UNCLASSIFIED

AECU-3259

PHYSICS

I

UNITED STATES ATOMIC ENERGY COMMISSION

APPLICATIONS OF MONTE CARLO

By
Herman Kahn

April 19, 1954

RAND Corporation
Santa Monica, California

Technical Information Service Extension, Oak Ridge, Tenn.

UNCLASSIFIED

DISCLAIMER

II

Other issues of this report may bear the number RM-1237-AEC.

This report has been reproduced directly from the best available copy.

Printed in USA, Price $1.25. Available from the Office of Technical Services, Department of Commerce, Washington 25, D. C.

AEC, Oak Ridge, Tenn.

Prepared Under Contract With
The U. S. Atomic Energy Commission Contract No. AT(11-1)-135
Project Agreement No. 1
And the U. S. Air Force Project RAND

RESEARCH MEMORANDUM

APPLICATIONS OF MONTE CARLO

Herman Kahn

19 April 1954
Revised 27 April 1956

The RAND Corporation
1700 MAIN ST. • SANTA MONICA • CALIFORNIA

FOREWORD

This document discusses the general principle of doing Monte Carlo calculations with particular emphasis on reducing the amount of work involved. It does not discuss, but for a few exceptions, relationships between probabilistic problems and deterministic ones, and how either can be chosen to model the other. More importantly, it does not include any important specific applications. Both of these other subjects are widely discussed in Monte Carlo literature by many people. At a later date the author hopes to put out a book on the subject which will supersede this report and include applications.

The work that preceded this report has been supported by the U.S. Air Force and several laboratories of the A.E.C. In addition, I would like to express my appreciation to the Reactor Division of the A.E.C. for their sympathetic and long range support of basic studies in the Monte Carlo method.

A short description of the Monte Carlo method can be given as follows. The expected score of a player in any reasonable game of chance, however complicated, can in principle be estimated by averaging the results of a large number of plays of the game. Such estimation can be rendered more efficient by various devices which replace the original game with another known to have the same expected score. The new game may lead to a more efficient estimate by being less erratic, that is, having a score of lower variance or by being cheaper to play with the equipment on hand.

There are obviously many problems about probability that can be viewed as problems of calculating the expected score of a game. Still more, there are problems that do not concern probability but are none the less equivalent for some purposes to the calculation of an expected score. The Monte Carlo method refers simply to the exploitation of these remarks.

The method has been extensively used by statisticians and others under the name of Model Sampling. Many of the variance reducing techniques discussed in this report have been developed by statisticians for use in Survey Sampling.

John von Neumann and Stanley Ulam seem to be mainly responsible, both as practitioners and propagandists, for the present widespread use in physics and engineering. They also seem to have been the first to have advocated the idea of systematically inverting the usual situation and treating determinate mathematical problems by first finding a probabilistic analogue and then solving this analogue by some experimental sampling procedure. In this report though, most of the applications are to problems which have been derived from probabilistic situations. The name of Monte Carlo is used rather than Model Sampling partly because we wish to differentiate the relatively sophisticated sampling techniques used in the former from the straightforward approach that seems to be customary in the usual applications of the latter, and partly because the more picturesque name of Monte Carlo has just about replaced its predecessor in physical applications.

In writing a report of this nature it is difficult to apportion credits and acknowledgments in a reasonable manner. The author has spent about half of his time betwwen 1948 and 1952 on applications of the method. Some of the applications with which he has been concerned have been fairly large problems involving the collaboration of several organizations and many individuals. Because major emphasis has always been on physics or engineering, and not statistics, and also because most of the problems are classified, it is difficult to pinpoint many individual contributions. Therefore, except for Part I (inspired by John von Neumann) and for specific statistical suggestions, there will be almost no specific acknowledgments made. Instead, a simple listing of the individuals who have contributed to the problems upon which we learned how to do Monte Carlo will be given.

The following either originated problems or collaborated on their design: Hans Bethe, Jim Coon, Robert Day, Walter Goad, Herbert Goldstein, Frederic de Hoffmann, Frank Hoyt, Richard Latter, Louis Nelson, Lothar Nordheim, Milton Plesset, Fred Reines, Paul Stein, Edward Teller, Robert Thomas and Carl Wahlske.

I am indebted to the following for helpful discussions: George Brown, Herman Feschbach, Francis Friedman, Gerald Goertzel, Mario Juncosa, John von Neumann, Melvin Peisakoff, Leonard J. Savage, John W. Tukey and Theodore Welton.

Most of the actual work of programming, coding and computing was done by Barbara Batchelder, Barbara Cohen, Ruth Ann Engvall, Lois Foster, Esther Gersten, Irwin Greenwald, Jean Hall, Clyde Hauff,

Herbert Hilton, Robert Johnson, Winifred Jonas, David Langfield, Don Madden, Wes Melahn, Cynthia Mercer, Leona Otfinoski, Josephine Powers, Frieda Rosenberg, Cliff Shaw, and Charles Swift. Without their high morale, professional skill, and enthusiasm, it would have been impossible to have met many of our deadlines on the always capricious and sometimes malignant computing equipment available from 1948 to 1952.

Finally, an inadequate thanks to Theodore Harris and Andrew Marshall, with whom the author has collaborated extensively and on whom he has always been able to lean for a learned opinion on statistics and probability. Some of the ideas in this report have previously appeared in joint papers by them and the author.

I would also like to thank Leonard J. Savage for reading an earlier version of this report and making prolific comments. This version doesn't show the full effect of his comments as I am saving many of them for a future book.

INTRODUCTION

The Monte Carlo Method is concerned with the application of random sampling to problems of applied mathematics. While subtle or difficult questions may arise in applications, most problems can be treated without using much statistical theory. Nevertheless statistical theory can be very helpful. This report presents an elementary exposition of some of the ideas and techniques that have proved useful in problems with which the author has been concerned. In this case, the word elementary implies that the author has tried to make the presentation intelligible to a mathematician, physicist, or engineer with only a slight formal background in probability theory. There will be a strong flavor of the "cookbook" about many selections. The author can only suggest judicious skipping.

It will be assumed that the reader has in intuitive notion of the idea of probability (even though philosophers may argue). That is, that he knows what is meant by the statement "The probability that a 'fair' coin lands heads up when tossed is 1/2," and that he knows and has had some basic experience with the simplest rules of the calculus of probabilities.[1] In any case most of the statistical ideas that are used will be presented or reviewed in the first two chapters.

---

1 These rules are of the following types. The probability that one or the other of two mutually exclusive events occurs is the sum of the separate probabilities. The probability that two independent events occur is the product of their separate probabilities, etc.

AECU-3259

PART I

TECHNIQUES WITH RANDOM VARIABLES

PART I

TABLE OF CONTENTS

I. TECHNIQUES WITH RANDOM VARIABLES

1. Random Variables

In the following a random variable (generally denoted by a capital letter) will mean a numerical quantity (or quantities) associated with a game of chance in such a way that as the various events or possible outcomes of the game occur, the random variable takes on definite values. Thus one could associate a random variable C with the coin tossing process by saying that when a head comes up, C = 0, and when a tail comes up, C = 1. C then has a probability of 1/2 of being zero and 1/2 of being 1. All other values have zero probability.

Associated with any random variable X is a cumulative distribution function (c.d.f.) which will be called "F(x)". F(x) is defined as the probability that the random variable X will assume values less than or equal to x. If F(x) is the integral, at least in some regions, of a function f(x), the random variable is said to have a probability density then and f(x) is called the probability density function (p.d.f.). If F(x) makes a finite jump at some point x_0, there is a non-zero probability of x_0 occurring. Thus in the coin tossing problem mentioned above

$$\begin{aligned} F(C) &= 0 & C &< 0 \\ &= 1/2 & 0 &\leq C < 1 \\ &= 1 & 1 &\leq C < \infty \end{aligned}$$

If $f(x)$ exists everywhere, $F(x)$ must be continous, and the random variable has a zero probability of taking on any particular value.[1] It is then customary to speak of the probability that the random variable lies in the interval between x and $x + \Delta x$. This probability is $F(x + \Delta x) - F(x)$, for positive Δx, or approximately $f(x)\Delta x$ if Δx is small. A common but elliptical statement, "the probability that X takes on the value x is $f(x)$ [or $f(x)\Delta x$]," is to be interpreted in the above sense. In the case of a finite interval (a,b) the probability that $a < X \leq b$ is $F(b) - F(a)$ or $\int_a^b f(x)dx$ if $f(x)$ exists. In the future the qualification "if $f(x)$ exists" will not be used but should always be understood.

It is sometimes necessary to associate two or more random variables with the same process. One then has a joint c.d.f., $F(x,y)$, which is defined to be the probability that the event $(X \leq x, Y \leq y)$ occurs. The function $f(x,y)$ defined by

$$f(x,y) = \frac{\partial^2 F}{\partial x \partial y} = \frac{\partial^2 F}{\partial y \partial x}$$

is called the joint p.d.f. for x and y. $f(x,y)\Delta x\Delta y$ is approximately the probability that the event $(x \leq X \leq x + \Delta x,\ y \leq Y \leq y + \Delta y)$ occurs. Some other important definitions and concepts are

$$F(x) = F(x, \infty)$$

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

$$= \frac{\partial F(x,\infty)}{\partial x}$$

---

1 It is still possible to use p.d.f.'s when $F(x)$ is discontinuous by using the formalism of the Dirac delta function. This will occasionally be done when it simplifies the appearance of formulae.

= p.d.f. of x (called marginal p.d.f. of x in this context.)

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

$$= \frac{\partial F(\infty,y)}{\partial y}$$

= marginal p.d.f. of y

$$f(x:y) = f(x,y)/g(y)$$

= p.d.f. for X given that Y has the value y (sometimes called the conditional p.d.f. of x)

$$g(y:x) = f(x,y)/f(x)$$

= p.d.f. for Y given that X has the value x

The same for F(x:y), G(y:x), and the extensions to more than two variables.

The p.d.f. of a random variable restricted to a portion of its full domain is sometimes used, for example the p.d.f. of X for $a < x$ is just $\frac{f(x)}{1-F(a)}$; i.e., proportional to the old density in the region $a < x$ but renormalized, and zero elsewhere.

If F(x,y) happens to be equal to F(x)G(y), the random variables are said to be independent of each other. If this is not true, the random variables are said to be dependent. Three random variables are called independent if F(x,y,z) = F(x)G(y)H(z); it is not enough that the variables be independent in pairs.

A random variable has associated with it a so-called <u>expected value</u>. This notion is central to our considerations and we will discuss it more in what follows. If f(x) is the p.d.f. of X, the expected value of X is defined as

$$\bar{X} = \int_{-\infty}^{\infty} x\, f(x)dx$$

The reader will readily notice that this is a generalization of the ordinary arithmetical average or mean. Monte Carlo is concerned almost exclusively with the calculation of such averages.

2. Transformations of Random Variables and Their Realization

Consider two random variables X and Y and the monotonic increasing transformation $Y = T(X)$. If X has the known c.d.f. $F(x)$, it is a simple matter to calculate $G(y)$, the c.d.f. for y. Since Y is less than or equal to y if and only if X is less than or equal to $T^{-1}(y)$ the probability of these two events occurring must be the same. Therefore if x and y are corresponding values,

$$F(x) = G(y)$$

But

$$x = T^{-1}(y)$$

so

$$G(y) = F\left[T^{-1}(y)\right] \tag{1}$$

A crucial step in the Monte Carlo method is the realization of a given distribution function $F(x)$. By that is meant the construction of an actual game of chance with which is associated a sequence of independent random variables $X_1, X_2, \ldots, X_n$, each with the c.d.f. $F(x)$. It is the empirical values $x_1, x_2, \ldots, x_n$, in a single actual play of the game that constitute the statistical data for a Monte Carlo calculation.

The construction of some of the necessary games of chance is discussed in the sections which follow. The point to be made here is that some distributions can be realized more easily than others so that it is important to study the process of constructing a realization of $G(y)$, given a realization of $F(x)$. How important may be judged from the fact that if $F(x)$ is continuous, then for any $G(y)$ there is a T such that (1) holds.

The most obvious, and often the best, way to realize G(y) on the basis of a realization of F(x) is simply to take for the sequence y_i,

$$y_i = T(x_i) \tag{2}$$

In actual computations on high speed machines it may, however, be quite difficult to evaluate $T(x_i)$. It may then be convenient to use instead an approximate transformation $\bar{T}(x_i)$ or one of the other techniques to be discussed.

Before equation (2) can be used to realize G(y) it is necessary first to generate independent values distributed according to F(x). For this purpose it is often convenient to use as a basic distribution the uniform distribution between 0 and 1; i.e., with

$$\begin{aligned} f(x) &= 0 \quad \text{or} \quad F(x) = 0 && x \leq 0 \\ &= 1 && = x && 0 \leq x \leq 1 \\ &= 0 && = 1 && 1 \leq x \end{aligned}$$

A discussion of various techniques for producing independent values with this distribution is found in Appendix I. These values are referred to as random numbers (sometimes reasonable facsimiles called pseudo random numbers are used instead), and denoted by R_i.[1] By using equation (2) which now takes the equivalent forms

$$\begin{aligned} G(y_i) &= R_i \\ y_i &= G^{-1}(R_i) = T(R_i) \\ \int_{-\infty}^{y_i} g(y)dy &= R_i \end{aligned} \tag{3}$$

---

1 Because of previous commitments, these independent random variables and the independent variable of their p.d.f. will both be denoted by a capital letter. It is hoped that this will not cause confusion.

it is possible to generate a set of independent random variables $Y_1, \ldots Y_n$ with an arbitrary c.d.f. G(y).

Sometimes it is necessary to represent a multidimensional p.d.f. For instance, equation (3) can be generalized to handle three variables as follows:

From f(x,y,z) the p.d.f.'s f(x), g(y:x), and h(z:x,y) are obtained. A random (x,y,z) can be determined by first picking three random numbers and then solving the following equations consecutively:

$$\begin{aligned} \int_{-\infty}^{x} f(x')dx' &= R_1 \\ \int_{-\infty}^{y} g(y':x)dy' &= R_2 \\ \int_{-\infty}^{z} h(z':x,y)dz' &= R_3 \end{aligned} \qquad (4)$$

3. The Rejection Technique

It has been mentioned that equations (1) and (2) may be awkward to use in a high speed computing device. An alternate method of producing independent sample values of a distribution F(x) is by the use of the rejection technique.

For a simple example of this technique a p.d.f. f(x) with the following properties will be considered (See Figure 1, page 12).

$$f(x) = 0 \qquad x < a,\ a + b < x$$

$$0 \leq f(x) \leq M \qquad a \leq x \leq a + b$$

The rejection technique as it applies here can be explained graphically with reference to Figure 1 as follows. Let a point be chosen uniformly at random from the rectangle with base of length b and height M. If this point falls below the graph of f(x) accept the abscissa as a sample value. If not, reject it and try again. The full technical meaning of these instructions may be expressed analytically thus.

1. Obtain two random numbers, R_1 and R_2,
2. If R_1 is less than or equal to $\frac{f(a+bR_2)}{M}$, let $X = a+bR_2$,
3. If R_1 is greater than $\frac{f(a+bR_2)}{M}$, pick two new random numbers, R_1 and R_2, and try again.

If no rejection procedure had been used, X would have been uniformly distributed between a and a+b. However, only those x's were saved that happened to have $R_1 \leq \frac{f(x)}{M}$, an event that has a probability $\frac{f(x)}{M}$, of occurring (since if k is less than 1, the probability that $R_1 \leq k$ is just k). Therefore, in view of the ever tacit assumption

that R_1 is independent of R_2, the probability of selecting a value of X in the region x to $x+\Delta x$ is equal to the probability of originally getting a value in this region $(\Delta x/b)$ times the probability of saving this x value $\left[f(x)/M\right]$.

The probability of obtaining a satisfactory x on the first trial is the sum of the probabilities of selecting an x in any one of the separate Δx_i regions, or approximately

$$\sum_i \frac{f(x_i)\Delta x_i}{Mb}$$

In the limit, as $\Delta x_i \to 0$, this is just

$$\int_a^{a+b} \frac{f(x)dx}{Mb}$$

Since $\int_a^{a+b} f(x)dx = 1$ the above expression is just $1/bM$. The probability of accepting some value the first time is called the efficiency of the technique, because of its obvious economic implication for applications, and is denoted by E. 1-E is the probability that the first value picked will be rejected. The probability that the process will fail n-1 times and then succeed on the $n^{\underline{th}}$ trial is $(1-E)^{n-1}E$. The expected number of trials, $\bar{n}$, is then

$$\bar{n} = \sum_{n=1}^{\infty} n(1-E)^{n-1} E \qquad (5)$$

$$= -E \sum_{n=1}^{\infty} \frac{d}{dE} (1-E)^n$$

$$= -E \frac{d}{dE} \left[\sum_{n=1}^{\infty} (1-E)^n\right]$$

$$= -E \frac{d}{dE} \frac{(1-E)}{1-(1-E)}$$

$$= \frac{1}{E}$$

The principle of the rejection technique can be illustrated by the following diagram.

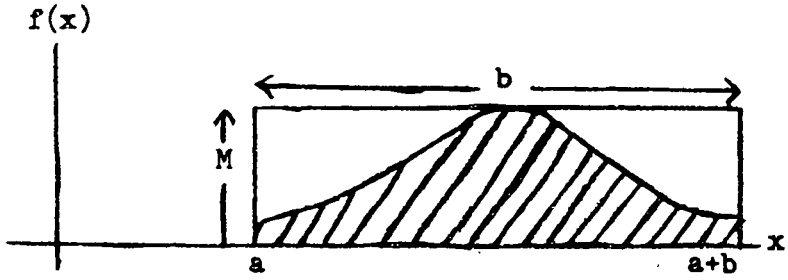


Figure 1

In Figure 1 a rectangle of area bM encloses the p.d.f. f(x). The shaded portion under f(x) has unit area. If a number of points are selected in the rectangle at random from a uniform distribution, but only those points saved that fall within the shaded portion, then the probability that any of these saved values lies between x and x + Δx will be $f(x)\Delta x/bM$. The fraction of points saved will be given by (shaded area)/(total area) or $1/bM$.

The rejection technique may be generalized as follows. Let n(x) and m(y) be p.d.f.'s and let U(x) be an arbitrary function. Then

1. Select an x out of the p.d.f. n(x)
2. Select independently a y out of the p.d.f. m(y) $\left[\text{c.d.f. } M(y)\right]$
3. If $y \leq U(x)$ accept x. Otherwise repeat steps 1 and 2.

It is often computationally convenient to write the inequality $y \leq U(x)$ in the form $s(y) \leq t(x)$ where

$$T(x) = s^{-1}\left[t(x)\right]$$

The a priori probability of getting an x in the region $(x, x + \Delta x)$ is, of course, $n(x)\Delta x$. The probability of accepting x, $\left[\text{probability that } y \leq U(x)\right]$, is $M\left[T(x)\right]$. Therefore, the

probability of selecting an x in the region dx and accepting it is

$$M\left[T(x)\right] n(x)dx$$

The probability of getting any x at all on the first iteration is

$$E = \int_{-\infty}^{\infty} M\left[T(x)\right] n(x)\Delta x \qquad (6)$$

By choosing m, n, and T appropriately it is usually possible to design a numerically convenient and efficient process for selecting an x from the p.d.f. $f(x) = M\left[T(x)\right] n(x)/E$.

If, in a special case, Y is the same as R, M is then the distribution of R. If also U(x) is bounded such that $U(x) \leq 1$, we can say

$$M\left[U(x)\right] = U(x)$$

The technique now becomes:

1. Select an x out of the p.d.f. n(x)
2. Select an R
3. If $R \leq \frac{f(x)}{K\, n(x)}$, where K is larger than or equal to the maximum value of $\frac{f(x)}{n(x)}$, accept x. Otherwise repeat steps 1 and 2.

The efficiency of the technique is now 1/K. Hence E can be equal to, but not larger than, the minimum value of $\frac{n(x)}{f(x)}$. If it happens that only a lower bound for this minimum value is known, than the efficiency will be less than it would have been.

Since the areas under the curves f(x) and n(x) are the same, the requirement that the efficiency be high (i.e., close to 1) imposes a serious restriction on n(x). One way to meet it is to choose n(x) "similar" to f(x). It must also be simple to select from, or there

would be no point in using a rejection technique. The choice of $n(x)$ is a compromise between these two criteria.

Variations of the basic rejection technique

In certain cases, realization of the variations mentioned below may give rise to considerable savings in computing time.

1. Select x out of $n(x)$, y_1 out of $m_1(y)$, and y_2 out of $m_2(y)$ and accept x if either $y_1 \leq T_1(x)$ or $y_2 \leq T_2(x)$. The probability of accepting x now becomes

$$n(x)\left\{M_1\left[T_1(x)\right] + M_2\left[T_2(x)\right] - M_1\left[T_1(x)\right] M_2\left[T_2(x)\right]\right\}$$

2. Break up the p.d.f. into the form

$$f(x) = \sum_i A_i M_i\left[T_i(x)\right] n_i(x)$$

With probability $\frac{A_i}{\sum_j A_j}$ pick x out of $n_i(x)$ and y out of $m_i(y)$ and make the test $y \leq T_i(x)$. If the test fails repeat the whole process. The expected number of iterations is $\sum A_i$; i.e., the efficiency is $1/\sum A_i$.

