4.38	3.52	3.13	2.90	2.74	2.63	2.54	2.48
20	4.35	3.49	3.10	2.87	2.71	2.60	2.51	2.45
21	4.32	3.47	3.07	2.84	2.68	2.57	2.49	2.42
22	4.30	3.44	3.05	2.82	2.66	2.55	2.46	2.40
23	4.28	3.42	3.03	2.80	2.64	2.53	2.44	2.37
24	4.26	3.40	3.01	2.78	2.62	2.51	2.42	2.36
25	4.24	3.39	2.99	2.76	2.60	2.49	2.40	2.34
26	4.23	3.37	2.98	2.74	2.59	2.47	2.39	2.32
27	4.21	3.35	2.96	2.73	2.57	2.46	2.37	2.31
28	4.20	3.34	2.95	2.71	2.56	2.45	2.36	2.29
29	4.18	3.33	2.93	2.70	2.55	2.43	2.35	2.28
30	4.17	3.32	2.92	2.69	2.53	2.42	2.33	2.27
40	4.08	3.23	2.84	2.61	2.45	2.34	2.25	2.18
60	4.00	3.15	2.76	2.53	2.37	2.25	2.17	2.10
120	3.92	3.07	2.68	2.45	2.29	2.17	2.09	2.02
∞	3.84	3.00	2.60	2.37	2.21	2.10	2.01	1.94

9	10	12	15	20	24	30	40	60	120	∞
240.5	241.9	243.9	245.9	248.0	249.1	250.1	251.1	252.2	253.3	254.3
19.38	19.40	19.41	19.43	19.45	19.45	19.46	19.47	19.48	19.49	19.50
8.81	8.79	8.74	8.70	8.66	8.64	8.62	8.59	8.57	8.55	8.53
6.00	5.96	5.91	5.86	5.80	5.77	5.75	5.72	5.69	5.66	5.63
4.77	4.74	4.68	4.62	4.56	4.53	4.50	4.46	4.43	4.40	4.36
4.10	4.06	4.00	3.94	3.87	3.84	3.81	3.77	3.74	3.70	3.67
3.68	3.64	3.57	3.51	3.44	3.41	3.38	3.34	3.30	3.27	3.23
3.39	3.35	3.28	3.22	3.15	3.12	3.08	3.04	3.01	2.97	2.93
3.18	3.14	3.07	3.01	2.94	2.90	2.86	2.83	2.79	2.75	2.71
3.02	2.98	2.91	2.85	2.77	2.74	2.70	2.66	2.62	2.58	2.54
2.90	2.85	2.79	2.72	2.65	2.61	2.57	2.53	2.49	2.45	2.40
2.80	2.75	2.69	2.62	2.54	2.51	2.47	2.43	2.38	2.34	2.30
2.71	2.67	2.60	2.53	2.46	2.42	2.38	2.34	2.30	2.25	2.21
2.65	2.60	2.53	2.46	2.39	2.35	2.31	2.27	2.22	2.18	2.13
2.59	2.54	2.48	2.40	2.33	2.29	2.25	2.20	2.16	2.11	2.07
2.54	2.49	2.42	2.35	2.28	2.24	2.19	2.15	2.11	2.06	2.01
2.49	2.45	2.38	2.31	2.23	2.19	2.15	2.10	2.06	2.01	1.96
2.46	2.41	2.34	2.27	2.19	2.15	2.11	2.06	2.02	1.97	1.92
2.42	2.38	2.31	2.23	2.16	2.11	2.07	2.03	1.98	1.93	1.88
2.39	2.35	2.28	2.20	2.12	2.08	2.04	1.99	1.95	1.90	1.84
2.37	2.32	2.25	2.18	2.10	2.05	2.01	1.96	1.92	1.87	1.81
2.34	2.30	2.23	2.15	2.07	2.03	1.98	1.94	1.89	1.84	1.78
2.32	2.27	2.20	2.13	2.05	2.01	1.96	1.91	1.86	1.81	1.76
2.30	2.25	2.18	2.11	2.03	1.98	1.94	1.89	1.84	1.79	1.73
2.28	2.24	2.16	2.09	2.01	1.96	1.92	1.87	1.82	1.77	1.71
2.27	2.22	2.15	2.07	1.99	1.95	1.90	1.85	1.80	1.75	1.69
2.25	2.20	2.13	2.06	1.97	1.93	1.88	1.84	1.79	1.73	1.67
2.24	2.19	2.12	2.04	1.96	1.91	1.87	1.82	1.77	1.71	1.65
2.22	2.18	2.10	2.03	1.94	1.90	1.85	1.81	1.75	1.70	1.64
2.21	2.16	2.09	2.01	1.93	1.89	1.84	1.79	1.74	1.68	1.62
2.12	2.08	2.00	1.92	1.84	1.79	1.74	1.69	1.64	1.58	1.51
2.04	1.99	1.92	1.84	1.75	1.70	1.65	1.59	1.53	1.47	1.39
1.96	1.91	1.83	1.75	1.66	1.61	1.55	1.50	1.43	1.35	1.25
1.88	1.83	1.75	1.67	1.57	1.52	1.46	1.39	1.32	1.22	1.00