A brief insight into the nature of this second variation can be obtained by considering the case when the $M_i(y) = y$: i.e., y is selected from the uniform distribution. Then $f(x)$ can be broken up into the form

$$f(x) = \sum_i r_i(x) n_i(x)$$

$$= \sum_i A_i \frac{r_i(x)}{A_i} n_i(x)$$

$$= \sum_i A_i T_i(x) n_i(x)$$

The A_i here are, it is clear, the probability of getting i multiplied by the maximum value of $T_i(x)$. The A_i must be large enough

to insure that $\frac{r_i(x)}{A_i} \leq 1$. As before the efficiency is $1/\sum A_i$ and an efficient process is one in which the $r_i(x)$ vary but little, in a sense. When the $r_i(x)$ are constants then the $\sum A_i = 1$ and the process is 100% efficient; it then just reduces to a convenient way to sample from a p.d.f.

If the i's with relatively uniform $r_i(x)$ have large A_i's while the ones with large variations have small A_i's, the process will still be efficient.

Sometimes as a special case of the above, it is desirable to take the $n_i(x)$ to be the same function; i.e., to break up $f(x)$ into the form

$$f(x) = \sum A_i T_i(x) n(x)$$

$$T(x) = \sum A_i T_i(x)$$

This is advantageous when it is difficult to find the maximum value of $T(x)$, but relatively easy to find the maximum value of the individual terms. However, breaking up $T(x)$ into separate terms always decreases the efficiency of the technique.

A special case of this last situation occurs very frequently when the p.d.f. $f(x)$ is fitted by sections. For example if

$$p_i = \int_{x_i}^{x_{i+1}} f(x)dx$$

is the probability that the event $x_i \leq X \leq x_{i+1}$ occurs and $f_i(x)$ is a fit to $\frac{f(x)}{p_i}$ in this segment of the x axis then

$$f(x) = \sum p_i f_i(x)$$

where the $f_i(x)$ are themselves properly normalized p.d.f.'s. The computer can then pick the i index with probability p_i and then pick x out of $f_i(x)$ by any convenient technique.

4. Manipulations with Distributions

The problem of generating values of random variables will now be considered from a slightly different point of view. Given two independent random variables x and y and their c.d.f.'s, F(x) and G(y), what is the c.d.f. of a function z(x,y)? There is perhaps no general answer easily given here. But a number of interesting special functions will be considered.

1.[1] Z = X + Y

The domain of X is considered broken into intervals by the points $x_1,\ldots,x_n$. The length of each interval is $\Delta x_i = x_{i+1} - x_i$.

The probability that $Z \leq z$ is equal to the sum of the probabilities of all the mutually exclusive ways in which X + Y can be less than z. Neglecting details of rigor, this can be obtained by multiplying the probability that $x_i < X \leq x_{i+1}$ $\left[F(x_{i+1}) - F(x_i)\right]$ by the probability that $Y \leq z - x_i$ $\left[G(z-x_i)\right]$, and summing over all possible x_i; so

$$H(z) \approx \sum_i G(z-x_i)\left[F(x_{i+1}) - F(x_i)\right] = \sum_i G(z-x_i)f(x_i)\Delta x_i \qquad (7)$$

The limit of the above expressions will be recognized as being the definition of the Stieltjes and Riemannian (ordinary) integrals[2] respectively.

$$H(z) = \int_{-\infty}^{\infty} G(z-t)dF(t) = \int_{-\infty}^{\infty} G(z-t)f(t)dt \qquad (8)$$
$$= \int_{-\infty}^{\infty} F(z-t)dG(t) = \int_{-\infty}^{\infty} F(z-t)g(t)dt$$

by symmetry.

---

1 In individual instances of this and some of the other functions it is often simpler in theory and practice to use Fourier and Laplace Transform techniques. For a discussion of these methods see e.g. Cramer, Mathematical Methods of Statistics, and Wilks, Mathematical Statistics.

2 See e.g. Widder, Advanced Calculus, for a discussion of the definitions of these integrals.

This can also be written

$$h(z) = \int_{-\infty}^{\infty} g(z-t)f(t)dt \qquad (9)$$

$$= \int_{-\infty}^{\infty} f(z-t)g(t)dt$$

2. $Z = XY$ $(0 \leq X,Y)$

The probability that $Z \leq z$ is the probability that X is on region Δt [$dF(t)$ or $f(t)\Delta t$] times the probability that $Y \leq \frac{z}{t}$ [$G(z/t)$] summed over all possible values of t; so

$$H(z) = \int_{0}^{\infty} G(\tfrac{z}{t})dF(t) = \int_{0}^{\infty} G(\tfrac{z}{t})f(t)dt \qquad (10)$$

$$= \int_{0}^{\infty} F(\tfrac{z}{t})dG(t) = \int_{0}^{\infty} F(\tfrac{z}{t})g(t)dt$$

$$h(z) = \int_{0}^{\infty} \tfrac{1}{t}\, g\,(\tfrac{z}{t})dF(t) = \int_{0}^{\infty} \tfrac{1}{t}\, g(\tfrac{z}{t})f(t)dt \qquad (11)$$

$$= \int_{0}^{\infty} \tfrac{1}{t}\, f(\tfrac{z}{t})dG(t) = \int_{0}^{\infty} \tfrac{1}{t} f(\tfrac{z}{t})g(t)dt$$

3. $Z = \frac{X}{Y}$ $(0 \leq X,Y)$

The probability that $Z \leq z$ is $dG(t)$ or $g(t)\Delta t$ [the probability that Y is in region Δt] times $F(zt)$ [the probability that $X \leq zt$] summed over all possible y; so

$$H(z) = \int_{0}^{\infty} F(zt)dG(t) = \int_{0}^{\infty} F(zt)g(t)dt \qquad (12)$$

$$h(z) = \int_{0}^{\infty} tf(zt)dG(t) = \int_{0}^{\infty} tf(zt)g(t)dt \qquad (13)$$

4. Z = smaller of X and Y

The probability that X is in the region Δx is of course $f(x)\Delta x$ and the probability that Y is larger than x is $1 - G(x)$; so the probability of getting X in the region Δx and accepting it (i.e., of its being the smaller) is $f(x)\Delta x \left[1 - G(x)\right]$. Similarly the probability of getting y in the region Δy and accepting it is $g(y)\Delta y \left[1 - F(y)\right]$. Since the two events are mutually exclusive ignoring ties, as may be done, the probability of one or the other is just the sum of the separate probabilities; so

$$h(z) = f(z)\left[1 - G(z)\right] + g(z)\left[1 - F(z)\right] \tag{14}$$
$$= f(z) + g(z) - f(z)G(z) - g(z)F(z)$$

A few more results follow without complete discussion.

5. Z = larger of X and Y

$$h(z) = f(z)G(z) + g(z)F(z) \tag{15}$$

6. Z > (smaller of X and Y)/(larger of X and Y) $(0 \leq X,Y)$

This is a corollary of example 3.

$h(z)\Delta z$ = probability that $(\frac{x}{y} = z$ or $\frac{y}{x} = z)$

Since the two possibilities are disjoint,

$$h(z) = \int_0^\infty t\left\{f(zt)g(t) + f(t)g(zt)\right\} dt \quad 0 \leq z \leq 1 \tag{16}$$

7. Z = (larger of X and Y)/(smaller of X and Y) $(0 \leq X,Y)$

Same distribution as 6, $\quad 1 \leq z$

8. W = the middle of X, Y, and Z

$$v(w) = f(w)\left[G(w) + H(w) - 2G(w)H(w)\right] \tag{17}$$
$$+ g(w)\left[F(w) + H(w) - 2F(w)H(w)\right]$$
$$+ h(w)\left[F(w) + G(w) - 2F(w)G(w)\right]$$

where $v(w)$ is of course the p.d.f. for W.

5. Examples

Introduction

The various methods that have been described are illustrated by the examples in this section. Some of these examples are actually useful for computational purposes, some have been included for pedagogical reasons, and some are included for the sake of completeness (in the handbook sense). In some cases the verification of the formulae involved is so simple that it is left out. It might be a useful exercise for inexperienced readers to actually carry through this verification for a few of the examples. Others may want to skip the whole section except for reference purposes.

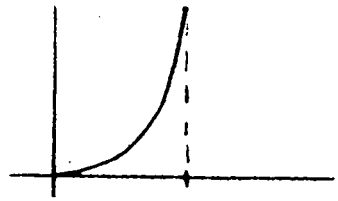
In many of the examples several methods are considered. Which method the computer should use depends on the application, the computing equipment available, and the relative importance of programming time, computing time, and memory.

It is often desirable to reflect a p.d.f. about a line $x = a$. This can always be done by replacing x by $2a-x$, as is occasionally explicity done in the examples which follow.

Primarily, however, the examples (consisting of the derivations which follow them) can be thought of as part of a library which will be useful in applications. This means that where in Section 4 the distribution was unknown, in this section we begin with a distribution, and consider the **most convenient method** which will realize it. More such examples and methods are of course invited.

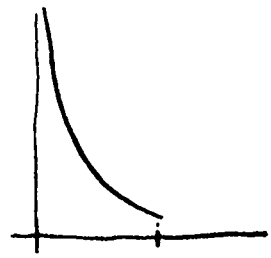
Table of Examples to be Considered[1]

1. nx^{n-1} $\quad 0 \leq x \leq 1$

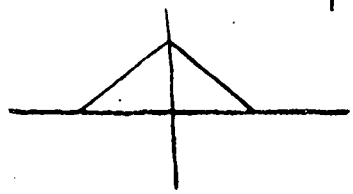


2. $n(1-x)^{n-1}$ $\quad 0 \leq x \leq 1$

3. $\frac{1}{n} x^{(1-n)/n}$ or $\frac{1}{n}(1-x)^{(1-n)/n}$ $\quad 0 \leq x \leq 1$

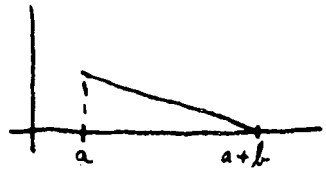


4. $1 - |x|$ $\quad -1 \leq x \leq 1$

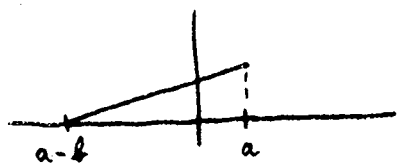


5. $2 - 2x$ $\quad 0 \leq x \leq 1$

6. $\frac{1}{b}\left[2 - \frac{2(x-a)}{b}\right]$ $\quad a \leq x \leq a + b$



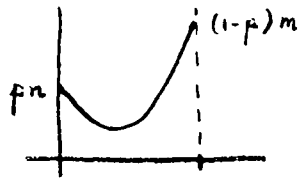
7. $\frac{1}{b}\left[2 - \frac{2(a-x)}{b}\right]$ $\quad a - b \leq x \leq a$



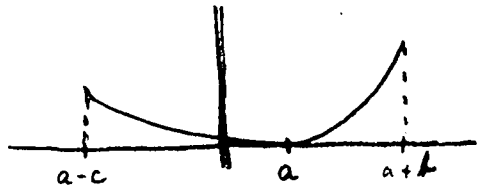
---

1 The order in which the p.d.f.'s are given has little significance. They are just grouped somewhat according to simplicity, method of generation, and field of application.

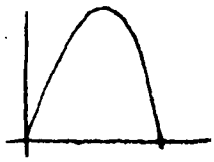
8. $pn(1-x)^{n-1} + (1-p)mx^{m-1} \quad 0 \le x \le 1$



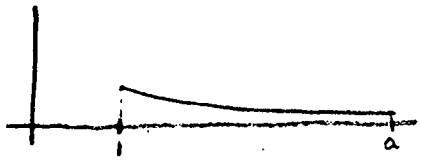
9. $\begin{cases} \dfrac{(1-p)m(a-x)^{m-1}}{c^m} & a - c \le x \le a \\ \dfrac{pn(x-a)^{n-1}}{b^n} & a \le x \le a + b \end{cases}$



10. $6(x-x^2) \qquad 0 \le x \le 1$



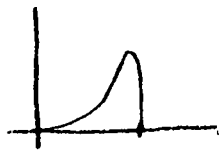
11. $\dfrac{1}{x \ln a} \qquad 1 \le x \le a$



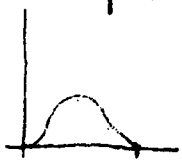
12. $\sqrt{\dfrac{2}{\pi}}\, e^{-x^2/2} \qquad 0 \le x < \infty$ (Gaussian)

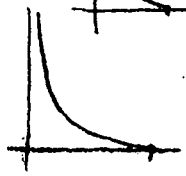
13. $n E_n(x) = n \displaystyle\int_1^\infty \frac{e^{-xy}}{y^n}\, dy \qquad 0 \le x < \infty$

14. $\dfrac{x^{1/b} - x^{1/a}}{(b-a)x} \qquad 0 \le x \le 1$

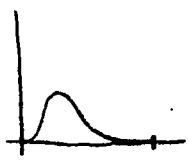


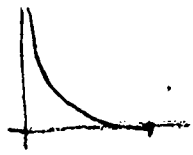
$-\dfrac{1}{a^2} x^{\frac{1}{a}-1} \ln x \qquad 0 \le x \le 1$





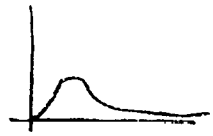
$\dfrac{x^{\frac{1}{a}-1}(-\ln x)^{n-1}}{a^n (n-1)!} \qquad 0 \le x \le 1$





15. $\frac{ab}{b-a}\left(e^{-ax} - e^{-bx}\right)$ $\quad 0 \leq x < \infty$

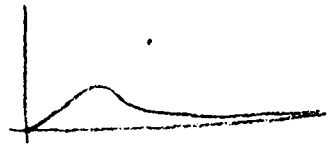
$\frac{a^n x^{n-1}}{(n-1)!} e^{-ax}$ $\quad 0 \leq x < \infty$



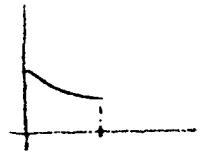
$ab\, K_0\left(2\sqrt{abx}\right) = ab \int_0^\infty \frac{1}{y} e^{-\sqrt{abx}\,(y + \frac{1}{y})} dy$ $\quad 0 \leq x < \infty$

$\frac{m}{(x+m)^2}$ $\quad 0 \leq x < \infty$

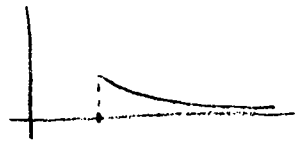
$ae^{-ax} + be^{-bx} - (a+b)e^{-(a+b)x}$ $\quad 0 \leq x < \infty$



$ab\left\{\frac{1}{(ax+b)^2} + \frac{1}{(a+bx)^2}\right\}$ $\quad 0 \leq x \leq 1$

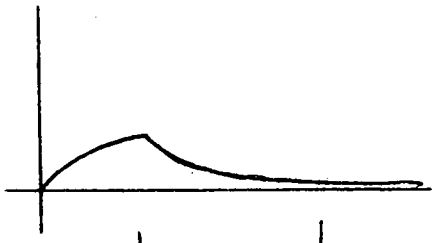


$ab\left\{\frac{1}{(ax+b)^2} + \frac{1}{(a+bx)^2}\right\}$ $\quad 1 \leq x < \infty$

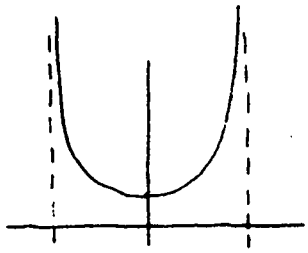


$(a+b)e^{-(a+b)x} + (b+c)e^{-(b+c)x} + (c+a)e^{-(c+a)x}$
$- 2(a+b+c)e^{-(a+b+c)x}$ $\quad 0 \leq x < \infty$

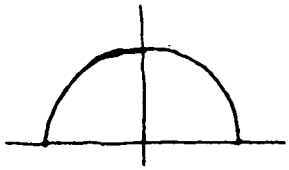
16. $\begin{cases} \frac{1}{a}(1-e^{-bx}) & 0 \le x \le a \\ \frac{1}{a}(e^{-b(x-a)}-e^{-bx}) & a \le x < \infty \end{cases}$



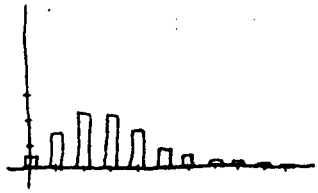
17. $\frac{1}{\pi\sqrt{1-x^2}}$ $\quad -1 \le x \le 1$



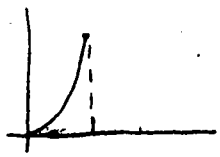
$\frac{4}{\pi}\sqrt{1-x^2}$ $\quad -1 \le x \le 1$



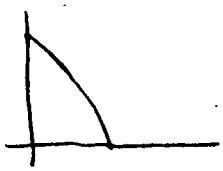
18. $\frac{a^i e^{-a}}{i!}$ for $0 < a$, $\quad i = 0, 1, 2, \ldots$ (Poisson)



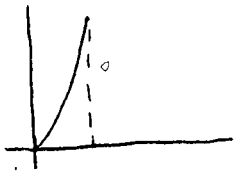
19. xe^x $\quad 0 \le x \le 1$



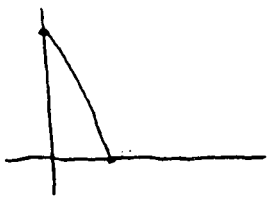
$e - e^x$ $\quad 0 \le x \le 1$



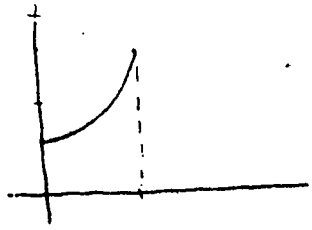
$\frac{e}{e-1}\, x \cosh x$ $\quad 0 \le x \le 1$



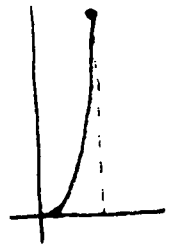
$\frac{e}{e-1}(\sinh 1 - \sinh x)$ $\quad 0 \le x \le 1$



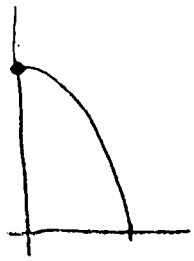
$\frac{1}{e-1} e^x$ $\quad 0 \leq x \leq 1$



ex sinh x $\quad 0 \leq x \leq 1$



e (cosh 1 - cosh x) $\quad 0 \leq x \leq 1$

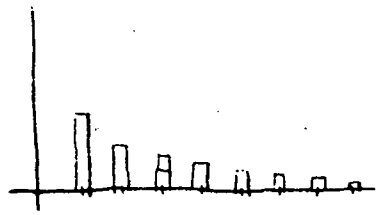


Also the following joint p.d.f.'s of (x,i):

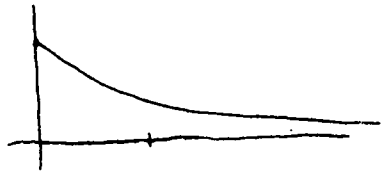
$$\frac{x^i}{(i-1)!}, \quad \frac{1-x^i}{i!}, \quad \frac{(i-x)^{i-1}}{(i-1)!} - \frac{(i-x)^i}{i!} \quad \begin{cases} 0 \leq x \leq 1 \\ i = 1, 2, \ldots \end{cases}$$

Also, the marginal p.d.f.:

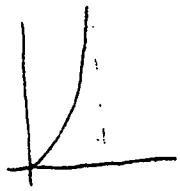
$\frac{1}{i!} - \frac{1}{(i+1)!}$ $\quad i = 1, 2, \ldots$



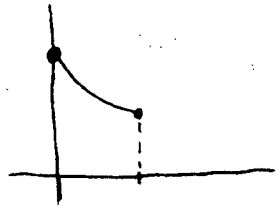
20. e^{-x} $\quad 0 \leq x < \infty$



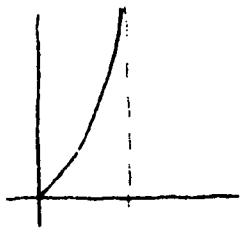
21. $-\ln(1-x)$ $\quad 0 \leq x \leq 1$



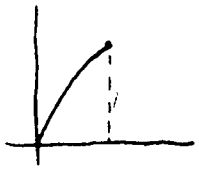
1.443 $\frac{1}{1+x}$ $\quad 0 \leq x \leq 1$



$.721 \ln \frac{1+x}{1-x}$ $\quad 0 \leq x \leq 1$



$3.259 \frac{x}{1+x}$ $\quad 0 \leq x \leq 1$

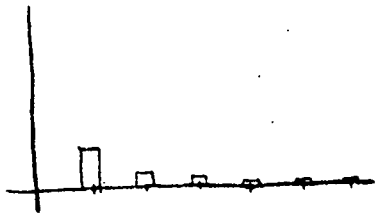


$-1.629 \ln (1-x^2)$ $\quad 0 \leq x \leq 1$

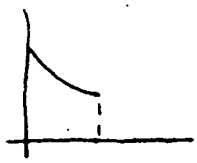
Also the following p.d.f.'s for (x,i) or i alone:

$x^{i-1} - x^i$, $\frac{1}{I} x^i$ $\quad \begin{cases} 0 \leq x \leq 1 \\ i = 1, 2, \ldots \end{cases}$

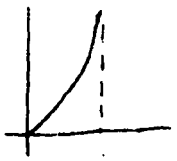
$\frac{1}{I(I+1)}$ $\quad i = 1, 2, \ldots$



22. $1.216 \frac{1}{x} \ln (1+x)$ $\quad 0 \leq x \leq 1$



$5.634 \left[1 - \frac{1}{x} \ln(1+x)\right]$ $\quad 0 \leq x \leq 1$



Also the joint p.d.f. for (x,i) and i alone:

$$\frac{x^{i-1}}{i} - \frac{x^{i}}{i+1} \qquad \begin{cases} 0 \leq x \leq 1 \\ i = 1, 2, \ldots \end{cases}$$

$$\frac{2i+1}{i^2(i+1)^2} \qquad i = 1, 2, \ldots$$

23. The Klein-Nishina Scattering Formula.

24. Neutron-deuteron elastic scattering.

25. Neutron-deuteron inelastic scattering.

26. General inelastic scattering of neutrons.

27. Fit to experimental data of elastic scattering of 14 MEV neutrons in copper.

* * *

Representations of the p.d.f.s Considered

In the discussion of the representations of each of the distributions below, it is assumed that there is a large store of (independent, uniformly distributed) random numbers, symbolized R, R_1, etc., available.

1. $h(z) = nz^{n-1}$ $\qquad 0 \leq z \leq 1$

Let Z be the largest of n random numbers.

The proof is by induction. Let X be the largest of n-1 random numbers and assume that its p.d.f. is $(n-1)x^{n-2}$, $0 \leq x \leq 1$. Let Y equal another random number and let Z be the larger of X and Y. Then as mentioned in Section 4,

$$h(z) = f(z)G(z) + g(z)F(z)$$

$$= (n-1)z^{n-2}z + z^{n-1}$$

$$= nz^{n-1}$$

Since Z is the largest of n-1 random numbers and another random number, it is the largest of n random numbers.

2. $h(z) = n(1-z)^{n-1}$ $\qquad 0 \leq z \leq 1$

Let Z be the smallest of n random numbers.

This is just a reflection of example 1 about the vertical line $z = 1/2$.

3. $f(x) = \frac{1}{n} x^{(1-n)/n}$ for $0 < n$ $\qquad 0 \leq x \leq 1$

Let $X = R^n$

The c.d.f. $F(x)$ can be found as follows:

$$F(x) = \text{probability that } X \leq x$$

$$= \text{probability that } R^n \leq x$$

$$= \text{probability that } R \leq x^{1/n}$$

$$= x^{1/n}$$

Then $f(x) = \frac{1}{n} x^{(1-n)/n}$

In actual practice, only the integral values of n are of interest. The p.d.f.s obtained by putting $n = 1/2, 1/3$, etc. are often more simply obtained by the method of example 1.

If $X = 1 - R^n$, all of the above curves are reflected about the line $x = 1/2$.

4. $f(x) = 1 - |x| \qquad -1 \leq x \leq 1$

Let $X = R_1 - R_2$

Then from example 1 of Section 4,

$$\begin{aligned} f(x) &= 0 && x \leq -1 \\ &= 1 + x && -1 \leq x \leq 0 \\ &= 1 - x && 0 \leq x \leq 1 \\ &= 0 && 1 \leq x \end{aligned}$$

If $X = R_1 + R_2$, the p.d.f. would have been translated one unit in the positive direction.

5. $f(x) = 2 - 2x \qquad 0 \leq x \leq 1$

Let $X = |R_1 - R_2|$ or let X = the smaller of R_1 and R_2.

Then the density of f(x) is the sum of the two disjoint possibilities that $R_1 - R_2 = x$ or that $R_2 - R_1 = x$. Using example 4, we have

$$f(x) = \begin{cases} 2 - 2x & 0 \leq x \leq 1 \\ 0 & \text{elsewhere} \end{cases}$$

6. $f(x) = \frac{1}{b}\left[2 - \frac{2(x-a)}{b}\right]$ $\qquad a \leq x \leq a + b$

Let $X = a + b\,|R_1 - R_2|$

This is just a translation and dilation of example 5. Use for the X of this example a + bY where Y is the variable of example 5.

7. $\frac{1}{b}\left[2 - \frac{2(a-x)}{b}\right]$ $\qquad a - b \leq x \leq a$

Let $X = a - b\,|R_1 - R_2|$

This is a reflection of example 6.

8. $pn(1-x)^{n-1} + (1-p)mx^{m-1}$ $\qquad 0 \leq x \leq 1$

Let X be, with probability p, the smallest of n random numbers; with probability (1-p), the largest of m random numbers.

This is a mixture of examples 1 and 2. With probability p (that is, after a test, R < p ?) use example 1. If not example 1, use example 2. Then

$$f(x) = pn(1-x)^{n-1} + (1-p)mx^{m-1} \qquad 0 \leq x \leq 1$$

If $p = 1/2$ and $m = n$,

$$f(x) = n/2\left[x^{n-1} + (1-x)^{n-1}\right]$$

which is symmetric about $x = 1/2$.

9. $$h(z) = \begin{cases} \dfrac{(1-p)m(a-z)^{m-1}}{c^m} & a - c \le z \le a \\ \dfrac{pn(z-a)^{n-1}}{b^n} & a \le z \le a + b \end{cases}$$

With probability p, pick X out of nx^{n-1} and let $Z = a + bX$.

With probability 1-p, pick X out of mx^{m-1} and let $Z = a - cX$.

One piece is like example 1 and the other is like example 2. If $p = 1/2$, $m = n$, and $b = c$, then the p.d.f. is symmetric about $z = a$ and

$$h(z) = n/2 \frac{|z-a|^{n-1}}{b^n} \qquad a - b \le z \le a + b$$

10. $h(x) = 6(x-x^2)$ $\qquad 0 \le x \le 1$

Let X be the middle of R_1, R_2, and R_3 (Section 4, example 8).

11. $f(x) = \dfrac{1}{x \ln a}$ $\qquad 1 \le x \le a$

The most obvious method is to solve the equation

$$\int_1^x \frac{1}{t \ln a}\, dt = R$$

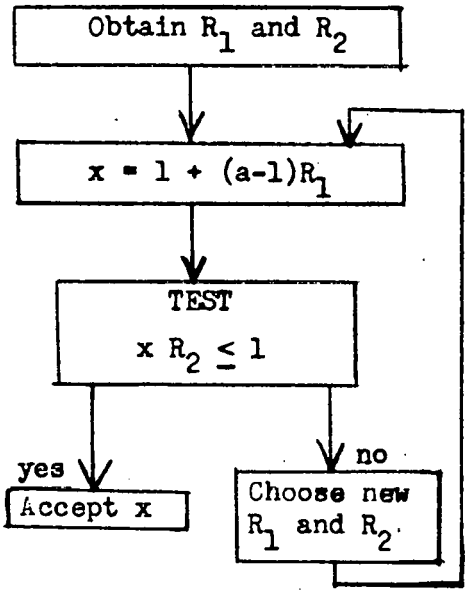
$$x = a^R$$

$$= e^{R \ln a}$$

This is inconvenient, because both the exponential and a logarithm must be calculated in most applications.

Five rejection methods for selecting from this p.d.f. will now be considered. The example will be given such a thorough treatment, not because there is a great practical importance in avoiding exponentials and logarithms, but because it gives a good opportunity to explain and illustrate devices heretofore mentioned only abstractly.

a. The straight-forward general method:



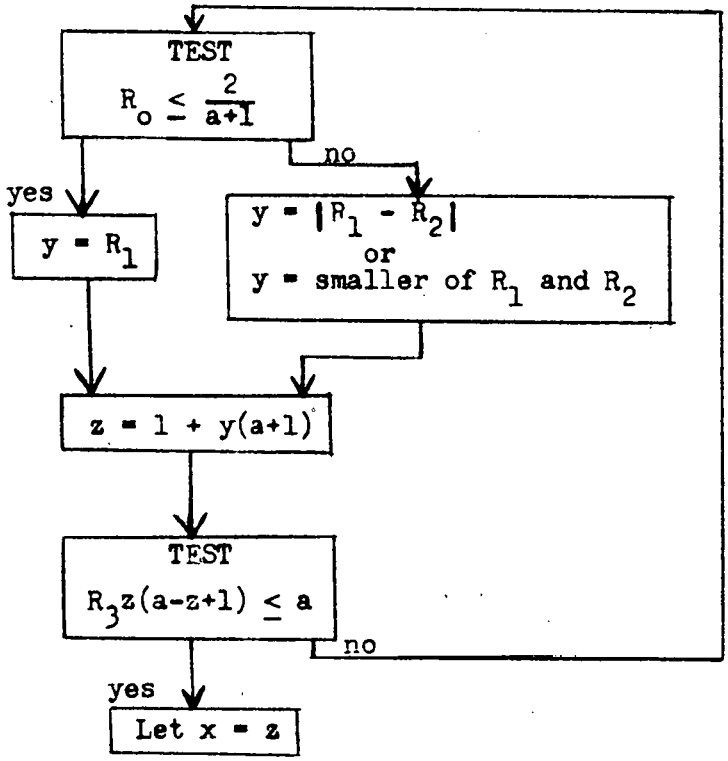
The a priori probability of arriving at a given value of x is $\frac{dx}{a-1}$ and the probability of accepting it is $\frac{1}{x}$, so the efficiency is:

$$E_a = \int_1^a \frac{1}{x} \frac{dx}{a-1} = \frac{\ln a}{a-1}$$

Thus for example, $E_a \approx .25$ for $a = 10$.

The computations required by this method are of the simplest sort from almost any calculational point of view, and the yield is $1/2\ E_a$ per random number used.

b.



With probability $\frac{2}{a+1}$, y is chosen uniformly; with probability $1 - \frac{2}{a+1} = \frac{a-1}{a+1}$, y is chosen from the p.d.f. 2(1-y). Weighting the two p.d.f.s with these probabilities gives

$$g(y) = \frac{a-1}{a+1}\, 2(1-y) + \frac{2}{a+1}$$

$$= \frac{2(a-ay+y)}{a+1}$$

Since

$$y = \frac{z-1}{a-1}$$

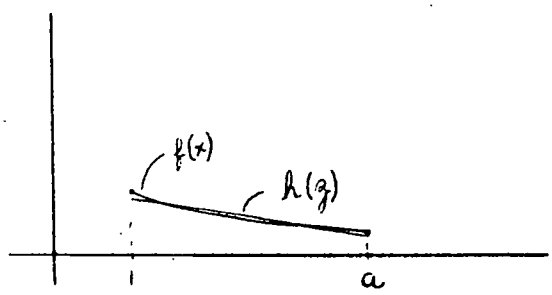
$$dy = \frac{dz}{a-1}$$

$$h(z)dz = g(\frac{z-1}{a-1})dy$$

$$h(z) = \frac{2\left[a - (a-1)\frac{z-1}{a-1}\right]}{a+1} \cdot \frac{1}{a-1}$$

$$= \frac{2}{a^2-1}(a-z+1)$$

h(z) is a straight line.



The probability in the first box was chosen so that

$$\frac{h(1)}{f(1)} = \frac{h(a)}{f(a)}$$

Because f(x) is convex in the interval of interest, this choice maximizes the efficiency E_a of this second method where the auxilliary p.d.f. is a straight line segment.

We now choose from h(z) and test whether $R \leq \frac{f(z)}{Kh(z)}$ where K is the maximum value of $\frac{f(z)}{h(z)}$. We have

$$K = \frac{f(1)}{h(1)} = \frac{1}{\ln a} / \frac{2a}{a^2-1} = \frac{a^2-1}{2a\ln a}$$

Hence the test is:

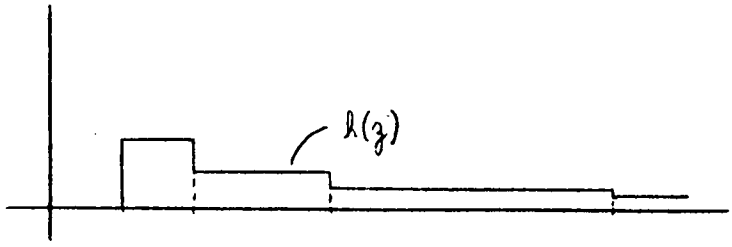
$$R \leq \frac{f(z)}{Kh(z)} = \frac{a}{z(a-z+1)}$$

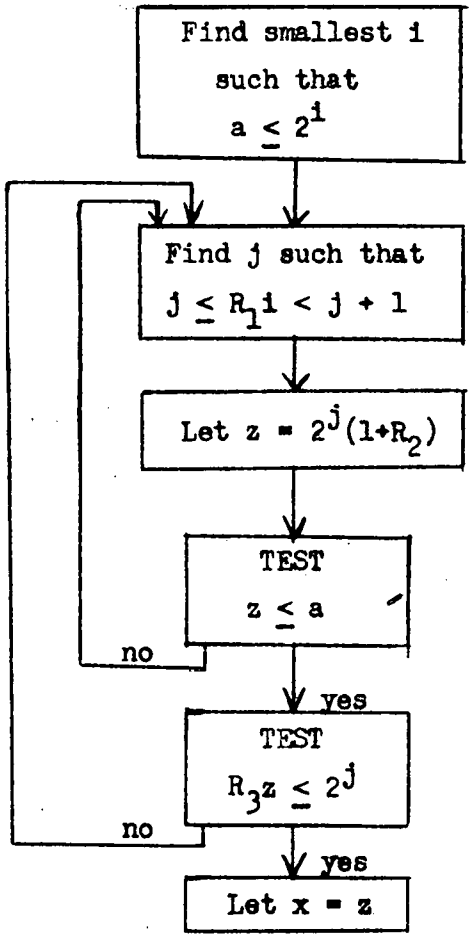
and

$$E_b = \frac{2a\ln a}{a^2-1}$$

The computations are again simple. In general E_b is about twice E_a.

c. In this case, h(z) is a step function.





(a choice dictated by efficiency)

(discrete uniform j)

(needed only if j = i - 1)

The probability of picking a given value of x is

$$E_c \cdot f(x) = \text{(prob. of picking j) (prob. of picking z) (prob. of accepting z)}$$

$$= \frac{1}{i} \cdot \frac{1}{2^j} \cdot \frac{2^j}{x}$$

$$= \frac{1}{ix}$$

$$= \frac{\ln a}{i} \cdot \frac{1}{x \ln a}$$

Therefore $E_c = \frac{\ln a}{i}$ or roughly ln2.

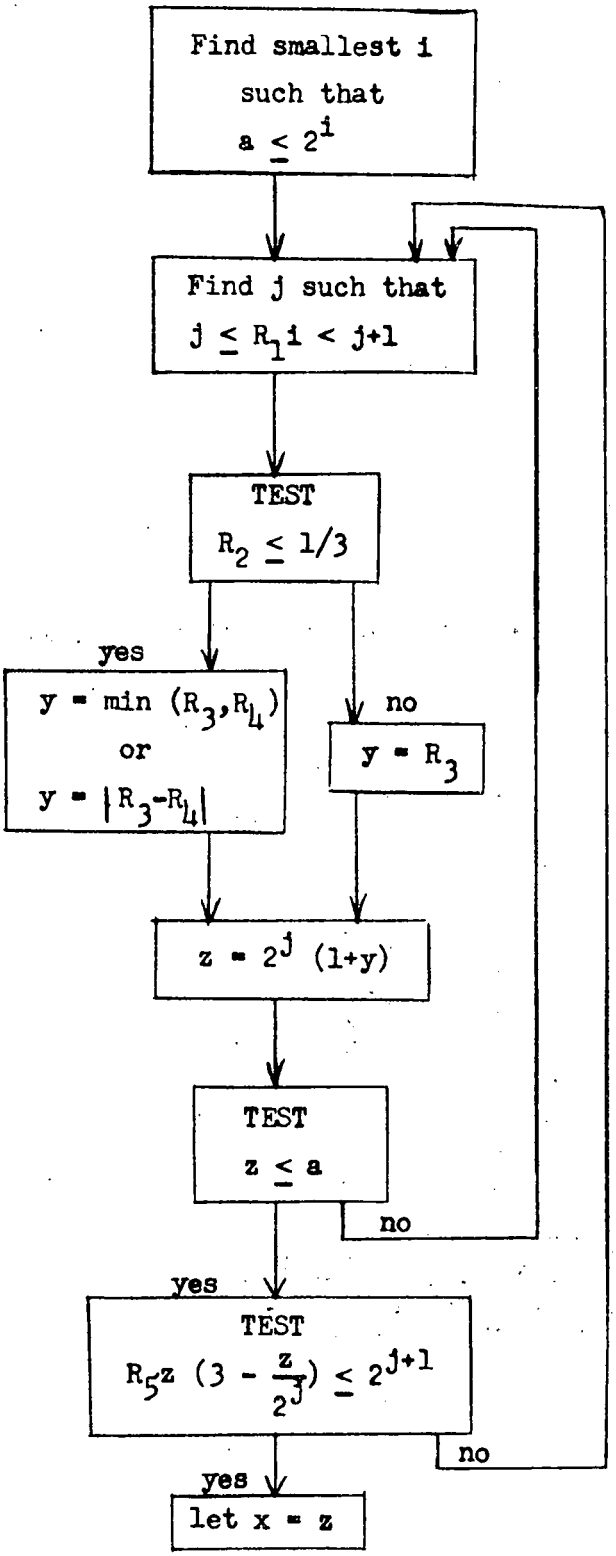
d. In this method, z is picked out of

$$h(z) = \frac{1}{3.2^{j-1}} \left(3 - \frac{z}{2^j}\right) \qquad 2^j \leq z \leq 2^{j+1}$$

instead of

$$h(z) = \frac{1}{2^j} \qquad 2^j \leq z \leq 2^{j+1}$$

as in method c.


Find smallest i such that $a \leq 2^i$
Find j such that $j \leq R_1 i < j+1$
TEST $R_2 \leq 1/3$
yes
$y = \min(R_3, R_4)$ or $y = |R_3 - R_4|$
no
$y = R_3$
$z = 2^j (1+y)$
TEST $z \leq a$
no
yes
TEST $R_5 z (3 - \frac{z}{2^j}) \leq 2^{j+1}$
no
yes
let x = z

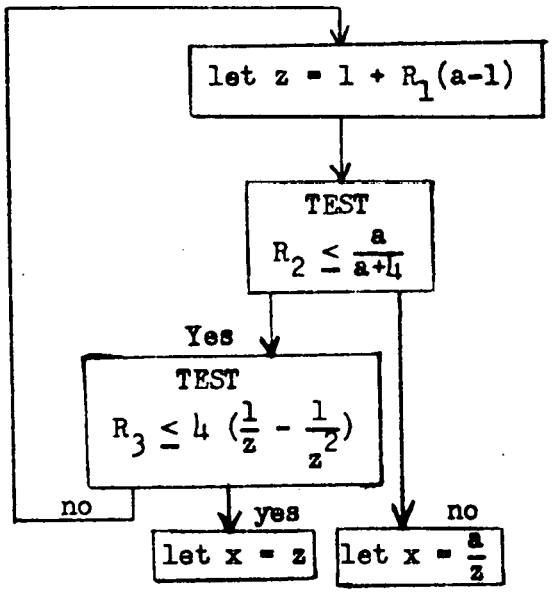
Similarly as in c,

$$E_d \cdot f(x) = \frac{1}{I} \cdot \frac{1}{3.2^{j-I}} \left(3 - \frac{x}{2^j}\right) \cdot \frac{2^{j+1}}{x\left(3 - \frac{x}{2^j}\right)}$$

$$= \frac{4}{3} \frac{1}{Ix}$$

$$E_d = \frac{4 \ln a}{3I} \approx \frac{4}{3} \ln 2 \approx .9$$

e. In this method, x is picked from f(x) with probability p and g(x) with probability 1 - p.



The probability of getting a given x is (prob. of 1st yes branch) (prob. that $z = x$) + (prob. of 1st no branch) (prob. that $z = \frac{a}{x}$).

Hence

$$E_e\, f(x) = \frac{a}{a+4} \cdot \frac{1}{a-1}\, 4 \left(\frac{1}{x} - \frac{1}{x^2}\right) + \frac{4}{a+4} \cdot \frac{1}{a-1} \left(\frac{a}{x^2}\right)$$

$$= \frac{4a}{(a+4)(a-1)} \cdot \frac{1}{x}$$

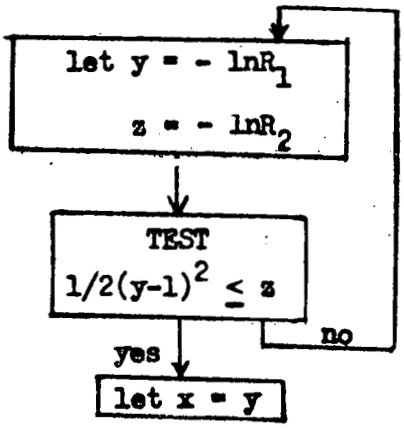
and

$$E_e = \frac{4a}{a+4} \cdot \frac{1}{a-1} \cdot E_a = \frac{4a}{a+4} E_a$$

For large a, E_e is about 4 E_a.

E_a, E_b, E_c, E_d, and E_e are shown for a range of $\underline{a}$ in graph number 1.

12. $f(x) = \sqrt{\frac{2}{\pi}}\, e^{-x^2/2}$ $\quad 0 \leq x < \infty$ the (half) Gaussian.



The probability of getting a given value of x is equal to the probability of picking that value of x times the probability of accepting it or

$$E \cdot f(x) = e^{-x} \cdot e^{-(x-1)^2/2}$$

$$= e^{-1/2} \cdot e^{-x^2/2}$$

$$E = \sqrt{\frac{\pi}{2}}\, e^{-1/2}$$

$$= .76 \text{ , which is remarkably high.}$$

A random sign can be attached to x to turn it in to a true Gaussian.