(Appendix D continues on next page)

Appendix D (Continued)

PERCENTILES OF THE F DISTRIBUTION

$$F_{.975}(n_1, n_2)$$

n_1 = degrees of freedom for numerator

n_2 = degrees of freedom for denominator

n_2 \ n_1	1	2	3	4	5	6	7	8	9
1	647.8	799.5	864.2	899.6	921.8	937.1	948.2	956.7	963.3
2	38.51	39.00	39.17	39.25	39.30	39.33	39.36	39.37	39.39
3	17.44	16.04	15.44	15.10	14.88	14.73	14.62	14.54	14.47
4	12.22	10.65	9.98	9.60	9.36	9.20	9.07	8.98	8.90
5	10.01	8.43	7.76	7.39	7.15	6.98	6.85	6.76	6.68
6	8.81	7.26	6.60	6.23	5.99	5.82	5.70	5.60	5.52
7	8.07	6.54	5.89	5.52	5.29	5.12	4.99	4.90	4.82
8	7.57	6.06	5.42	5.05	4.82	4.65	4.53	4.43	4.36
9	7.21	5.71	5.08	4.72	4.48	4.32	4.20	4.10	4.03
10	6.94	5.46	4.83	4.47	4.24	4.07	3.95	3.85	3.78
11	6.72	5.26	4.63	4.28	4.04	3.88	3.76	3.66	3.59
12	6.55	5.10	4.47	4.12	3.89	3.73	3.61	3.51	3.44
13	6.41	4.97	4.35	4.00	3.77	3.60	3.48	3.39	3.31
14	6.30	4.86	4.24	3.89	3.66	3.50	3.38	3.29	3.21
15	6.20	4.77	4.15	3.80	3.58	3.41	3.29	3.20	3.12
16	6.12	4.69	4.08	3.73	3.50	3.34	3.22	3.12	3.05
17	6.04	4.62	4.01	3.66	3.44	3.28	3.16	3.06	2.98
18	5.98	4.56	3.95	3.61	3.38	3.22	3.10	3.01	2.93
19	5.92	4.51	3.90	3.56	3.33	3.17	3.05	2.96	2.88
20	5.87	4.46	3.86	3.51	3.29	3.13	3.01	2.91	2.84
21	5.83	4.42	3.82	3.48	3.25	3.09	2.97	2.87	2.80
22	5.79	4.38	3.78	3.44	3.22	3.05	2.93	2.84	2.76
23	5.75	4.35	3.75	3.41	3.18	3.02	2.90	2.81	2.73
24	5.72	4.32	3.72	3.38	3.15	2.99	2.87	2.78	2.70
25	5.69	4.29	3.69	3.35	3.13	2.97	2.85	2.75	2.68
26	5.66	4.27	3.67	3.33	3.10	2.94	2.82	2.73	2.65
27	5.63	4.24	3.65	3.31	3.08	2.92	2.80	2.71	2.63
28	5.61	4.22	3.63	3.29	3.06	2.90	2.78	2.69	2.61
29	5.59	4.20	3.61	3.27	3.04	2.88	2.76	2.67	2.59
30	5.57	4.18	3.59	3.25	3.03	2.87	2.75	2.65	2.57
40	5.42	4.05	3.46	3.13	2.90	2.74	2.62	2.53	2.45
60	5.29	3.93	3.34	3.01	2.79	2.63	2.51	2.41	2.33
120	5.15	3.80	3.23	2.89	2.67	2.52	2.39	2.30	2.22
∞	5.02	3.69	3.12	2.79	2.57	2.41	2.29	2.19	2.11