It is possible to pick from an approximate Gaussian p.d.f. by using the Central Limit Theorem which states, in one of its forms, that the sum of a large number of independent and identically distributed random variables with a finite variance is asymtotically normally distributed (Gaussian). In particular, the random variable defined by the equation

$$X = \sum_{i=1}^{n} \pm R_i$$

becomes normally distributed with 0 mean and variance n/3 as $n \longrightarrow \infty$. (The variance is defined below, see Part II, P. 2). The exact p.d.f. and corresponding c.d.f. can be shown to be

$$f(x) = \frac{n}{2^n} \sum_{r=0}^{\left[\frac{n+x}{2}\right]} \frac{(-1)^r}{r!(n-r)!} (n + x - 2r)^{n-1}$$

$$F(x) = \frac{1}{2^n} \sum_{r=0}^{\left[\frac{n+x}{2}\right]} \frac{(-1)^r}{r!(n-r)!} (n + x - 2r)^{n}$$

The easiest way to obtain a random variable uniformly distributed from -1 to 1 is to take it equal to 2R-1. The formula for X then becomes

$$X = 2 \sum_{i=1}^{n} R_i - n$$

Another approximation to a two-sided Gaussian is given by the p.d.f.

$$f(x) = \frac{Be^{Bx}}{(1 + e^{Bx})^2} \qquad B > 0$$

f(x) has mean 0 and variance $\pi^2/3B^2$. To pick from this p.d.f., the standard technique

$$x = F^{-1}(R)$$

$$= -\frac{1}{B} \ln \left(\frac{1}{R} - 1\right)$$

can be used.

Curves for the p.d.f.'s for the Gaussian, the sum of 6 R_i, the sum of 12 R_i, and the approximate Gaussian are given in graph number 2. Graph number 3 shows the c.d.f.'s of the same distributions, plotted on cumulative probability paper. They have all been normalized to have variance 1.

13. Pick from $E_n(x) = \int_1^\infty \frac{e^{-xu}}{u^n}\,du \qquad 0 \le x < \infty$

Let the p.d.f. for Y be $ny^{n-1}, \qquad 0 \le y \le 1.$

Let Z have the p.d.f. $ae^{-az}, \qquad 0 \le z < \infty$. Let $X = YZ$.

As in section 4, the p.d.f. f(x) of X is given by:

$$f(x) = \int_0^1 \frac{1}{y}\,(ae^{-ax/y})ny^{n-1}dy$$

$$= an \int_0^1 e^{-ax/y}\, y^{n-2}dy$$

Letting $y = \frac{1}{u}$

$$f(x) = an \int_1^\infty \frac{e^{-axu}}{u^n}\,du$$

$$= an\, E_n(ax)$$

$$F(x) = \int_0^x f(t)dt$$

$$= 1 - n\, E_{n+1}(ax)$$

14. $$f(x) = \frac{x^{1/b} - x^{1/a}}{(b-a)x} \qquad 0 \le x \le 1$$

Let $X = R_1^{\,a} R_2^{\,b}$.

Then

$$F(x) = \frac{bx^{1/b} - ax^{1/a}}{b-a} \qquad 0 \le x \le 1$$

and f(x) is as given.

$$f(x) = -\frac{1}{a^2} x^{\frac{1}{a}-1} \ln x \qquad 0 \le x \le 1$$

As above, but let a = b.

Then

$$F(x) = x^{\frac{1}{a}}\left(1 - \frac{1}{a}\ln x\right) \qquad 0 \le x \le 1$$

$$f(x) = \frac{x^{\frac{1}{a}-1}(-\ln x)^{n-1}}{a^n(n-1)!} \qquad 0 \le x \le 1$$

Let $X = \prod_{i=1}^{n} R_i^{\,a}$

Then

$$F(x) = x^{\frac{1}{a}} \sum_{i=1}^{n} \frac{(-\ln x)^{n-1}}{a^{n-1}(n-1)!} \qquad 0 \le x \le 1$$

15. $f(x) = \frac{ab}{b-a}(e^{-ax} - e^{-bx}) \qquad 0 \leq x < \infty$

Let Y and Z have the p.d.f.'s ae^{-ay} and be^{-bz} respectively.

Let $X = Y + Z$.

Then

$$f(x) = \int_0^x ae^{-a(x-z)}be^{-bz}dz$$

$$= \frac{ab}{b-a}(e^{-ax} - e^{-bx}) \qquad 0 \leq x < \infty$$

If $a = b$, then the process yields

$$f(x) = a^2xe^{-ax} \qquad 0 \leq x < \infty$$

The sum of n random variables each with the p.d.f. ae^{-ay} is similarly shown to have the p.d.f.

$$f(x) = \frac{a^n x^{n-1}}{(n-1)!}e^{-ax} \qquad 0 \leq x < \infty$$

$$f(x) = ab\,K_0(2\sqrt{abx}) = ab\int_0^\infty \frac{1}{y}e^{-\sqrt{abx}(y + \frac{1}{y})}dy^1 \qquad 0 \leq x < \infty$$

Let $X = YZ$

Then $$f(x) = \int_0^\infty \frac{1}{z}ae^{-ax/z}be^{-bz}dz$$

$$= ab\int_0^\infty \frac{1}{z}e^{-(ax/z + bz)}dz \qquad \text{Let } y = \sqrt{\frac{a}{b}}\,x\,z$$

$$f(x) = ab\int_0^\infty \frac{1}{y}e^{-\sqrt{abx}(y + \frac{1}{y})}dy$$

$$= ab\,K_0(2\sqrt{abx}) \qquad 0 \leq x < \infty$$

---

1 See Watson, Theory of Bessel Functions, p. 181.

$$f(x) = \frac{m}{(x+m)^2} \qquad 0 \leq x < \infty$$

Let $X = \frac{Y}{Z}$

Then

$$f(x) = \int_0^\infty zae^{-axz}\, be^{-bz}$$

$$= \frac{ab}{(ax+b)^2}$$

$$= \frac{m}{(x+m)^2}$$

if $m = b/a$.

$$f(x) = ae^{-ax} + be^{-bx} - (a+b)e^{-(a+b)x} \qquad 0 \leq x < \infty$$

Let X = larger of Y and Z

$$f(x) = ab\left\{\frac{1}{(ax+b)^2} + \frac{1}{(a+bx)^2}\right\} \qquad 0 \leq x \leq 1$$

Let $X = \frac{\text{smaller of Y and Z}}{\text{larger of Y and Z}}$

$$f(x) = ab\left\{\frac{1}{(ax+b)^2} + \frac{1}{(a+bx)^2}\right\} \qquad 1 \leq x < \infty$$

Let $X = \frac{\text{larger of Y and Z}}{\text{smaller of Y and Z}}$

$$f(x) = (a+b)e^{-(a+b)x} + (b+c)e^{-(b+c)x} + (c+a)e^{-(c+a)x} - 2(a+b+c)e^{-(a+b+c)x} \qquad 0 \leq x < \infty$$

Let X = the middle of 3 random variables with the p.d.f.'s ae^{-ay}, be^{-bz}, and ce^{-cw}, respectively.

16. $$f(x) = \begin{cases} \frac{1}{a}(1 - e^{-bx}) & 0 \leq x \leq a \\ \frac{1}{a}(e^{-b(x-a)} - e^{-bx}) & a \leq x < \infty \end{cases}$$

Let Y have the p.d.f. $1/a$, $0 \leq x \leq a$, and Z the p.d.f. be^{-bz}.

Let $X = Y + Z$.

Then

$$f(x) = \int_0^x \frac{1}{a} be^{-bz}dz$$

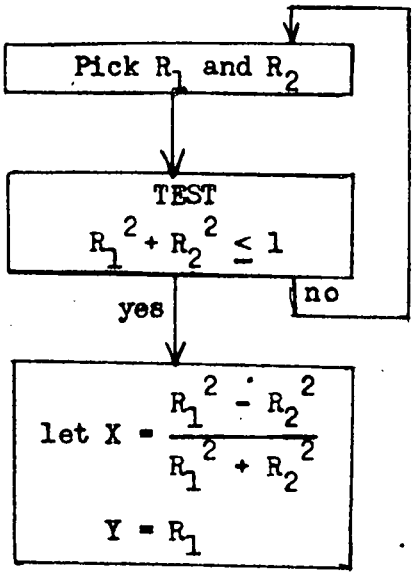
$$= \frac{1}{a}(1 - e^{-bx}) \qquad 0 \leq x \leq a$$

$$= \int_{x-a}^x \frac{1}{a} be^{-bz}dz$$

$$= \frac{1}{a}(e^{-b(x-a)} - e^{-bx}) \qquad a \leq x < \infty$$

17. $f(x) = \frac{1}{\pi\sqrt{1-x^2}} \qquad -1 \leq x \leq 1$

It is often useful to pick values from the random variable $X = \cos \pi R$, of which this is the p.d.f. The following technique is due to von Neumann.



The accepted R_1 and R_2 can be used to define a point $(x = R_1, y = R_2)$ in the first quadrant. These points have a uniform distribution in the 1/4 circle $0 \leq x \leq 1$, $0 \leq y \leq 1 - x^2$. Therefore the angle defined by $\eta = \tan^{-1} \frac{y}{x}$ has a uniform distribution between 0 and $\pi/2$. Since twice this angle is uniformly distributed between 0 and π, taking $X = \cos 2\eta$ will produce the desired p.d.f.

$$\cos 2\eta = \cos^2\eta - \sin^2\eta$$

$$\cos \eta = \frac{R_1}{\sqrt{R_1^2 + R_2^2}}$$

$$\sin \eta = \frac{R_2}{\sqrt{R_1^2 + R_2^2}}$$

So $$\cos 2\eta = \frac{R_1^2 - R_2^2}{R_1^2 + R_2^2}$$

The p.d.f. for Y is also of interest.

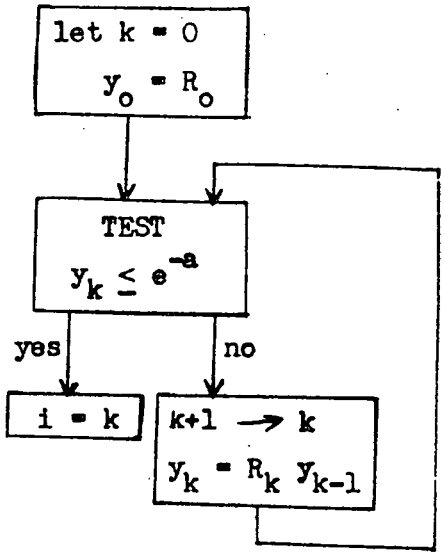
E . g(y) = (probability of y) (probability that $R_2 \leq \sqrt{1-y^2}$)

$$= \sqrt{1-y^2}$$

$$g(y) = \frac{4}{\pi}\sqrt{1-y^2}$$

and $E = \frac{\pi}{4}$.

18. $f(i) = \frac{a^i e^{-a}}{i!}$ for $0 < a$ $i = 0, 1, 2, \ldots$ (Poisson distribution)



Because $R_k < 1$, y_k is a monotonically decreasing function of k. Therefore the probability that y_k fails the test $y_k \leq e^{-a}$ is equal to the probability that a random variable

$$X_k = \prod_{j=0}^{k} R_j$$

is greater than e^{-a}. It was shown in example 14 that this probability is

$$1 - F(e^{-a}) = 1 - e^{-a} \sum_{j=0}^{k} \frac{a^j}{j!}$$

Since this probability decreases by an amount $\frac{a^k}{k!} e^{-a}$ after every test, the probability that i = k is just $\frac{a^k}{k!} e^{-a}$.

The average number of R_k used in each choice is a + 1.

19. The following joint p.d.f.'s will be obtained:

$$\frac{x^i}{(i-1)!}, \quad \frac{1-y^i}{i!}, \quad \frac{(1-z)^{i-1}}{(i-1)!} - \frac{(1-z)^i}{i!} \qquad 0 \le \left\{\begin{matrix} x \\ y \\ z \end{matrix}\right\} \le 1 \qquad i = 1, 2, \ldots$$

The following p.d.f. for i alone:

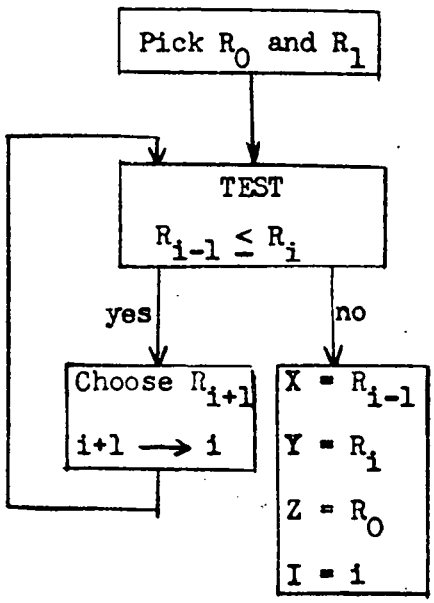
$$\frac{1}{i!} - \frac{1}{(i+1)!} \qquad i = 1, 2, \ldots$$

Also the following p.d.f.'s: xe^x, $e - e^y$,

$$\frac{e}{e-1} x \cosh x, \quad \frac{e}{e-1} (\sinh 1 - \sinh y), \quad \frac{1}{e-1} e^z, \qquad 0 \le \left\{\begin{matrix} x \\ y \\ z \end{matrix}\right\} \le 1$$

$$ex \sinh x, \quad e(\cosh 1 - \cosh y)$$

Start with R_0 and R_1 and iterate as follows.
If $R_{i-1} \le R_i$, increase the i index by one and test again. As soon as the inequality fails, take $X = R_{i-1}$, $Y = R_i$, $Z = R_0$, and $I = i$. Schematically,



Let the probability of making at least i tests be P_i. Then $P_{i+1} = P_i$. (probability that $R_{i-1} \leq R_i$). Since R_{i-1} is the largest of i random numbers, it has the p.d.f. iR_{i-1}^{i-1}. Therefore the probability that $R_{i-1} < R_i$ is R_i^i. The probability of the test succeeding is:

$$\int_0^1 R_i^i \, dR_i = \frac{1}{i+1}$$

So $$P_{i+1} = \frac{P_i}{i+1}$$

But $P_1 = 1$.

Then $$P_i = \frac{1}{i!}$$

The joint p.d.f. for I and X is product of the probability of making i tests $(1/i!)$ and the probability of getting a given x on the i^{th} test (ix^{i-1}) and the probability of then failing this i^{th} test (x); so

$$f(x,i) = \frac{x^i}{(i-1)!}$$

The joint p.d.f.'s for I and Y, and I and Z are similarly obtained by:

$$g(y,i) = \frac{1-y^i}{i!}$$

$$h(z,i) = \frac{i(1-z)^{i-1}}{i!} - \frac{(i+1)(1-z)^i}{(i+1)!}$$

$$= \frac{(1-z)^{i-1}}{(i-1)!} - \frac{(1-z)^i}{i!}$$

The marginal p.d.f. for i can be obtained by integrating any of the above. For example:

$$P_i = \int_0^1 \frac{x^i}{(i-1)!}\,dx$$

$$= \frac{1}{(i+1)} \cdot \frac{1}{(i-1)!}$$

$$= \frac{1}{i!} - \frac{1}{(i+1)!}$$

The marginal p.d.f.'s for X, Y, and Z can be obtained by summing the respective joint p.d.f.'s over i; so

$$f(x) = \sum_{i=1}^{\infty} \frac{x^i}{(i-1)!}$$

$$= xe^x \qquad 0 \le x \le 1$$

$$g(y) = \sum_{i=1}^{\infty} \frac{1-y^i}{i!}$$

$$= e - e^y \qquad 0 \le y \le 1$$

$$h(z) = \sum_{i=1}^{\infty} \left[\frac{(1-z)^{i-1}}{(i-1)!} - \frac{(1-z)^i}{i!}\right]$$

$$= 1 \qquad 0 \le z \le 1$$

By accepting x, y, or z only when i is odd the following p.d.f.'s are obtained:

$$E \cdot f(x) = x \sum_{0}^{\infty} \frac{x^{2i}}{(2i)!}$$

$$= x \cosh x \qquad 0 \leq x \leq 1$$

and $$E = \int_{0}^{1} x \cosh x \, dx$$

$$= 1 - e^{-1}$$

$$E \cdot g(y) = \sum_{0}^{\infty} \frac{(1-y^{2i+1})}{(2i+1)!}$$

$$= \sinh 1 - \sinh y \qquad 0 \leq y \leq 1$$

$$E = \int_{0}^{1} (\sinh 1 - \sinh y)dy$$

$$= \sinh 1 + 1 - \cosh 1$$

$$= 1 - e^{-1} \qquad \text{as before}$$

$$E \cdot h(z) = \sum_{0}^{\infty} \frac{(1-z)^{2i}}{2i!} - \sum_{0}^{\infty} \frac{(1-z)^{2i+1}}{(2i+1)!}$$

$$= \sum_{0}^{\infty} (-1)^{i} \frac{(1-z)^{i}}{i!}$$

$$= e^{-1} e^{z} \qquad 0 \leq z \leq 1$$

$$E = e^{-1}$$

By accepting only even i's one obtains:

$$E \cdot f(x) = x \sum_{0}^{\infty} \frac{x^{2i+1}}{2i+1}$$

$$= x \sinh x \qquad 0 \leq x \leq 1$$

$$E = \int_{0}^{1} x \sinh x$$

$$= e^{-1}$$

$$E \cdot g(y) = \sum_{1}^{\infty} \frac{1 - y^{2i}}{(2i)!}$$

$$= \sum_{0}^{\infty} \frac{1 - y^{2i}}{(2i)!}$$

$$= \cosh 1 - \cosh y \qquad 0 \leq y \leq 1$$

$$E = 1/e$$

$$E \cdot h(z) = \sum_{0}^{\infty} \frac{(1-z)^{2i+1}}{(2i+1)!} - \sum_{1}^{\infty} \frac{(1-z)^{2i}}{(2i)!}$$

$$= 1 - \sum_{0}^{\infty} \frac{(-1)^{i} (1-z)^{i}}{i!}$$

$$= 1 - e^{-1} e^{z} \qquad 0 \leq z \leq 1$$

$$E = 1/e$$

If the test $R_{i-1} \leq R_i$ is replaced by the test $R_{i-1} \geq R_i$, then it is easy to see that the only change in the result is to replace x by 1-x, y by 1-y, and z by 1-z, and the following p.d.f.'s obtained:

$$\frac{(1-x)^i}{(i-1)!}, \qquad \frac{1-(1-y)^i}{i!}, \qquad \frac{z^{i-1}}{(i-1)!} - \frac{z^i}{i!}$$

$$e(1-x)e^{-x}, \qquad e(1-e^{-y})$$

$$\frac{e}{1-e}(1-x)\cosh(1-x), \qquad \frac{e}{e-1}\left[\sinh 1 - \sinh(1-y)\right], \qquad \frac{e}{e-1}e^{-z}$$

$$e(1-x)\sinh(1-x), \qquad e\left[\cosh 1 - \cosh(1-y)\right]$$

20. The rejection technique illustrated in the last example was suggested by John von Neumann [1]. He also pointed out that the technique for picking out of

$$h(z) = \frac{e}{e-1}e^{-z} \qquad 0 \leq z \leq 1$$

with an efficiency of $\frac{e-1}{e}$ could be used to pick out of

$$f(x) = e^{-x} \qquad 0 \leq x < \infty$$

by simply taking $x = z + j$ where j is the number of times the test has failed. The probability that a trial will be rejected is e^{-1} and since

$$e^{-x}dx = e^{-1}\,e^{-x+1}dx$$

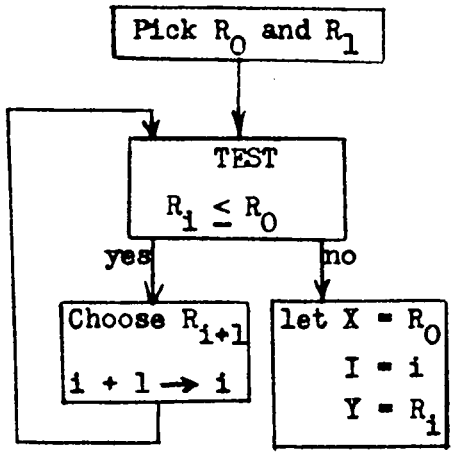
we are choosing from succeeding intervals with exactly the right probability.

The expected number of R_j in a single trial is $1 + e$, so the number of R_j for each x selected is about

$$(1 + e)\,\frac{e}{e-1} \approx 6$$

21.	$x^{i-1} - x^i$, $\quad \frac{1}{I}\, y^i$	$0 \le \left\{\begin{matrix} x \\ y \end{matrix}\right\} \le 1$ $i = 1, 2, \ldots$
	$\frac{1}{i(i+1)}$	$i = 1, 2, \ldots$
	$-\ln(1-y)$	$0 \le y \le 1$
	$1.443\,\frac{1}{1+x}$, $\quad .721 \ln \frac{1+y}{1-y}$	$0 \le \left\{\begin{matrix} x \\ y \end{matrix}\right\} \le 1$
	$3.259\,\frac{x}{1+x}$, $\quad -1.629 \ln(1-y^2)$	$0 \le \left\{\begin{matrix} x \\ y \end{matrix}\right\} \le 1$

Start with an R_0 and R_1 and iterate as follows. If $R_i \le R_0$, increase the index by one and test again. As soon as the inequality fails, take $X = R_0$, $I = i$, and $Y = R_i$. Schematically:



The joint p.d.f. for X and I is

$$f(x,i) = x^{i-1}(1 - x)$$

The probability of getting a given x times the probability of passing the first i - 1 tests times the probability of failing the $i^{\underline{th}}$ test. The marginal p.d.f. of x has not been changed by the processing and is still uniform.