10	12	15	20	24	30	40	60	120	∞
968.6	976.7	984.9	993.1	997.2	1001	1006	1010	1014	1018
39.40	39.41	39.43	39.45	39.46	39.46	39.47	39.48	39.49	39.50
14.42	14.34	14.25	14.17	14.12	14.08	14.04	13.99	13.95	13.90
8.84	8.75	8.66	8.56	8.51	8.46	8.41	8.36	8.31	8.26
6.62	6.52	6.43	6.33	6.28	6.23	6.18	6.12	6.07	6.02
5.46	5.37	5.27	5.17	5.12	5.07	5.01	4.96	4.90	4.85
4.76	4.67	4.57	4.47	4.42	4.36	4.31	4.25	4.20	4.14
4.30	4.20	4.10	4.00	3.95	3.89	3.84	3.78	3.73	3.67
3.96	3.87	3.77	3.67	3.61	3.56	3.51	3.45	3.39	3.33
3.72	3.62	3.52	3.42	3.37	3.31	3.26	3.20	3.14	3.08
3.53	3.43	3.33	3.23	3.17	3.12	3.06	3.00	2.94	2.88
3.37	3.28	3.18	3.07	3.02	2.96	2.91	2.85	2.79	2.72
3.25	3.15	3.05	2.95	2.89	2.84	2.78	2.72	2.66	2.60
3.15	3.05	2.95	2.84	2.79	2.73	2.67	2.61	2.55	2.49
3.06	2.96	2.86	2.76	2.70	2.64	2.59	2.52	2.46	2.40
2.99	2.89	2.79	2.68	2.63	2.57	2.51	2.45	2.38	2.32
2.92	2.82	2.72	2.62	2.56	2.50	2.44	2.38	2.32	2.25
2.87	2.77	2.67	2.56	2.50	2.44	2.38	2.32	2.26	2.19
2.82	2.72	2.62	2.51	2.45	2.39	2 33	2.27	2.20	2.13
2.77	2.68	2.57	2.46	2.41	2.35	2.29	2.22	2.16	2.09
2.73	2.64	2.53	2.42	2.37	2.31	2.25	2.18	2.11	2.04
2.70	2.60	2.50	2.39	2.33	2.27	2.21	2.14	2.08	2.00
2.67	2.57	2.47	2.36	2.30	2.24	2.18	2.11	2.04	1.97
2.64	2.54	2.44	2.33	2.27	2.21	2.15	2.08	2.01	1.94
2.61	2.51	2.41	2.30	2.24	2.18	2.12	2.05	1.98	1.91
2.59	2.49	2.39	2.28	2.22	2.16	2.09	2.03	1.95	1.88
2.57	2.47	2.36	2.25	2.19	2.13	2.07	2.00	1.93	1.85
2.55	2.45	2.34	2.23	2.17	2.11	2.05	1.98	1.91	1.83
2.53	2.43	2.32	2.21	2.15	2.09	2.03	1.96	1.89	1.81
2.51	2.41	2.31	2.20	2.14	2.07	2.01	1.94	1.87	1.79
2.39	2.29	2.18	2.07	2.01	1.94	1.88	1.80	1.72	1.64
2.27	2.17	2.06	1.94	1.88	1.82	1.74	1.67	1.58	1.48
2.16	2.05	1.94	1.82	1.76	1.69	1.61	1.53	1.43	1.31
2.05	1.94	1.83	1.71	1.64	1.57	1.48	1.39	1.27	1.00