The marginal p.d.f. for i is

$$\int_0^1 (x^{i-1} - x^i)dx = \frac{1}{i} - \frac{1}{i+1} = \frac{1}{i(i+1)}$$

Since the joint p.d.f. for R_0 and I at the $i^{\underline{th}}$ test is $R_0{}^{i-1}$, the probability of making the $i^{\underline{th}}$ test is

$$\int_0^1 R_0{}^{i-1}dR_0 = \frac{1}{i}$$

The joint p.d.f. for Y and I is given by (prob. of making $i^{\underline{th}}$ test) . (prob. of getting a given y) . (prob. that $R_0 < y$).

$$= \frac{1}{i} \cdot 1 \cdot y^i = \frac{y^i}{i}$$

The marginal p.d.f. of Y is

$$g(y) = \sum_1^\infty \frac{y^i}{i}$$

$$= \sum_1^\infty \int_0^y t^{i-1}dt$$

$$= \int_0^y dt \sum_1^\infty t^{i-1}$$

$$= \int_0^y \frac{dt}{1-t}$$

$$= -\ln(1-y)$$

If only the odd i are accepted,

$$E \cdot f(x) = \sum_0^\infty x^{2i} - \sum_0^\infty x^{2i+1}$$

$$= \sum_0^\infty (-1)^i x^i$$

$$= \frac{1}{1+x} \qquad 0 \le x \le 1$$

$$E = \ln 2$$

$$E \cdot g(y) = \sum_0^\infty \frac{y^{2i+1}}{2i+1}$$

$$= \sum_0^\infty \int_0^y t^{2i} dt$$

$$= \int_0^y \sum_0^\infty t^{2i} dt$$

$$= \int_0^y \frac{1}{1-t^2} dt$$

$$= \frac{1}{2} \ln \frac{1+y}{1-y} \qquad 0 \le y \le 1$$

$$E = \ln 2$$

If only the even i are accepted,

$$E \cdot f(x) = \sum_{0}^{\infty} x^{2i+1} - \sum_{1}^{\infty} x^{2i}$$

$$= 1 + \sum_{0}^{\infty} (-1)^{i+1} x^{i}$$

$$= \frac{x}{1+x} \qquad 0 \le x \le 1$$

$$E = 1 - \ln 2$$

$$E \cdot g(y) = \sum_{1}^{\infty} \frac{y^{2i}}{2\,1}$$

$$= \sum_{1}^{\infty} \int_{0}^{y} t^{2i-1} dt$$

$$= \int_{0}^{y} \sum_{1}^{\infty} t^{2i-1} dt$$

$$= \int_{0}^{y} \frac{t}{1-t^2} dt$$

$$= -\frac{1}{2} \ln(1-y^2) \qquad 0 \le y \le 1$$

If the inequality is changed to $R_i \ge R_0$, the p.d.f.'s become:

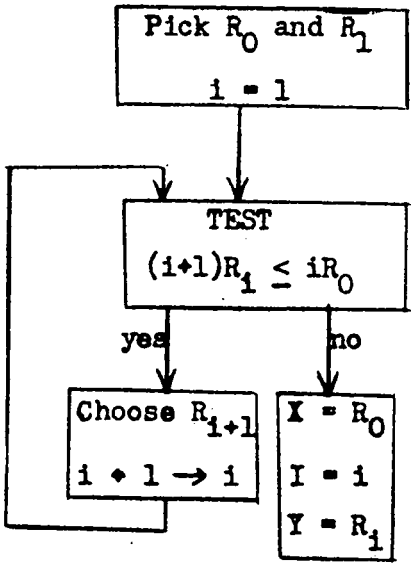
$x(1-x)^{i-1}$,	$\frac{1}{1}(1-y)^{i}$	$0 \le \left\{\begin{matrix} x \\ y \end{matrix}\right\} \le 1$
		$i = 1, 2, \ldots$
$-\ln y$		
$1.443 \frac{1}{2-x}$,	$.721 \ln (\frac{2}{y} - 1)$	
$3.259 \frac{1-x}{2-x}$,	$-1.629 \ln y(2-y)$	

22. $1.216\,\frac{1}{x}\ln(1+x)$, $\quad 5.634\left[1-\frac{1}{x}\ln(1+x)\right]$ $\quad 0 \le x \le 1$

Number 21 can be modified slightly by making the comparison

$$R_i \le \frac{i}{i+1} R_0$$

Schematically:



Given R_0, the probability of passing $i-1$ tests is $\frac{R_0^{i-1}}{i}$. Since R_0 is initially uniformly distributed this is just the joint p.d.f. of R_0 and i entering the i^{th} test. The probability of failing the i^{th} test is $1 - \frac{i}{i+1} R_0$ so

$$f(x,i) = \frac{x^{i-1}}{i}\left(1 - \frac{i}{i+1}x\right)$$

$$= \frac{x^{i-1}}{i} - \frac{x^i}{i+1}$$

The marginal p.d.f. for X is uniform.

The p.d.f. for I is

$$\int_0^1 f(x,i)dx = \frac{1}{i^2} - \frac{1}{(i+1)^2} = \frac{2i+1}{i^2(i+1)^2}$$

The joint p.d.f. for Y and I is

$$g(y,i) = \begin{cases} \frac{1}{i^2}\frac{(i+1)^i}{i^i}y^i & \text{for } y \le \frac{i}{i+1} \\ \frac{1}{i^2} & \frac{i}{i+1} \le y \end{cases}$$

The marginal p.d.f. for Y seems too difficult to bother with.

If only the odd values of i are accepted:

$$E \cdot f(x) = \sum_0^\infty \frac{(-1)^i x^i}{i+1}$$

$$= \frac{1}{x}\sum_0^\infty (-1)^i \int_0^x t^i dt$$

$$= \frac{1}{x}\int_0^x dx \sum_0^\infty (-1)^i t^i$$

$$= \frac{1}{x}\int_0^x \frac{dt}{1+t}$$

$$= \frac{\ln(1+x)}{x}$$

$$E = \int_0^1 \frac{\ln(1+x)}{x}\,dx$$

$$\approx .8225$$

If only the even values are accepted:

$$E \cdot f(x) = 1 - \frac{\ln(1+x)}{x}$$

$$E \approx .1775$$

22. Picking from the Klein-Nishina Scattering Formula

It can be shown that if a γ ray of energy α (in mc^2) is traveling in a cloud of free electrons, then it has a probability $g(x,\alpha)dxdl$ of having a collision in the distance dl and emerging from this collision with an energy α' such that

$$\frac{\alpha}{x} \leq \alpha' \leq \frac{\alpha}{x} + \frac{\alpha}{x^2}\, dx$$

$$g(x,\alpha)dx = \begin{cases} \dfrac{n\pi a_0^{\,2}}{\alpha}\left(\cos^2\theta - 1 + x + \dfrac{1}{x}\right)\dfrac{dx}{x^2} & 1 \leq x \leq 1 + 2\alpha \\ 0 & x \leq 1,\ 1 + 2\alpha \leq x \end{cases}$$

where $\cos\theta = 1/\alpha = x/\alpha + 1$ = cosine of angle of scattering.

a_0 = classical radius of electron

$= 2.81833 \times 10^{-13}$ cm

$\pi a_0^2 = .249536 \times 10^{-24}$ cm^2

n = number of electrons per cc

$\alpha' = x\alpha$ = energy of γ ray after collision.

If $\sigma(\alpha) = \int_1^{1+2\alpha} g(\alpha,x)dx$ then $\frac{\sigma(\alpha)}{n}$ is the so-called Compton scattering cross section and is tabulated in R-170 [2], Tables 5 and 6. The probability that the γ ray will have any kind of scattering collision in the distance dl is then $\sigma(\alpha)dl$. $g(\alpha,x)$ can now be written in the form:

$$g(\alpha,x) = n\sigma(\alpha)f(\alpha,x)$$

where $$f(\alpha,x) = \frac{1}{x^2}(\cos^2\theta - 1 + x + \frac{1}{x})/K(\alpha)$$

and $$K(\alpha) = \int_1^{1+2\alpha} (\cos^2\theta - 1 + x + \frac{1}{x})\frac{dx}{x^2}$$

$f(\alpha,x)$ is then the p.d.f. for the energy ratio x of a γ ray which enters collison with energy α. The normalizing factor, $K(\alpha)$, is shown in Graph 4.

Graphs and Tables of the equation

$$R = \int_1^x f(\alpha,x)dx$$

can also be found in R-170.[1]

Empirical fits to these functions could be made, but it is undesirable to have to fit a two variable function unless absolutely necessary.

Several exact methods for picking out of the Klein Nishina p.d.f. will now be discussed. This is partly pedagogy and partly because the method used may depend on the particular section being picked from or the available machine.

---

1 Actually cos θ and $1/\alpha'$ as a function of R and α are tabulated, not x.

First, techniques in which x is drawn from a p.d.f. m(x) and then accepted if R is $\leq T(x)$ will be considered. This implies that $E \cdot f(\alpha,x) = m(x)T(x)$.

a. Let $m(x) = \frac{1}{2\alpha}$ $\qquad 1 \leq x \leq 1 + 2\alpha.$

$$T(x) = \frac{1}{x^2}\left(\cos^2\theta - 1 + x + \frac{1}{x}\right)$$

It is clear that the expression to the right of the proportion sign is ≤ 2, since $\frac{(\cos^2\theta - 1)}{x^2} \leq 0$ and $\frac{1}{x^2}(x + \frac{1}{x}) \leq 2$ in the region $1 \leq x \leq 1 + 2\alpha$.

So if

$$T(x) = \frac{1}{2x^2}\left(\cos^2\theta - 1 + x + \frac{1}{x}\right)$$

the inequality $0 \leq T(x) \leq 1$ is satisfied. The efficiency is

$$E_a = \frac{m(x)T(x)}{f(x)}$$

$$= \frac{K(\alpha)}{4\alpha}$$

b.[1] Let $m(x) = \frac{1}{x\ln(1+2\alpha)}$ $\qquad 1 \leq x \leq 1 + 2\alpha$

$$T(x) = \frac{1}{2x}\left(\cos^2\theta - 1 + x + \frac{1}{x}\right)$$

$$E_b = \frac{K(\alpha)}{2\ln(1+2\alpha)}$$

---

1 See example 11 for technique of picking out of $1/x\ln(1+2\alpha)$

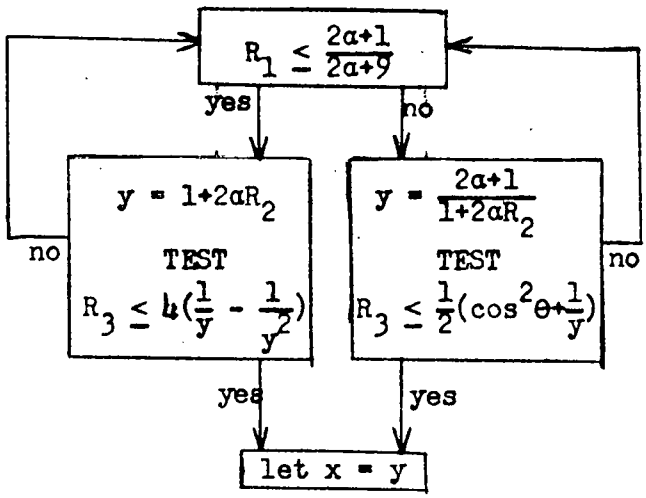
c. Let $m(x) = \frac{1+2\alpha}{a\alpha}\ \frac{1}{x^2}$ $\qquad 1 \le x \le 1 + 2\alpha$

$$T(x) = (\cos^2\theta - 1 + x + \frac{1}{x})/(1 + 2\alpha + \frac{1}{1+2\alpha})$$

$$E_c = \frac{(1+2\alpha)^2\ K(\alpha)}{(2\alpha)\left[1 + (1+2\alpha)^2\right]}$$

That $0 \le T(x) \le 1$ can be verified by noting that $x + \frac{1}{x}$ is a monotonically increasing function in the region $1 \le x$ and that $\cos^2\theta - 1$ has a maximum value of 0. Therefore the function $(\cos^2\theta - 1 + x + \frac{1}{x}) \le x + \frac{1}{x} \le 1 + 2\alpha + \frac{1}{1+2\alpha}$ if $1 \le x \le 1 + 2\alpha$.

d. It is also possible to break up $f(x,\alpha)$ into the sum of two p.d.f.'s; for example:



As always.

$$E_d \cdot f(x) = \frac{2\alpha+1}{2\alpha+9}\ \frac{1}{2\alpha}\ 4(\frac{1}{x} - \frac{1}{x^2}) + \frac{8}{2\alpha+9} \cdot \frac{2\alpha+1}{2\alpha x^2}\ \frac{1}{2}(\cos^2\theta + \frac{1}{x})$$

$$= \frac{2\alpha+1}{2\alpha+9} \cdot \frac{2}{\alpha}\ (\frac{1}{x} - \frac{1}{x^2} + \frac{1}{x^3} + \frac{\cos^2\theta}{x^2})$$

$$E_d = \frac{(2\alpha+1)}{(2\alpha+9)}\ \frac{2K(\alpha)}{\alpha}$$

The efficiencies E_a through E_d are shown in graph number 5.

23. Pick from elastic n-d scattering

See Figure 2 (p. 67) for schematic which gives the simplest rejection technique for picking an angle of scatter out of the n-d elastic scattering cross section. It has been obtained by careful fitting to the best theoretical and experimental data [3] available. The efficiency of the technique is of course a function of α and is $\frac{1}{2M(\alpha)}$. This is shown in graph number 6.

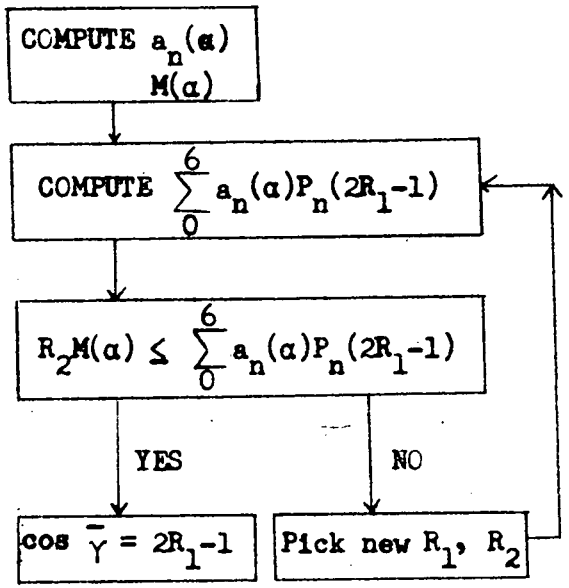
The angle of scatter γ in the lab system and the new energy α' are obtained as follows:

$$\alpha' = \frac{\alpha}{3}\sqrt{5 + 4\cos\bar{\gamma}}$$

$$\cos\gamma = \frac{1 + 2\cos\bar{\gamma}}{\sqrt{5 + 4\cos\bar{\gamma}}}$$

24. Approximate inelastic n-d scattering

The energy spectrum of inelastically scattered neutrons is not very well known. A reasonable approximation is to subtract the binding energy of the deuteron from the incident neutron and then assume that the two neutrons and proton coming off share the remaining energy, each particle having a uniform energy from 0 to the maximum available. Let α, $\bar{\alpha}$, $\bar{\alpha}'$, α' be the square root of the incident energy in lab, incident energy in C. of M., final energy in C. of M., and final energy in lab, respectively.



NOTE:

$a_0 = 1/2$

$$a_n(\alpha) = \sum_{i=0}^{5} C_i^n \alpha^i$$

$$M(\alpha) = .49912762 + .19661182\alpha + .36139778\alpha^2 - .21189016\alpha^3 + .039941747\alpha^4 - .0018623547\alpha^5$$

$P_0(x) = 1$

$P_1(x) = x$

$$P_n(x) = \frac{1}{n}\left[(2n-1)xP_{n-1} - (n-1)P_{n-2}\right]$$

TABLE OF C_i^n

n \ i	0	1	2	3	4	5	RANGE OF α		RANGE OF α
1	0.10897	-0.60059	0.25289	0.1441	-0.078966	0.0095411	$.2 < \alpha \leq \sqrt{14}$	$a_1 = 0$;	$0 \leq \alpha \leq .2$
2	0.049252	-0.44156	1.10016	-0.6494	0.15812	-0.01394	$.3 < \alpha \leq \sqrt{14}$	$a_2 = 0$;	$0 \leq \alpha \leq .3$
3	-0.15639	0.60643	-0.68341	0.26465	-0.047307	0.003672	$.9 < \alpha \leq \sqrt{14}$	$a_3 = 0$;	$0 \leq \alpha \leq .9$
4	0.02342	-0.071859	0.035517	0.025435	-0.010014	0.0008593	$.9 < \alpha \leq \sqrt{14}$	$a_4 = 0$;	$0 \leq \alpha \leq .9$
5	1.50914	-3.56725	3.29214	-1.45866	0.3021	-0.023347	$1.395 < \alpha \leq \sqrt{14}$	$a_5 = 0$;	$0 \leq \alpha \leq 1.395$
6	-0.07806	0.37108	-0.54035	0.32282	-0.079385	0.006843	$1.395 < \alpha \leq \sqrt{14}$	$a_6 = 0$;	$0 \leq \alpha \leq 1.395$

$\alpha = \sqrt{\text{Energy in MEV}}$

Figure 2

To pick the new energy of the first neutron

$$\bar{a} = \frac{2}{3} a$$

$$\bar{a}'^2 = R_1(\bar{a}^2 - 2.18) \qquad 2.18 = \text{binding energy of deuteron}$$

$$\cos \bar{\gamma} = 2R_2 - 1 \qquad \text{assumes scattering is isotropic in C. of M.}$$

$$a' = \sqrt{\frac{a^2}{9} + \bar{a}'^2 + \frac{2a\,\bar{a}'}{3} \cos \bar{\gamma}}$$

$$\cos \gamma = \frac{a/3 + \bar{a}' \cos \bar{\gamma}}{a'}$$

The energy of the second neutron can now be picked from the energy that is left by the first neutron. For the purpose of calculating expected values this is not necessary--the first neutron can be given a weight of 2 and the second neutron ignored--even though this is physical nonsense.

25. Approximate general inelastic scattering

A useful approximation to inelastic scattering of neutrons is to assume that the neutron loses at least a minimum amount of energy δ to the excited nucleus and that its energy is uniformly distributed between 0 and the maximum possible.

If a, $\bar{a}$, $\bar{a}'$, a' are the square roots of the incident energy (lab), incident energy (C. of M.), final energy (C. of M.), and final energy (lab) respectively then:

$$\bar{a} = \frac{A}{A+1} a$$

$$\bar{a}'^2 = R_1(\bar{a}^2 - \delta)$$

where A is the atomic weight.

The angle of scattering ($\bar{\gamma}$) in the C. of M. is to be picked out of its distribution. For want of better information this is usually taken as isotropic.

$$\cos \bar{\gamma} = 2R_2 - 1$$

$$\alpha' = \sqrt{\frac{\alpha^2}{(A+1)^2} + \bar{\alpha}'^2 + \frac{2\alpha \bar{\alpha}'}{A+1} \cos \bar{\gamma}}$$

$$\cos \gamma = \frac{\frac{\alpha}{A+1} + \bar{\alpha}' \cos \bar{\gamma}}{\alpha'}$$

γ, of course, is the angle of scattering in the lab system.

26. Fit to experimental data of n-copper scattering (graph number 7).

Picking from another empirical p.d.f., the angular scattering of 14 MEV neutrons on copper, is now discussed. If x = the cosine of angle of scatter, then this p.d.f. can be represented in the form

$$f(x) = h_i(x) e^{-a_i(1-x)} \qquad x_i \leq x \leq x_{i-1}$$

where the $h_i(x)$ satisfy the inequality

$$0 \leq h_i(x) \leq M_i \qquad \text{when } x_i \leq x \leq x_{i-1}$$

The parameters are as follows:

$x_o = 1$

$x_1 = .98$

$x_2 = .93$

$x_3 = .71$

$x_4 = -.1$ (The scattering for $x < -.1$ is essentially zero.)

$a_1 = a_2 = a_3 = 16.146952$

$a_4 = 4.520990$

$h_1(x) = 6826.237250x^2 - 13411.70412x + 6603.930212$

$h_2(x) = 4.271122975x + 12.19273318$

$h_3(x) = 130921.6031 - 813913.1074x + 2023593.429x^2 - 2513392.773x^3 + 1558716.733x^4 - 385960.6254x^5$

$h_4(x) = 1.05474959 - 1.33330155x + 2.12496606x^2 - 2.63973279x^3 + .72947297x^4 + 2.58277190x^5$

$M_1 = 18.5$

$M_2 = 16.4$

$M_3 = 25.8$

$M_4 = 1.25$

A set of p_i can be defined by the equation

$$p_i = \int_{x_i}^{1} f(x)dx$$

Then $p_i - p_{i-1}$ is the probability that the event $(x_i \leq x \leq x_{i-1})$ occurs.

$P_1 = .29096398$

$p_2 = .69549204$

$p_3 = .95437174$

If now in addition a set of b_i's is defined by

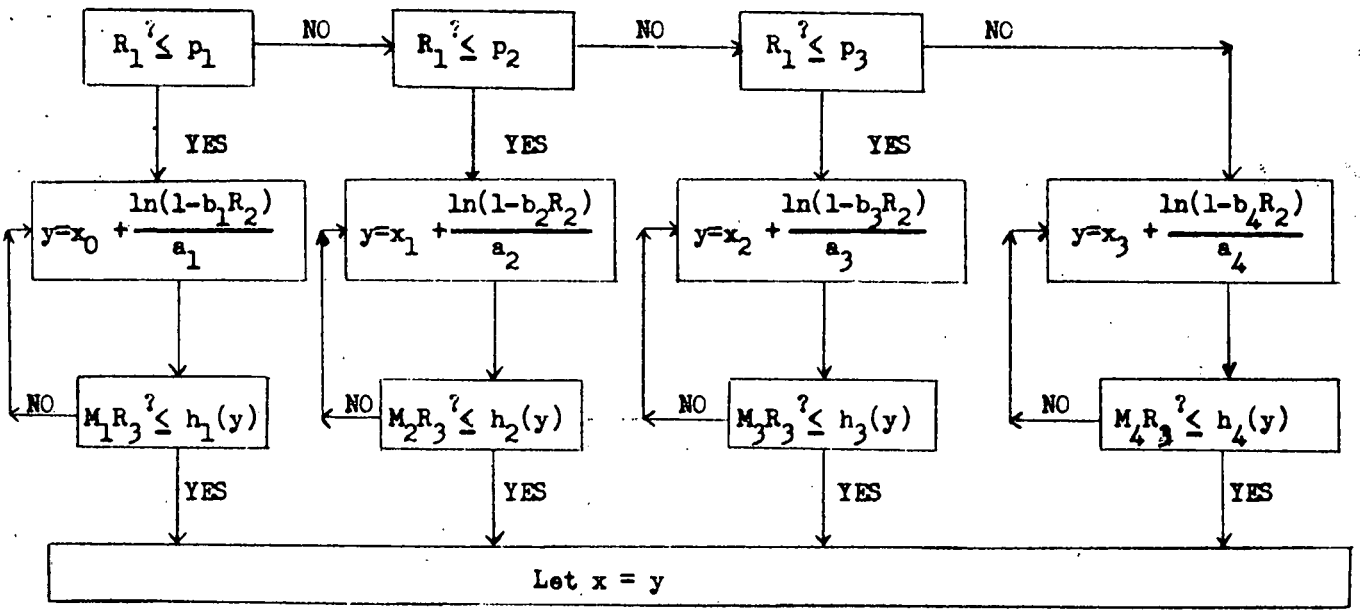
$b_1 = 1-e^{+a_1(x_1-x_0)} = .2759820108$

$b_2 = 1-e^{+a_2(x_2-x_1)} = .5539604260$

$b_3 = 1-e^{+a_3(x_3-x_2)} = .9713421948$

$b_4 = 1-e^{+a_4(x_4-x_3)} = .9743189497$

Then the following schematic indicates how to pick from f(x).



The method can be verified as follows. The probability of going down the i'th branch is $p_i - p_{i-1}$. As R_2 varies from 0 to 1, y varies from x_{i-1} to x_i. The probability of acceptance in any interval is proportional to $h_i(x)e^{-a_i(1-x)}$ and the p_i have been chosen to make everything properly normalized.

REFERENCES

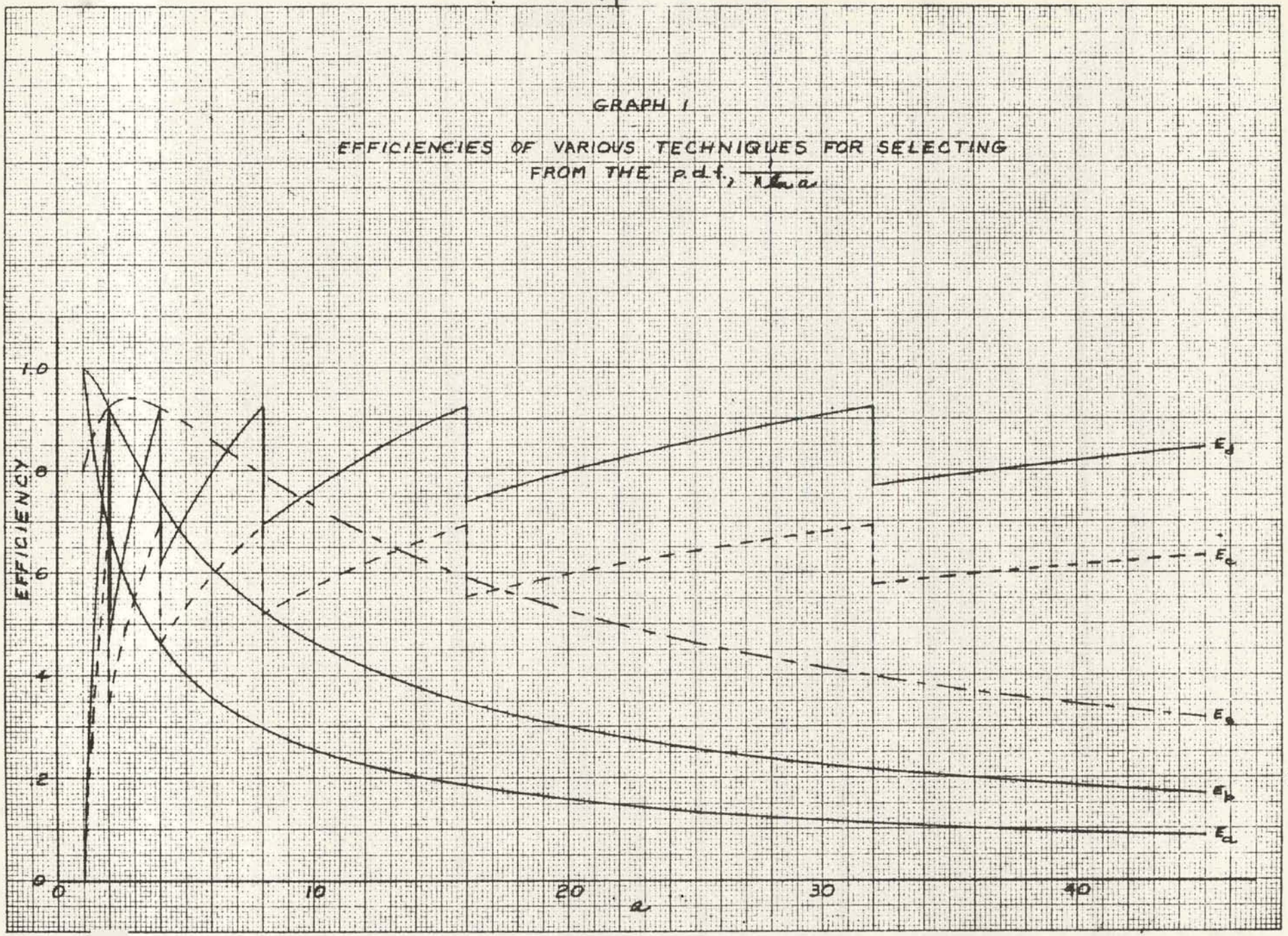
1. Monte Carlo Method, U. S. Department of Commerce, National Bureau of Standards, Applied Mathematics Seminar 12, June 11, 1951.

2. Latter, R., and Kahn, H., RAND Report R-170, Gamma-Ray Absorption Coefficients, September 19, 1949.

3. Zirin, H., RAND Research Memorandum RM-1203-AEC, Polynomial Approximations To Neutron-Deuteron Differential Angular Cross Sections, June 5, 1953.

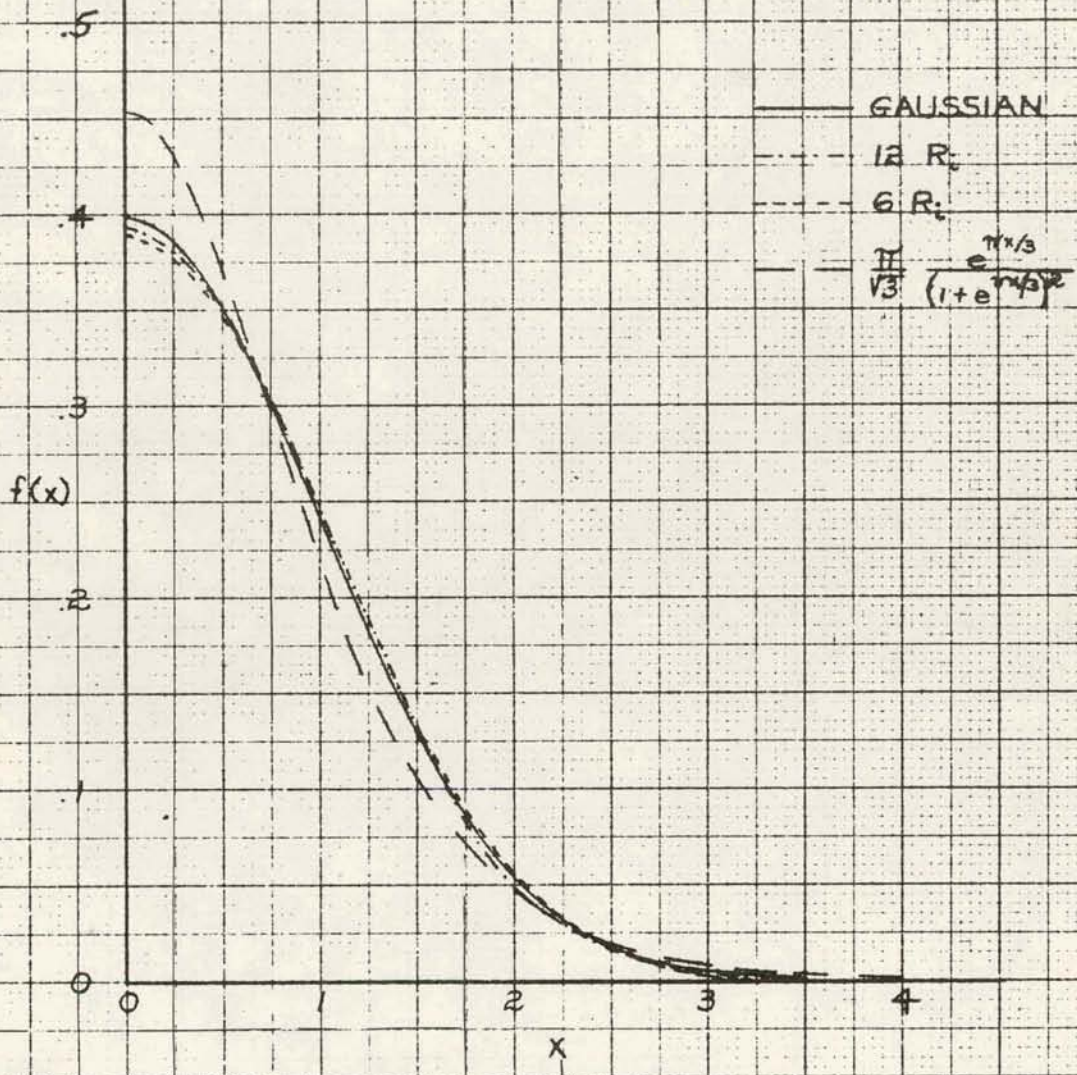
GRAPH 1

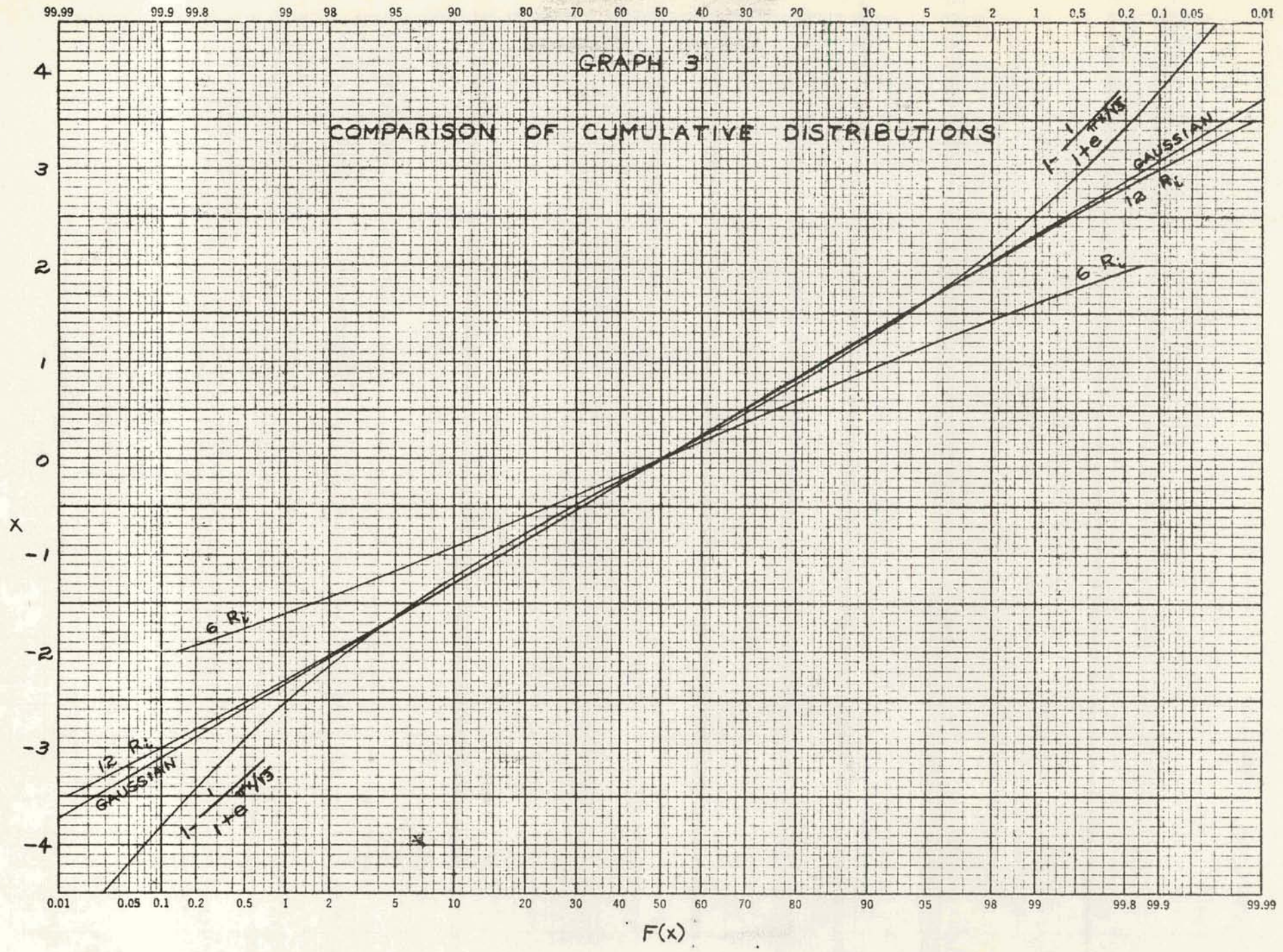
EFFICIENCIES OF VARIOUS TECHNIQUES FOR SELECTING FROM THE p.d.f., $\frac{1}{\pi(1+a^2)}$



GRAPH 2

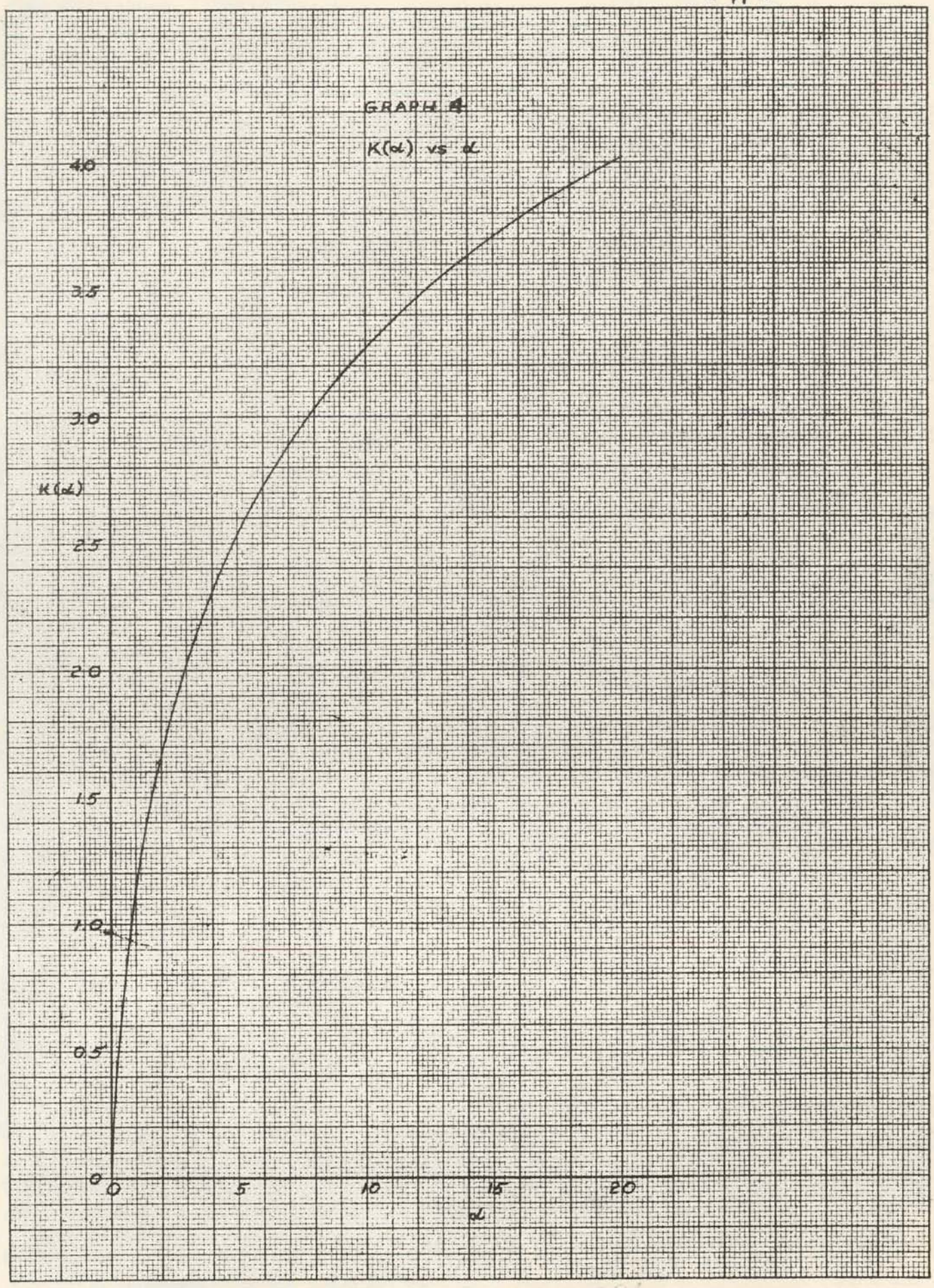
COMPARISON OF APPROXIMATE GAUSSIANS

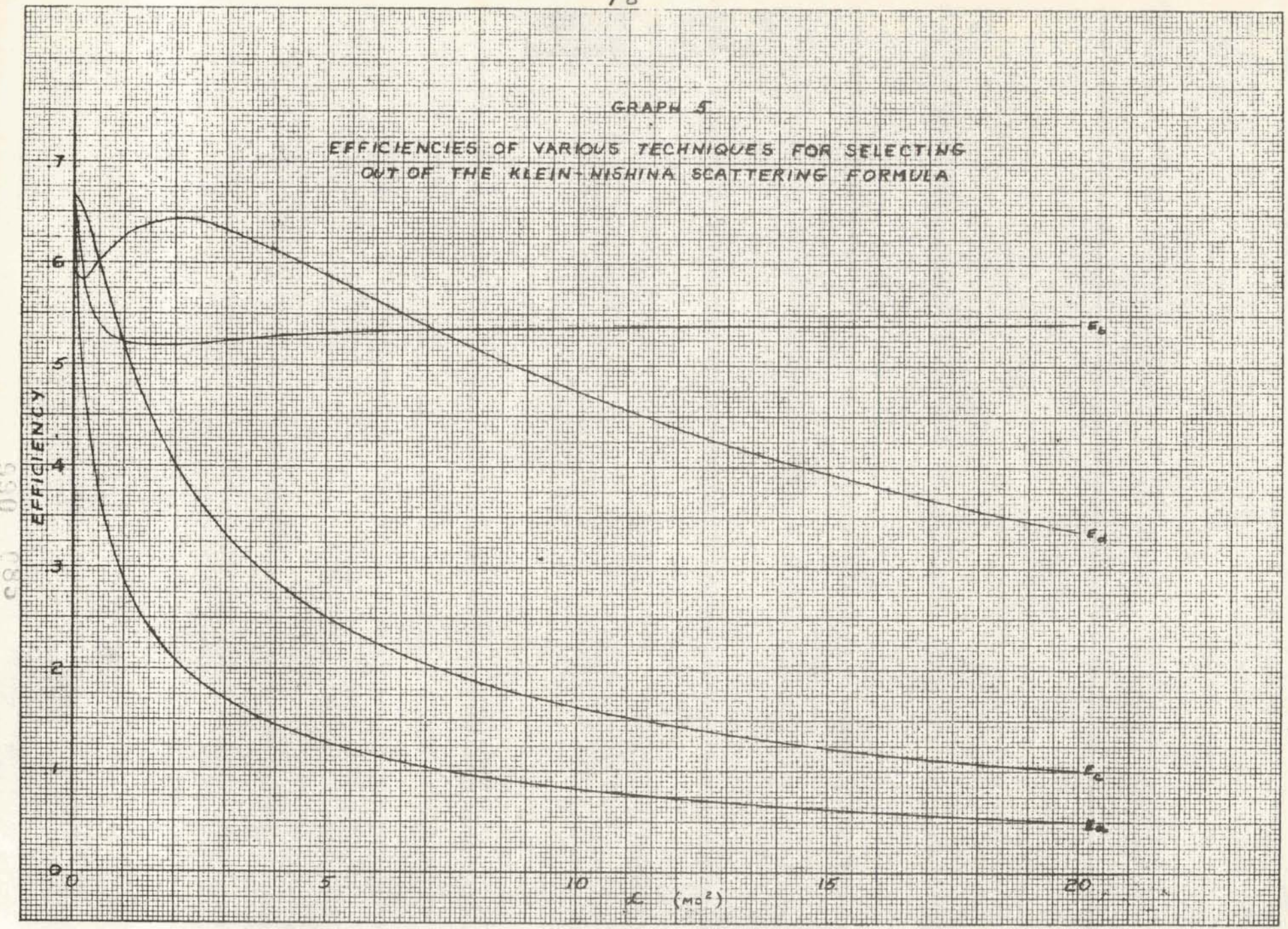



GRAPH 3
COMPARISON OF CUMULATIVE DISTRIBUTIONS
99.99 99.9 99.8 99 98 95 90 80 70 60 50 40 30 20 10 5 2 1 0.5 0.2 0.1 0.05 0.01
4 3 2 1 0 -1 -2 -3 -4
X
0.01 0.05 0.1 0.2 0.5 1 2 5 10 20 30 40 50 60 70 80 90 95 98 99 99.8 99.9 99.99
F(x)
6 Ri
12 Ri
GAUSSIAN
1 - 1/(1+e^(πx/√3))
6 Ri
12 Ri
GAUSSIAN
1 - 1/(1+e^(πx/√3))