(Appendix D continues on next page)

Appendix D (Continued)

PERCENTILES OF THE F DISTRIBUTION

$F_{.99}(n_1,n_2)$

n_1 = degrees of freedom for numerator

n_2 = degrees of freedom for denominator

n_2 \ n_1	1	2	3	4	5	6	7	8	9
1	4052	4999.5	5403	5625	5764	5859	5928	5982	6022
2	98.50	99.00	99.17	99.25	99.30	99.33	99.36	99.37	99.39
3	34.12	30.82	29.46	28.71	28.24	27.91	27.67	27.49	27.35
4	21.20	18.00	16.69	15.98	15.52	15.21	14.98	14.80	14.66
5	16.26	13.27	12.06	11.39	10.97	10.67	10.46	10.29	10.16
6	13.75	10.92	9.78	9.15	8.75	8.47	8.26	8.10	7.98
7	12.25	9.55	8.45	7.85	7.46	7.19	6.99	6.84	6.72
8	11.26	8.65	7.59	7.01	6.63	6.37	6.18	6.03	5.91
9	10.56	8.02	6.99	6.42	6.06	5.80	5.61	5.47	5.35
10	10.04	7.56	6.55	5.99	5.64	5.39	5.20	5.06	4.94
11	9.65	7.21	6.22	5.67	5.32	5.07	4.89	4.74	4.63
12	9.33	6.93	5.95	5.41	5.06	4.82	4.64	4.50	4.39
13	9.07	6.70	5.74	5.21	4.86	4.62	4.44	4.30	4.19
14	8.86	6.51	5.56	5.04	4.69	4.46	4.28	4.14	4.03
15	8.68	6.36	5.42	4.89	4.56	4.32	4.14	4.00	3.89
16	8.53	6.23	5.29	4.77	4.44	4.20	4.03	3.89	3.78
17	8.40	6.11	5.18	4.67	4.34	4.10	3.93	3.79	3.68
18	8.29	6.01	5.09	4.58	4.25	4.01	3.84	3.71	3.60
19	8.18	5.93	5.01	4.50	4.17	3.94	3.77	3.63	3.52
20	8.10	5.85	4.94	4.43	4.10	3.87	3.70	3.56	3.46
21	8.02	5.78	4.87	4.37	4.04	3.81	3.64	3.51	3.40
22	7.95	5.72	4.82	4.31	3.99	3.76	3.59	3.45	3.35
23	7.88	5.66	4.76	4.26	3.94	3.71	3.54	3.41	3.30
24	7.82	5.61	4.72	4.22	3.90	3.67	3.50	3.36	3.26
25	7.77	5.57	4.68	4.18	3.85	3.63	3.46	3.32	3.22
26	7.72	5.53	4.64	4.14	3.82	3.59	3.42	3.29	3.18
27	7.68	5.49	4.60	4.11	3.78	3.56	3.39	3.26	3.15
28	7.64	5.45	4.57	4.07	3.75	3.53	3.36	3.23	3.12
29	7.60	5.42	4.54	4.04	3.73	3.50	3.33	3.20	3.09
30	7.56	5.39	4.51	4.02	3.70	3.47	3.30	3.17	3.07
40	7.31	5.18	4.31	3.83	3.51	3.29	3.12	2.99	2.89
60	7.08	4.98	4.13	3.65	3.34	3.12	2.95	2.82	2.72
120	6.85	4.79	3.95	3.48	3.17	2.96	2.79	2.66	2.56
∞	6.63	4.61	3.78	3.32	3.02	2.80	2.64	2.51	2.41