GRAPH 4

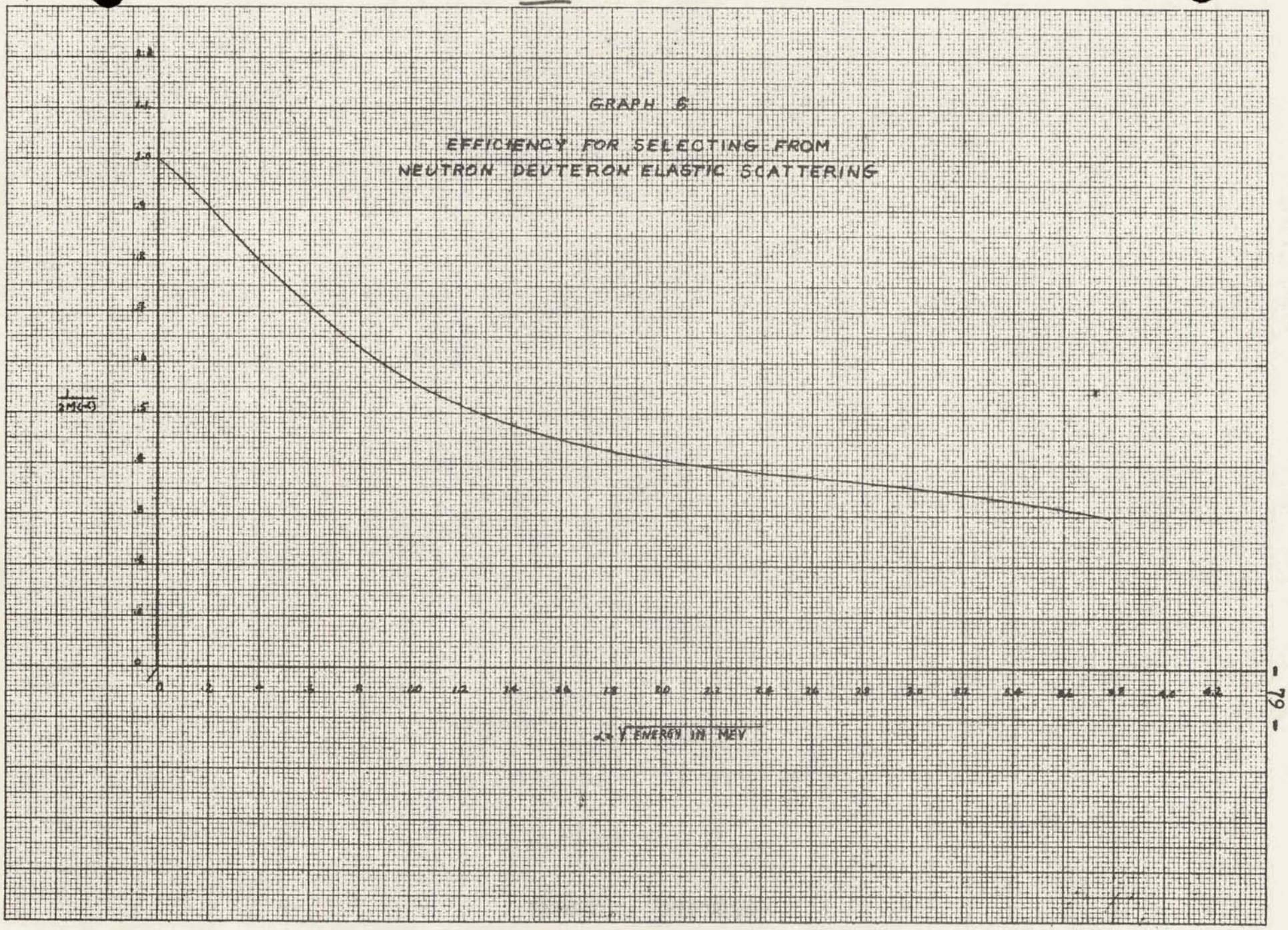
K(α) vs α




GRAPH 5
EFFICIENCIES OF VARIOUS TECHNIQUES FOR SELECTING OUT OF THE KLEIN-NISHINA SCATTERING FORMULA
EFFICIENCY
0
1
2
3
4
5
6
7
0
5
10
15
20
α (m_0c^2)
ε_b
ε_d
ε_c
ε_a

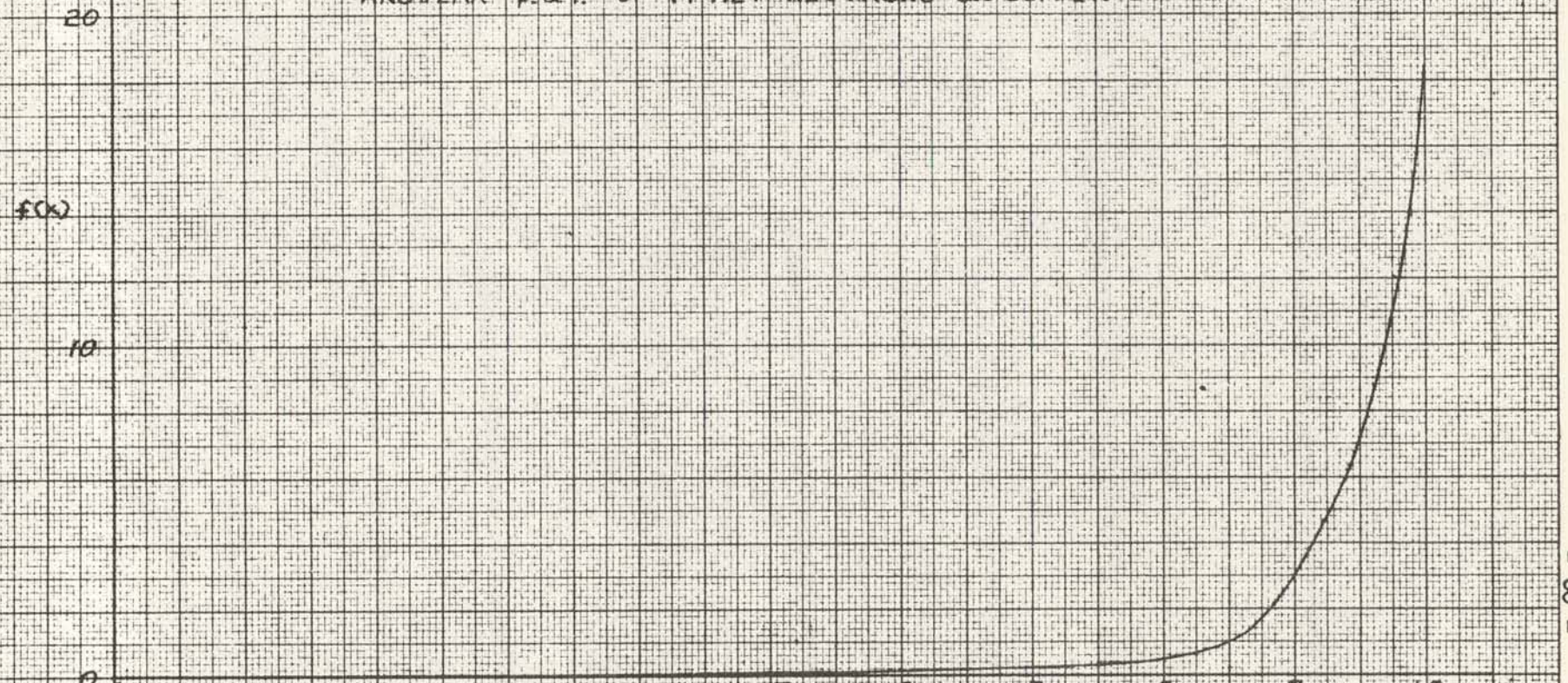
GRAPH 6

EFFICIENCY FOR SELECTING FROM
NEUTRON DEUTERON ELASTIC SCATTERING



GRAPH 17

ANGULAR p.d.f. OF 14 MEV NEUTRONS ON COPPER



PART II

EVALUATING INTEGRALS

PART II

TABLE OF CONTENTS

II. EVALUATING INTEGRALS

1. Introduction

The simplest application of Monte Carlo is the evaluation of integrals. While in actual practice it is rarely efficient to use Monte Carlo unless the integral is rather highly multi-dimensional, this chapter is restricted to one- or two-dimensional integrals. The generalizations to more dimensions, however, are obvious. In fact most of the discussion is unchanged if the variables of integration (x,y) are each considered to represent multidimensional spaces. The rare instances in which this interpretation is not legitimate will be clear from the context.

The application to integration and, in fact, most applications of Monte Carlo depend on the following two theorems which will be stated without proof.

Theorem I (The Strong Law of Large Numbers)[1]

If a sequence of N random variables x_1 to x_N are picked from the p.d.f. f(x) and a random variable $\hat{z}_N$ defined by the equation

$$\hat{z}_N = \frac{1}{N} \sum_{1}^{N} z(x_i) \tag{1}$$

and if the integral

$$\bar{z} = \int_{-\infty}^{\infty} z(x)f(x)dx \tag{2}$$

---

1 See Doob, Stochastic Processes.

exists in the ordinary sense, $\hat{z}_N$ will, almost always, approach $\bar{z}$ as a limit as N approaches ∞.

The integral (2) is called the expected value[1] of the function $z(x)$, and $\hat{z}_N$ is called an estimate of $\bar{z}$. If $\overline{z^2}$, the expected value of $z^2(x)$, also exists, an estimate can be made about the amount that $\hat{z}_N$ deviates from $\bar{z}$ for large N. Denote the variance of $z(x)$ by either σ^2 or V; define it by the equation

$$\begin{aligned}\sigma^2 = V &= \overline{(z - \bar{z})^2} \\ &= \int (z - \bar{z})^2 f(x)dx \\ &= \int z^2 f(x)dx - 2\bar{z}\int zf(x)dx + \bar{z}^2 \int f(x)dx \\ &= \overline{z^2} - 2\bar{z}^2 + \bar{z}^2 \\ &= \overline{z^2} - \bar{z}^2 \end{aligned} \qquad (3)$$

and then apply Theorem II.

Theorem II (The Central Limit Theorem)[2]

For large N the probability that the event $\bar{z} - \delta \leq \hat{z} \leq \bar{z} + \delta$ occurs is asymptotically independent of the exact nature of $z(x)$ or $f(x)$ but depends only on N and σ^2. In fact,

$$\text{Prob.}\left\{\hat{z} \leq \bar{z} + \delta\right\} = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\frac{\delta}{\sigma}\sqrt{N}} e^{-x^2/2}dx + \text{terms of order } \frac{1}{\sqrt{N}} \qquad (4)$$

---

1 Most readers will be familiar with the fact that the "expected value" may be very unexpected. For example in the coin tossing example of Part I the expected value of C was 1/2 though C can take on only the values 0 and 1.

2 Almost any book on statistics discusses this theorem. Cramer, Mathematical Methods of Statistics, is especially full and interesting on this theorem and its variants.

The probability that the deviation of $\hat{z}$ from $\bar{z}$ will exceed $\pm \lambda\sigma\sqrt{N}$ is given in the following abbreviated table of $\sqrt{\frac{2}{\pi}} \int_{\lambda}^{\infty} e^{-x^2/2} dx$:

λ	Probability
.6745	.5000
1.0000	.3173
2.0000	.0455
3.0000	.0027
4.0000	.0001

It can be seen from the above table that deviations greater than $\pm \sigma/\sqrt{N}$ will be frequent, deviations greater than $\pm 2\sigma/\sqrt{N}$ not uncommon, and deviations greater than $\pm 3\sigma/\sqrt{N}$ so uncommon that if the table applies[1] the possibility that this last event may occur can usually be ignored. $\sigma/\sqrt{N}$ is called the standard deviation (s.d.) of the estimate $\hat{z}_N$.

The reason that sampling is useful in evaluating multiple integrals of a high order is that neither of the theorems depend on the dimensionality of the integral. The number of points required to evaluate a multidimensional integral to a fixed level of accuracy depends only on σ, or $\sigma/\bar{z}$ if a fixed percent accuracy is desired, once there are enough so that the Central Limit Theorem is reliable. While it is true that in this perverse world σ or $\sigma/\bar{z}$ seems to increase with the dimensionality, there is no reason in principle why this should be so. By contrast, in almost all standard techniques the number of points required to evaluate an integral go up in geometrical progression

---

1 As discussed in Appendix II, the table is almost consistently optimistic for the p.d.f.'s and N's actually used in practice. In fact, its "sweet bye and bye" form does not always admit too confident an application. It is therefore to be considered as suggestive and not categorical.

with its dimensionality. In part this undoubtedly is due to a defect in the theory of integration in many dimensions,[1] but partially it seems to be unavoidable. This exponential increase almost never occurs if the integration is done by Monte Carlo. The other occasional advantage of Monte Carlo lies in that it may be cheaper to compute points by Monte Carlo than in the standard ways. This shows up most sharply in trying to solve certain Green's function types of problems.[2] On the whole, though, it must be admitted that Monte Carlo has not shown up very well in competition with standard techniques, when the standard techniques were at all reasonable. It has been used most successfully where the standard numerical techniques completely fail. In this sense it is a method of last resort.

The results of Theorem II depend on N being large enough and the variance being known. Of course, it is rare that the variance should be known and $\bar{z}$ unknown. The question "What is large enough?" is discussed in Appendix II.

---

1 One way to calculate $\int \cdots \int z(x_1,\ldots,x_n)dx_1\ldots dx_n$ would be to evaluate z at the M^n points obtained by dividing each x_i space into M intervals and taking the midpoints of these intervals. If instead the function $z(x_1,\ldots,x_n)$ were expanded in the form $\sum_{k=1}^{K} \prod_{i=1}^{n} \phi_{ik}(x_i)$ then the corresponding numerical integration would only require MnK points. Routine methods exist for making such expansions, but if the function $z(x_1,\ldots,x_n)$ is in any way rough, a very large K may be needed to make the expansion accurate enough. In general, in any definite problem special techniques can be used to reduce the number of points to less than M^n but in a large class of problems not enough less to make the classical numerical integration competitive with the number of points required by Monte Carlo (see equation (8)). However, it also seems to be true in the past that Monte Carlo has been most useful in evaluating integrals that have arisen out of probabilistic situations. The author knows of no serious non-probabilistic integrals evaluated by Monte Carlo. It is hard to say whether this is coincidental or symptomatic.

2 J. H. Curtiss, "Comparison of Efficiency of Monte Carlo Methods with that of Classical Methods for Linear Computation Problems," Symposium on Monte Carlo Methods, John Wiley and Sons, 1956.

The variance[1] can be estimated by

$$\hat{V} = \frac{N}{N-1}\left(\hat{z^2} - \hat{z}^2\right) \tag{5}$$

where of course

$$\hat{z^2} = \frac{1}{N}\sum_{1}^{N} z^2(x_i)$$
$$\hat{z} = \frac{1}{N}\sum_{1}^{N} z(x_i) \tag{6}$$

In general, whenever it is desirable to estimate values of formulae in which $\overline{z^2}$ and $\bar{z}$ involved, the expected value can be replaced by $\hat{z^2}$ and $\hat{z}$ respectively. While the estimate will almost always be biased, the amount of the bias is usually proportional to $\frac{1}{N}$ and can be ignored if N is reasonably large.

The estimate of V in equation (5) is often unreliable unless N is very large. If $\hat{V}$ is not known to be reliable, the computer may be able, by exploiting special properties of the problem, to obtain an upper bound for V or $(V-\hat{V})$. In other cases the computer may beable to depend on experience, intuition, or just plain faith for his belief in the accuracy of the answer. This point bears a lot of discussion, some of which can be found in Appendix II.

The estimate in equation (6) is useful if only because it may give negative information. If the estimated $\hat{V}$ is larger than the computer can tolerate, this information, at least is usually reliable and the computer must either increase the number of samples or change the sampling technique.

---

1 While the expected values of $\hat{z^2}$ and $\hat{z}^2$ are $\overline{z^2}$ and $\bar{z}^2$ respectively, the expected value of $(\hat{z^2} - \hat{z}^2)$ is not V but $\frac{N-1}{N}V$. This occurs because the expected value of $\hat{z}^2$ is $\frac{1}{N}\overline{z^2} + (1 - \frac{1}{N})\bar{z}^2$. It is customary to prevent a bias from occurring in the estimate of V by multiplying the intuitive estimate by $\frac{N}{N-1}$. Unfortunately, even if this is done the expected value of $\sqrt{V}$ will not be σ but will also be biased by terms of the order of $\frac{1}{N}$. The bias however, is practically never significant.

2. The Economics of Sampling

The error in the estimate of $\bar{z}$ is measured by $\sigma/\sqrt{N}$. There are two ways to make this error small--to increase N or to change the sampling technique to make σ small. The extent to which each of these alternatives should be used depends on the relative cost of each for the problem to be done. Before going into a description of the sampling techniques available for reducing σ, it is worthwhile to consider briefly how much of the work should be allocated to decrease σ and how much into making N large.

It is assumed, for simplicity, in what follows that the computer is interested in obtaining the greatest accuracy possible at a fixed cost or--what is in this context much the same thing--the minimum cost for a fixed accuracy; the truth will generally lie between these extremes, but either of them affords a basis for the analysis. The desired accuracy is set by requiring that $\sigma/\sqrt{N}$ be equal to a preassigned ε.

The cost of doing a problem can be divided into three parts, the cost of:

a. designing the sampling including the cost of extra analysis if fancy methods are to be used.

b. programming, coding, and code checking.[1] This cost is usually determined by the sampling design. It is listed separately because even though it can be very important, it is often ignored. For small problems it may be the largest part of the cost.

---

1 Programming refers to the details of putting the problem into a form that is suitable for machine computation. Coding refers to the semiclerical job of translating these details into the instructions that the machine will follow and to the recording of these instructions on a medium which the machine can read. Code checking is the perilous job of finding all the mistakes. Anything the computer can do to simplify these time consuming steps may result in a large reduction in the cost of doing the problem.

c. the computing machine on which the problem is done. Except for the time used for code checking and therefore already counted in (b), this cost is usually considered to be proportional to N. Since the proportionality constant will vary with different sampling methods it is also a function of (a).

If the cost of (a) and (b) is denoted by C_1, the cost of (c) by C_2N, and the total cost by C then

$$C = C_1 + C_2(C_1)N \tag{7}$$

C_1 and N are under the control of the computer, but it is usually impossible to predict in advance, even approximately, the form of $\sigma(C_1)$. The analysis from this point on therefore takes on a certain fictional character.

The error is

$$\varepsilon = \frac{\sigma(C_1)}{\sqrt{N}} \tag{8}$$

Solving equation (8) for N and substituting in (7),

$$C = C_1 + \frac{C_2\sigma^2}{\varepsilon^2} \tag{9}$$

$$\frac{dC}{dC_1} = 1 + 2\frac{\sigma C_2}{\varepsilon^2}\frac{d\sigma}{dC_1} + \frac{\sigma^2}{\varepsilon^2}\frac{dC_2}{dC_1} = 0 \tag{10}$$

In most cases $\frac{dC_2}{dC_1}$ can be ignored and (10) becomes

$$\frac{d\sigma}{dC_1} = -\frac{\varepsilon^2}{2\sigma C_2} \tag{11}$$

By solving equation (11) for C_1, the $\sigma(C_1)$ of the sampling plan and therefore the sampling plan itself is determined. N is also determined

since it is equal to σ^2/ε^2. The less said about how sampling plans are chosen in actual practice the better.

The only place in this report where the cost will be brought in explicitly will be in the discussion of the device of Russian Roulette and Splitting where it will be shown that a modification of equation (10) can be used to determine the sampling scheme. Even though it is not mentioned explicitly the computer must always keep costs at least roughly in mind when designing or evaluating sampling schemes.