10	12	15	20	24	30	40	60	120	∞
6056	6106	6157	6209	6235	6261	6287	6313	6339	6366
99.40	99.42	99.43	99.45	99.46	99.47	99.47	99.48	99.49	99.50
27.23	27.05	26.87	26.69	26.60	26.50	26.41	26.32	26.22	26.13
14.55	14.37	14.20	14.02	13.93	13.84	13.75	13.65	13.56	13.46
10.05	9.89	9.72	9.55	9.47	9.38	9.29	9.20	9.11	9.02
7.87	7.72	7.56	7.40	7.31	7.23	7.14	7.06	6.97	6.88
6.62	6.47	6.31	6.16	6.07	5.99	5.91	5.82	5.74	5.65
5.81	5.67	5.52	5.36	5.28	5.20	5.12	5.03	4.95	4.86
5.26	5.11	4.96	4.81	4.73	4.65	4.57	4.48	4.40	4.31
4.85	4.71	4.56	4.41	4.33	4.25	4.17	4.08	4.00	3.91
4.54	4.40	4.25	4.10	4.02	3.94	3.86	3.78	3.69	3.60
4.30	4.16	4.01	3.86	3.78	3.70	3.62	3.54	3.45	3.36
4.10	3.96	3.82	3.66	3.59	3.51	3.43	3.34	3.25	3.17
3.94	3.80	3.66	3.51	3.43	3.35	3.27	3.18	3.09	3.00
3.80	3.67	3.52	3.37	3.29	3.21	3.13	3.05	2.96	2.87
3.69	3.55	3.41	3.26	3.18	3.10	3.02	2.93	2.84	2.75
3.59	3.46	3.31	3.16	3.08	3.00	2.92	2.83	2.75	2.65
3.51	3.37	3.23	3.08	3.00	2.92	2.84	2.75	2.66	2.57
3.43	3.30	3.15	3.00	2.92	2.84	2.76	2.67	2.58	2.49
3.37	3.23	3.09	2.94	2.86	2.78	2.69	2.61	2.52	2.42
3.31	3.17	3.03	2.88	2.80	2.72	2.64	2.55	2.46	2.36
3.26	3.12	2.98	2.83	2.75	2.67	2.58	2.50	2.40	2.31
3.21	3.07	2.93	2.78	2.70	2.62	2.54	2.45	2.35	2.26
3.17	3.03	2.89	2.74	2.66	2.58	2.49	2.40	2.31	2.21
3.13	2.99	2.85	2.70	2.62	2.54	2.45	2.36	2.27	2.17
3.09	2.96	2.81	2.66	2.58	2.50	2.42	2.33	2.23	2.13
3.06	2.93	2.78	2.63	2.55	2.47	2.38	2.29	2.20	2.10
3.03	2.90	2.75	2.60	2.52	2.44	2.35	2.26	2.17	2.06
3.00	2.87	2.73	2.57	2.49	2.41	2.33	2.23	2.14	2.03
2.98	2.84	2.70	2.55	2.47	2.39	2.30	2.21	2.11	2.01
2.80	2.66	2.52	2.37	2.29	2.20	2.11	2.02	1.92	1.80
2.63	2.50	2.35	2.20	2.12	2.03	1.94	1.84	1.73	1.60
2.47	2.34	2.19	2.03	1.95	1.86	1.76	1.66	1.53	1.38
2.32	2.18	2.04	1.88	1.79	1.70	1.59	1.47	1.32	1.00

Appendix E

TABLE OF CRITICAL VALUES FOR T (ONE-SIDED TEST) WHEN STANDARD DEVIATION IS CALCULATED FROM THE SAME SAMPLE

Number of Observations n	5% Significance Level	2.5% Significance Level	1% Significance Level
3	1.15	1.15	1.15
4	1.46	1.48	1.49
5	1.67	1.71	1.75
6	1.82	1.89	1.94
7	1.94	2.02	2.10
8	2.03	2.13	2.22
9	2.11	2.21	2.32
10	2.18	2.29	2.41
11	2.23	2.36	2.48
12	2.29	2.41	2.55
13	2.33	2.46	2.61
14	2.37	2.51	2.66
15	2.41	2.55	2.71
16	2.44	2.59	2.75
17	2.47	2.62	2.79
18	2.50	2.65	2.82
19	2.53	2.68	2.85
20	2.56	2.71	2.88
21	2.58	2.73	2.91
22	2.60	2.76	2.94
23	2.62	2.78	2.96
24	2.64	2.80	2.99
25	2.66	2.82	3.01
30	2.75	2.91	
35	2.82	2.98	
40	2.87	3.04	
45	2.92	3.09	
50	2.96	3.13	
60	3.03	3.20	
70	3.09	3.26	
80	3.14	3.31	
90	3.18	3.35	
100	3.21	3.38	

$$T_n = \frac{x_n - \bar{x}}{s} \qquad s = \left\{\frac{\Sigma(x_i - \bar{x})^2}{n-1}\right\}^{1/2} = \left\{\frac{n\Sigma x_i^2 - (\Sigma x_i)^2}{n(n-1)}\right\}^{1/2}$$

$$T_1 = \frac{\bar{x} - x_1}{s} \qquad x_1 \leq x_2 \leq \ldots \leq x_n$$

From Frank E. Grubbs, Procedures for Detecting Outlying Observations in Samples, *Technometrics*, 2(1): 4 (1969).

Appendix F

TABLE OF COEFFICIENTS $\{a_{n-i+1}\}$ USED IN W TEST FOR NORMALITY, FOR $n = 3(1)50$

i \ n	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	0.7071	0.6872	0.6646	0.6431	0.6233	0.6052	0.5888	0.5739	0.5601	0.5475	0.5359	0.5251	0.5150	0.5056	0.4968	0.4886
2		0.1677	0.2413	0.2806	0.3031	0.3164	0.3244	0.3291	0.3315	0.3325	0.3325	0.3318	0.3306	0.3290	0.3273	0.3253
3				0.0875	0.1401	0.1743	0.1976	0.2141	0.2260	0.2347	0.2412	0.2460	0.2495	0.2521	0.2540	0.2553
4						0.0561	0.0947	0.1224	0.1429	0.1586	0.1707	0.1802	0.1878	0.1939	0.1988	0.2027
5								0.0399	0.0695	0.0922	0.1099	0.1240	0.1353	0.1447	0.1524	0.1587
6										0.0303	0.0539	0.0727	0.0880	0.1005	0.1109	0.1197
7												0.0240	0.0433	0.0593	0.0725	0.0837
8														0.0196	0.0359	0.0496
9																0.0163

i \ n	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
1	0.4808	0.4734	0.4643	0.4590	0.4542	0.4493	0.4450	0.4407	0.4366	0.4328	0.4291	0.4254	0.4220	0.4188	0.4156	0.4127
2	0.3232	0.3211	0.3185	0.3156	0.3126	0.3098	0.3069	0.3043	0.3018	0.2992	0.2968	0.2944	0.2921	0.2898	0.2876	0.2854
3	0.2561	0.2565	0.2578	0.2571	0.2563	0.2554	0.2543	0.2533	0.2522	0.2510	0.2499	0.2487	0.2475	0.2463	0.2451	0.2439
4	0.2059	0.2085	0.2119	0.2131	0.2139	0.2145	0.2148	0.2151	0.2152	0.2151	0.2150	0.2148	0.2145	0.2141	0.2137	0.2132
5	0.1641	0.1686	0.1736	0.1764	0.1787	0.1807	0.1822	0.1836	0.1848	0.1857	0.1864	0.1870	0.1874	0.1878	0.1880	0.1882
6	0.1271	0.1334	0.1399	0.1443	0.1480	0.1512	0.1539	0.1563	0.1584	0.1601	0.1616	0.1630	0.1641	0.1651	0.1660	0.1667
7	0.0932	0.1013	0.1092	0.1150	0.1201	0.1245	0.1283	0.1316	0.1346	0.1372	0.1395	0.1415	0.1433	0.1449	0.1463	0.1475
8	0.0612	0.0711	0.0804	0.0878	0.0941	0.0997	0.1046	0.1089	0.1128	0.1162	0.1192	0.1219	0.1243	0.1265	0.1284	0.1301
9	0.0303	0.0422	0.0530	0.0618	0.0696	0.0764	0.0823	0.0876	0.0923	0.0965	0.1002	0.1036	0.1066	0.1093	0.1118	0.1140
10		0.0140	0.0263	0.0368	0.0459	0.0539	0.0610	0.0672	0.0728	0.0778	0.0822	0.0862	0.0899	0.0931	0.0961	0.0988
11				0.0122	0.0228	0.0321	0.0403	0.0476	0.0540	0.0598	0.0650	0.0697	0.0739	0.0777	0.0812	0.0844
12						0.0107	0.0200	0.0284	0.0358	0.0424	0.0483	0.0537	0.0585	0.0629	0.0669	0.0706
13								0.0094	0.0178	0.0253	0.0320	0.0381	0.0435	0.0485	0.0530	0.0572
14										0.0084	0.0159	0.0227	0.0289	0.0344	0.0395	0.0441
15												0.0076	0.0144	0.0206	0.0262	0.0314
16														0.0068	0.0131	0.0187
17																0.0062

i \ n	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50
1	0 4096	0 4068	0 4040	0 4015	0 3989	0 3964	0 3940	0 3917	0 3894	0 3872	0 3850	0 3830	0 3808	0 3789	0 3770	0 3751
2	0 2834	0 2813	0 2794	0 2774	0 2755	0 2737	0 2719	0 2701	0 2684	0 2667	0 2651	0 2635	0 2620	0 2604	0 2589	0 2574
3	0 2427	0 2415	0 2403	0 2391	0 2380	0 2368	0 2357	0 2345	0 2334	0 2323	0 2313	0 2302	0 2291	0 2281	0 2271	0 2260
4	0 2127	0 2121	0 2116	0 2110	0 2104	0 2098	0 2091	0 2085	0 2078	0 2072	0 2065	0 2058	0 2052	0 2045	0 2038	0 2032
5	0 1883	0 1883	0 1883	0 1881	0 1880	0 1878	0 1876	0 1874	0 1871	0 1868	0 1865	0 1862	0 1859	0 1855	0 1851	0 1847
6	0 1673	0 1678	0 1683	0 1686	0 1689	0 1691	0 1693	0 1694	0 1695	0 1695	0 1695	0 1695	0 1695	0 1693	0 1692	0 1691
7	0 1487	0 1496	0 1505	0 1513	0 1520	0 1526	0 1531	0 1535	0 1539	0 1542	0 1545	0 1548	0 1550	0 1551	0 1553	0 1554
8	0 1317	0 1331	0 1344	0 1356	0 1366	0 1376	0 1384	0 1392	0 1398	0 1405	0 1410	0 1415	0 1420	0 1423	0 1427	0 1430
9	0 1160	0 1179	0 1196	0 1211	0 1225	0 1237	0 1249	0 1259	0 1269	0 1278	0 1286	0 1293	0 1300	0 1306	0 1312	0 1317
10	0 1013	0 1036	0 1056	0 1075	0 1092	0 1108	0 1123	0 1136	0 1149	0 1160	0 1170	0 1180	0 1189	0 1197	0 1205	0 1212
11	0 0873	0 0900	0 0924	0 0947	0 0967	0 0986	0 1004	0 1020	0 1035	0 1049	0 1062	0 1073	0 1085	0 1095	0 1105	0 1113
12	0 0739	0 0770	0 0798	0 0824	0 0848	0 0870	0 0891	0 0909	0 0927	0 0943	0 0959	0 0972	0 0986	0 0998	0 1010	0 1020
13	0 0610	0 0645	0 0677	0 0706	0 0733	0 0759	0 0782	0 0804	0 0824	0 0842	0 0860	0 0876	0 0892	0 0906	0 0919	0 0932
14	0 0484	0 0523	0 0559	0 0592	0 0622	0 0651	0 0677	0 0701	0 0724	0 0745	0 0765	0 0783	0 0801	0 0817	0 0832	0 0846
15	0 0361	0 0404	0 0444	0 0481	0 0515	0 0546	0 0575	0 0602	0 0628	0 0651	0 0673	0 0694	0 0713	0 0731	0 0748	0 0764
16	0 0239	0 0287	0 0331	0 0372	0 0409	0 0444	0 0476	0 0506	0 0534	0 0560	0 0584	0 0607	0 0628	0 0648	0 0667	0 0685
17	0 0119	0 0172	0 0220	0 0264	0 0305	0 0343	0 0379	0 0411	0 0442	0 0471	0 0497	0 0522	0 0546	0 0568	0 0588	0 0608
18		0 0057	0 0110	0 0158	0 0203	0 0244	0 0283	0 0318	0 0352	0 0383	0 0412	0 0439	0 0465	0 0489	0 0511	0 0532
19				0 0053	0 0101	0 0146	0 0188	0 0227	0 0263	0 0296	0 0328	0 0357	0 0385	0 0411	0 0436	0 0459
20						0 0049	0 0094	0 0136	0 0175	0 0211	0 0245	0 0277	0 0307	0 0335	0 0361	0 0386
21								0 0045	0 0087	0 0126	0 0163	0 0197	0 0229	0 0259	0 0288	0 0314
22										0 0042	0 0081	0 0118	0 0153	0 0185	0 0215	0 0244
23												0 0039	0 0076	0 0111	0 0143	0 0174
24														0 0037	0 0071	0 0104
25																0 0035

From Gerald J. Hahn and S. S. Shapiro, *Statistical Models in Engineering,* John Wiley & Sons, Inc , New York, 1967.

Appendix G
PERCENTAGE POINTS OF W TEST FOR NORMALITY FOR $n = 3(1)50$

n	1	2	5	10	50
3	0.753	0.756	0.767	0.789	0.959
4	0.687	0.707	0.748	0.792	0.935
5	0.686	0.715	0.762	0.806	0.927
6	0.713	0.743	0.788	0.826	0.927
7	0.730	0.760	0.803	0.838	0.928
8	0.749	0.778	0.818	0.851	0.932
9	0.764	0.791	0.829	0.859	0.935
10	0.781	0.806	0.842	0.869	0.938
11	0.792	0.817	0.850	0.876	0.940
12	0.805	0.828	0.859	0.883	0.943
13	0.814	0.837	0.866	0.889	0.945
14	0.825	0.846	0.874	0.895	0.947
15	0.835	0.855	0.881	0.901	0.950
16	0.844	0.863	0.887	0.906	0.952
17	0.851	0.869	0.892	0.910	0.954
18	0.858	0.874	0.897	0.914	0.956
19	0.863	0.879	0.901	0.917	0.957
20	0.868	0.884	0.905	0.920	0.959
21	0.873	0.888	0.908	0.923	0.960
22	0.878	0.892	0.911	0.926	0.961
23	0.881	0.895	0.914	0.928	0.962
24	0.884	0.898	0.916	0.930	0.963
25	0.888	0.901	0.918	0.931	0.964
26	0.891	0.904	0.920	0.933	0.965
27	0.894	0.906	0.923	0.935	0.965
28	0.896	0.908	0.924	0.936	0.966
29	0.898	0.910	0.926	0.937	0.966
30	0.900	0.912	0.927	0.939	0.967
31	0.902	0.914	0.929	0.940	0.967
32	0.904	0.915	0.930	0.941	0.968
33	0.906	0.917	0.931	0.942	0.968
34	0.908	0.919	0.933	0.943	0.969
35	0.910	0.920	0.934	0.944	0.969
36	0.912	0.922	0.935	0.945	0.970
37	0.914	0.924	0.936	0.946	0.970
38	0.916	0.925	0.938	0.947	0.971
39	0.917	0.927	0.939	0.948	0.971
40	0.919	0.928	0.940	0.949	0.972
41	0.920	0.929	0.941	0.950	0.972
42	0.922	0.930	0.942	0.951	0.972
43	0.923	0.932	0.943	0.951	0.973
44	0.924	0.933	0.944	0.952	0.973
45	0.926	0.934	0.945	0.953	0.973
46	0.927	0.935	0.945	0.953	0.974
47	0.928	0.936	0.946	0.954	0.974
48	0.929	0.937	0.947	0.954	0.974
49	0.929	0.937	0.947	0.955	0.974
50	0.930	0.938	0.947	0.955	0.974

From Gerald J. Hahn and S. S. Shapiro, *Statistical Models in Engineering*, John Wiley & Sons, Inc., New York, 1967.

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