3. Methods of Sampling

The sampling techniques most often used in Monte Carlo problems are called:

1. Straightforward Sampling
2. Importance Sampling
3. Systematic Sampling
4. Stratified Sampling (Quota Sampling)
5. Use of Expected Values
6. Correlation
7. Russian Roulette and Splitting

In order to introduce and compare the different techniques, a brief discussion of how each one would be used by itself in connection with a typical problem is given in Sections 4 to 10. After the general discussion there is a more detailed explanation of each technique in Sections 13 to 19. It is of course possible, and often advisable, to use two or more of the techniques simultaneously.

The problem that will be used to illustrate the various techniques is to estimate the integral

$$\bar{z} = \iint_A z(x,y)f(x,y)dxdy \qquad (12)$$

where $f(x,y)$ is a p.d.f.[1] The area A over which the integration is done, is divided into J mutually exclusive areas, A_1 to A_J. It is the different characteristics of the integrand in these regions which will be exploited in the methods which follow.

---

1 This implies only that $f(x,y) \geq 0$ and that $\iint_A f(x,y)dxdy = 1$.

The following quantities are defined for each value of j:

the probability of A_j

$$p_j = \iint_{A_j} f(x,y)dxdy \tag{13}$$

probability density of (x,y) given A_j

$$f_j(x,y) = \begin{cases} f(x,y)/p_j & \text{if } (x,y) \text{ is in } A_j \\ 0 & \text{if } (x,y) \text{ is not in } A_j \end{cases} \tag{14}$$

conditional expected value of z given A_j

$$\begin{aligned} \bar{z}_j &= \iint_A z(x,y)f_j(x,y)dxdy \\ &= \iint_{A_j} z(x,y)f(x,y)dxdy \Big/ \iint_{A_j} f(x,y)dxdy \end{aligned} \tag{15}$$

conditional expected square

$$\begin{aligned} \overline{z_j^2} &= \iint_A z^2(x,y)f_j(x,y)dxdy \\ &= \iint_{A_j} z^2(x,y)f(x,y)dxdy \Big/ \iint_{A_j} f(x,y)dxdy \end{aligned} \tag{16}$$

conditional variance

$$\sigma_j^2 = \overline{z_j^2} - \bar{z}_j^2 \tag{17}$$

p_j is the probability that a point (x,y), picked at random out of the p.d.f. f(x,y), will be in the region A_j; $f_j(x,y)$ is a properly normalized p.d.f.; and f(x,y) is equal to $\sum p_j f_j(x,y)$. $\bar{z}_j$ is the average value of

$z(x,y)$ in A_j. The expected value of $z(x,y)$ over A is the expected value of the $\bar{z}_j$.

$$\bar{z} = \overline{\bar{z}_j} = \sum p_j \bar{z}_j \tag{18}$$

Similarly

$$\overline{z^2} = \overline{\overline{z_j^2}} = \sum p_j \overline{z_j^2} \tag{19}$$

Finally σ_j^2 measures the fluctuation of the random variable $z(x,y)$ given that (x,y) is in A_j. It is shown in Section 4 (equation 24) that the variance of $z(x,y)$ is the weighted sum of the values of these conditional variances and a variance due to the fluctuation of $\bar{z}_j$ from one j to another.

The same formulation can be used to treat a slightly more general problem than the simple evaluation of an integral. For example, consider the evaluation of the expected value of a random variable W that is generated by the following process:

a. Let p_j be the probability of a $j^{\underline{th}}$ event occurring.

b. If the $j^{\underline{th}}$ event occurs let the p.d.f. for (x,y) be $g_j(x,y)$ and let $W = w_j(x,y)$

$$\bar{w} = \sum_{j=1}^{J} p_j \iint w_j(x,y) g_j(x,y)\,dx\,dy \tag{20}$$

$$= \sum_{j=1}^{J} p_j \bar{w}_j$$

$$= \overline{\bar{w}_j}$$

where the obvious definitions for $\bar{w}_j$ and $\overline{\bar{w}_j}$ apply. All the techniques to be described can be used as easily to evaluate a $\bar{w}$, defined by equation (20), as to evaluate a $\bar{z}$, defined by equation (12). In fact, some of the techniques are unnecessarily complicated for the simple integral, but are useful for the more general problem, particularly if the p_j's are defined implicitly instead of explicitly.

4. Straightforward Sampling (A)

This is the sampling which was already discussed in section 1. N samples are picked from the p.d.f. $f(x,y)$ and an estimate of $\bar{z}$ is defined by

$$\hat{z}_1 = \frac{1}{N}\sum_{1}^{N} z(x_i, y_i) \tag{21}$$

The variance of the estimate is

$$V_1 = \frac{1}{N}\overline{\left[z(x,y) - \bar{z}\right]^2} = \frac{1}{N}\left(\overline{z^2} - \bar{z}^2\right) \tag{22}$$

It can be written

$$V_1 = \frac{1}{N}\left[\iint \left[z(x,y) - \bar{z}\right]^2 f(x,y)\,dxdy\right] \tag{23}$$

$$= \frac{1}{N}\left[\sum_j p_j \iint \left[z - \bar{z}\right]^2 f_j(x,y)\,dxdy\right]$$

$$= \frac{1}{N}\left[\sum_j p_j \iint \left[(z - \overline{z_j}) + (\overline{z_j} - \bar{z})\right]^2 f_j(x,y)\,dxdy\right]$$

$$= \frac{1}{N}\left[\sum_j p_j \sigma_j^2 + \sum_j p_j (\bar{z}_j - \bar{z})^2\right]$$

since

$$\iint (z - z_j)^2 f_j(x,y)\,dxdy = \sigma_j^2$$

$$2\iint (z - \bar{z}_j)(\bar{z}_j - \bar{z}) f_j(x,y)\,dxdy = 0$$

$$\iint (\bar{z}_j - \bar{z})^2 f_j(x,y)\,dxdy = (\bar{z}_j - \bar{z})^2$$

Therefore

$$V_1 = \frac{1}{N}\left[\overline{\sigma_j^2} + \overline{(\bar{z}_j - \bar{z})^2}\right] \tag{24}$$

5. Importance Sampling (A)

Another method of evaluating $\bar{z}$ by sampling would be to:

(a) pick a j out of a set of probabilities p_j^* instead of p_j

(b) once j is picked, pick an (x,y) out of $f_j(x,y)$

(c) with this (x,y) evaluate the function

$$z^*(x,y) = z_j^*(x,y) = \frac{p_j}{p_j^*} z(x,y)$$

The p_j^* can be chosen completely arbitrarily except for the usual conditions:

$$0 \leq p_j^* \leq 1 \tag{25}$$

$$\sum_j p_j^* = 1$$

together with the condition that

$$p_j^* = 0 \text{ (unless } p_j = 0)$$

The first two conditions guarantee that the p_j^* shall be a set of probabilities, the last one that p_j/p_j^* is never infinite.

Despite the arbitrariness of p_j^*, the expected value of $z^*(x,y)$ is easily seen to be $\bar{z}$:

$$\overline{z^*(x,y)} = \sum p_j^* \iint z_j^*(x,y) f_j(x,y)\,dxdy \tag{26}$$

$$= \sum p_j^* \iint \frac{p_j}{p_j^*} z(x,y) f_j(x,y)\,dxdy$$

$$= \sum p_j \iint z(x,y) f_j(x,y)\,dxdy$$

$$= \iint z(x,y) f(x,y)\,dxdy$$

$$= \bar{z}$$

However, $\overline{[z^*(x,y)]^2}$ is not equal to $\overline{z^2}$.

$$\overline{[z^*(x,y)]^2} = \sum p_j^* \iint z_j^{*2}(x,y) f_j(x,y)\,dx\,dy \qquad (27)$$

$$= \sum \iint \frac{p_j^2}{p_j^*} z^2(x,y) f_j(x,y)\,dx\,dy$$

$$= \sum \frac{p_j^2}{p_j^*} \overline{z_j^2}$$

So
$$V_2 = \frac{1}{N}\left[\overline{z^{*2}(x,y)} - \bar{z}^2\right] \qquad (28)$$

$$= \frac{1}{N}\left[\sum \frac{p_j^2 \overline{z_j^2}}{p_j^*} - \bar{z}^2\right]$$

There are, therefore, an infinite number of sampling schemes here that can be used to estimate $\bar{z}$ — each with a different variance. The computer would presumably like to use a set of p_j^*'s that minimizes this variance. To minimize V_2 it is sufficient to minimize $\overline{z^{*2}(x,y)}$. The term, $\bar{z}^2$, is not affected by changing the p_j^*. Of course the minimizing on p_j^* must be done subject to the conditions of equation (25).

As shown in Appendix III, this is equivalent to finding the values of p_j^* that minimize

$$\sum \frac{p_j^2 \overline{z_j^2}}{p_j^*} + \lambda \sum p_j^*$$

for a suitable λ to be determined later.

The unique minimizing set is given by

$$p_j^* = \frac{1}{\sqrt{\lambda}} p_j \sqrt{z_j^2} \tag{29}$$

To make the summation of the p_j^* equal to one, it is necessary to take

$$\sqrt{\lambda} = \sum p_j \sqrt{z_j^2} \tag{30}$$

If the sampling is done with this optimum set of p_j^*'s, the variance becomes

$$V_2 = \frac{1}{N}\left\{\left[\sum p_j \sqrt{z_j^2}\right]^2 - \bar{z}^2\right\} \tag{31}$$

$$= \frac{1}{N}(\lambda - \bar{z}^2)$$

The improvement over straightforward sampling is measured by

$$V_1 - V_2 = \frac{1}{N}\left\{\sum p_j z_j^2 - \left[\sum p_j \sqrt{z_j^2}\right]^2\right\} \tag{32}$$

$$= \frac{1}{N}\sum_{j=1}^{J} p_j \left[\sqrt{z_j^2} - \sum_{k=1}^{J} p_k \sqrt{z_k^2}\right]^2$$

$$= \overline{\left[\sqrt{z_j^2} - \sqrt{z_k^2}\right]^2}$$

The variance is reduced by the variance of a random variable which has a probability p_j of taking on the value $\sqrt{z_j^2}$.

It is slightly misleading to call sampling with the p_j^* Importance Sampling. The importance of any region in contributing to the answer is, in a sense, measured by $p_j|\bar{z}_j|$ but the sampling should be done by a set of probabilities proportional to $p_j \sqrt{z_j^2}$. However $\overline{z_j^2} = \bar{z}_j^2 + \sigma_j^2$, so if σ_j^2

is small compared to $\bar{z}_j^2$, $\sqrt{\overline{z_j^2}} \approx |\bar{z}_j|$. In fact in certain optimum situations the quantity corresponding to σ_j is zero; in which case the sampling probabilities should be taken exactly proportional to the importance of the various regions. In any case it is usually easier for the computer to conjure up estimates of $\bar{z}_j$ than $\sqrt{\overline{z_j^2}}$.

If the $\bar{z}_j$ are all positive and the p_j^* are taken proportional to $\bar{z}_j$ then

$$p_j^* = \frac{p_j \bar{z}_j}{\bar{z}} \tag{33}$$

$$V_2 = \frac{1}{N}\left[\bar{z}\sum p_j \frac{\overline{z_j^2}}{\bar{z}_j} - \bar{z}^2\right] \tag{34}$$

$$= \frac{1}{N}\bar{z}\sum p_j \frac{\sigma_j^2}{\bar{z}_j}$$

$$= \frac{1}{N}\bar{z}\left[\overline{\frac{\sigma_j^2}{\bar{z}_j}}\right]$$

and

$$V_1 - V_2 = \frac{1}{N}\left\{\overline{\sigma_j^2\left(1 - \frac{\bar{z}}{\bar{z}_j}\right)} + \overline{(\bar{z}_j - \bar{z})^2}\right\} \tag{35}$$

$$= \left[\overline{z_j^2\left(1 - \frac{\bar{z}}{\bar{z}_j}\right)}\right] \tag{36}$$

It is clear that sampling proportional to $|\bar{z}_j|$ may be poor if any of the terms $p_j\sigma_j^2/|\bar{z}_j|$ is large. The computer can protect himself against this possibility if whenever his estimate of $\bar{z}_j$ is very small he replaces

it with a larger number in the calculation of p_j. Exactly how far the computer should go in this direction is strongly dependent on the problem that is being done.

The problem of estimating $\overline{z_j^2}$ or $\bar{z}_j$ is crucial if importance sampling is to be done, Intuition, approximate calculations, experiments, or previous Monte Carlo calculations can be used to get information about $\overline{z_j^2}$ and $\bar{z}_j$. In most problems it is easy for the computer to get some idea of the relative importance of different regions. When it is necessary though, it is worthwhile to go to some effort to get reasonable estimates of $\overline{z_j^2}$ or $\bar{z}_j$ for, as shown in Appendix II, there are real disasters possible if the assumed importance functions are very badly chosen.

6. Systematic Sampling (A)

If it has been decided in advance how large N is to be and the p_j's are known explicitly, then instead of choosing a random j for each sample, the expected number of samples can be assigned to each region.

Denoting these expected numbers by $\bar{n}_j$, then

$$\bar{n}_j = p_j N \tag{37}$$

The estimate of $\bar{z}$ is

$$\hat{z}_3 = \sum_{j=1}^{J} \frac{p_j}{\bar{n}_j} \sum_{i=1}^{\bar{n}_j} z(x_{ij}, y_{ij}) \tag{38}$$

where (x_{ij}, y_{ij}) is the $i^{\underline{th}}$ sample value picked in the $j^{\underline{th}}$ region and $\frac{1}{\bar{n}_j} \sum_{i=1}^{\bar{n}_j} z(x_{ij}, y_{ij})$ is an estimate of $\bar{z}_j$.

The variance is given by

$$V_3 = \overline{(\hat{z}_3 - \bar{z})^2} \tag{39}$$

$\bar{z}$ can be written

$$\bar{z} = \sum_{j=1}^{J} \frac{p_j}{\bar{n}_j} \sum_{i=1}^{n_j} \bar{z}_j \tag{40}$$

Substituting equations (38) and (40) into (39),

$$V_3 = \overline{\left\{\sum_{j=1}^{J} \frac{p_j}{\bar{n}_j} \sum_{i=1}^{\bar{n}_j} \left[z(x_{ij},y_{ij}) - \bar{z}_j\right]\right\}^2} \qquad (41)$$

$$= \sum_{j=1}^{J} \frac{p_j^2}{\bar{n}_j^2} \overline{\sum_{i=1}^{\bar{n}_j} \left[z(x_{ij},y_{ij}) - \bar{z}_j\right]^2}$$

+ cross product terms which drop out when the averaging is done.

$$= \sum_{j=1}^{J} \frac{p_j^2}{\bar{n}_j^2} \sum_{i=1}^{\bar{n}_j} \sigma_j^2$$

$$= \sum_{j=1}^{J} \frac{p_j^2 \sigma_j^2}{\bar{n}_j}$$

$$= \frac{1}{N} \sum_{j=1}^{J} p_j \sigma_j^2 = \frac{1}{N} \overline{\sigma_j^2}$$

and

$$V_1 - V_3 = \frac{1}{N}\left[\sum_{j=1}^{J} p_j (\bar{z}_j - \bar{\bar{z}})^2\right] \qquad (42)$$

The variance is reduced by the variance of the average values of the different j regions, one of the terms of equation (24). Whether or not the gain in doing systematic sampling is large will depend on the amount of this variance, but as it rarely involves any extra work, if the p_j are already known, it is almost always desirable.

7. Stratified Sampling (Quota Sampling) (A)

As in Systematic Sampling, each region is assigned a definite number of samples instead of a random amount. However, instead of just taking this number equal to $p_j N$, it is chosen to minimize the variance of the estimate. In this respect Stratified Sampling is similar to Importance Sampling.

If n_j^* samples are taken in each region, then the estimate of $\bar{z}$ is given by

$$\hat{z}_4 = \sum_{j=1}^{J} \frac{p_j}{n_j^*} \sum_{i=1}^{n_j^*} z(x_{ij}, y_{ij}) \tag{43}$$

As usual, (x_{ij}, y_{ij}) is the i^{th} sample value in the j^{th} region and $\frac{1}{n_j^*} \sum_{i=1}^{n_j^*} z(x_{ij}, y_{ij})$ is an estimate of $\bar{z}_j$.

By following the procedure in the previous section on Systematic Sampling, the variance is shown to be

$$V_4 = \sum_{j=1}^{V} \frac{p_j^2 \sigma_j^2}{n_j^*} \tag{44}$$

To minimize V_4, subject to the restriction that $\sum_{j=1}^{J} n_j^* = N$, it is necessary to take the unrestricted minimum of

$$\sum_{j=1}^{J} \frac{p_j^2 \sigma_j^2}{n_j^*} + \lambda \sum_{j=1}^{J} n_j^* \tag{45}$$

This minimum occurs when

$$n_j^* = \frac{p_j \sigma_j}{\sqrt{\lambda}} \tag{46}$$

where

$$\sqrt{\lambda} = \frac{1}{N} \sum p_j \sigma_j \tag{47}$$

$$= \frac{\overline{\sigma_j}}{N}$$

therefore

$$n_j^* = \frac{N p_j \sigma_j}{\overline{\sigma_j}} \tag{48}$$

The result is reminiscent of Importance Sampling except that the importance of a region is measured by $p_j \sigma_j$ rather than $p_j \sqrt{\overline{z_j^2}}$

The variance becomes

$$V_4 = \frac{1}{N} \left(\sum p_j \sigma_j \right)^2 \tag{49}$$

$$= \frac{1}{N} \overline{\sigma_j}^2$$

$$V_1 - V_4 = \frac{1}{N} \left[\sum p_j (\sigma_j - \overline{\sigma_j})^2 + \sum p_j (\bar{z}_j - \bar{\bar{z}})^2 \right] \tag{50}$$

As in Systematic Sampling, the variance due to the variation in $\overline{z_j}$ is eliminated. In addition a variance due to the variation in σ_j is also eliminated.

As might be expected, $\hat{\bar{z}}_4$ is more accurate than $\hat{\bar{z}}_2$.

$$V_2 - V_4 = \frac{1}{N} \left[\sum \frac{p_j^2 \overline{z_j^2}}{p_j^*} - \bar{\bar{z}}^2 - \sum \frac{p_j^2 \sigma_j^2}{p_j^*} \right] \tag{51}$$

Substituting $\sigma_j^2 = \overline{z_j^2} - \bar{z}_j^2$ one gets

$$V_2 - V_4 = \frac{1}{N}\left[\sum \frac{p_j^2}{p_j^*}\bar{z}_j^2 - \bar{z}^2\right] \qquad (52)$$

$$= \frac{1}{N}\left[\sum p_j^*\left(\frac{p_j\bar{z}_j}{p_j^*}\right)^2 - \bar{z}^2\right]$$

$$= \frac{1}{N}\sum p_j^*\left(\frac{p_j\bar{z}_j}{p_j^*} - \bar{z}\right)^2$$

which is greater than 0.

The problem may be such that the p_j's are not known explicitly. It can then be very inconvenient to try to force, in advance, the region in which the point (x,y) is to fall. In this extremity a variation of the above sampling technique can be used.

a. A point (x,y) is picked at random and the j region to which it belongs identified.

b. If n_j^* points in this j region have already been picked, the point is discarded and a new choice made.

c. If less than n_j^* points have been picked then the evaluation $z(x_{ij},y_{ij})$ is made and the value recorded.

The above process can only be useful if the cost of picking a point is completely negligible compared to the cost of evaluating z(x,y). If the cost of picking the point (x,y) is not negligible, the process in principle, should be changed. The decision whether or not to discard a point should depend on how many points have already been picked in all the regions, and/or on the relative costs of picking and evaluating. Further discussion on this point will be found in Section 19.

If, as is often true, the computer has good estimate of $\bar{z}_j$ available, he may wish to take n_j^* proportional to this quantity.

$$n_j^* = \frac{Np_j\bar{z}_j}{\bar{z}} \tag{53}$$

In this case

$$V_4 = \frac{1}{N}\bar{z}\sum p_j \frac{\sigma_j^2}{\bar{z}_j} \tag{54}$$

$$V_1 - V_4 = \frac{1}{N}\left[\sum p_j\sigma_j^2(1 - \frac{\bar{z}}{\bar{z}_j}) + \sum p_j(\bar{z}_j - \bar{z})^2\right] \tag{55}$$

Since equations (54) and (34) are identical, there is no advantage to be gained by doing Systematic Sampling, or Stratified Sampling proportional to $\bar{z}_j$, when Importance Sampling proportional to $\bar{z}_j$ has already been used.

8. Using Expected Values (A)

Sometimes it is a simple matter to evaluate $\bar{z}_j$ analytically. Than if the p_j are known one can write $\bar{z} = \sum p_j \bar{z}_j$ and there is no necessity to do Monte Carlo. Sometimes though the p_j are not given explicitly and but only a complicated way of sampling for them is given. There is then no point in using Monte Carlo to do that part of the problem which can be done analytically. Only the j value should be drawn at random and then $\bar{z}_j$ used for the estimate:

$$z_5 = \frac{1}{N} \sum_{i=1}^{N} \bar{z}_{j(i)} \tag{56}$$

$\bar{z}_{j(i)}$ is the analytically calculated expected value of z(x,y) in the j region that was picked on the $i^{\underline{th}}$ sample. The variance is

$$V_5 = \frac{1}{N} \sum p_j (\bar{z}_j - \bar{z})^2 \tag{57}$$

$$V_1 - V_5 = \sum p_j \sigma_j^2 \tag{58}$$

As would be intuitively expected, the variation due to the fluctuation of z(x,y) within a j region has been eliminated. In many problems this variance eliminated is very large compared to V_5.

9. Correlation (A)

It is sometimes desirable to do two or more problems simultaneously. This occurs, in particular, when one of the following three conditions hold:

a. The answer to one of the problems is known. The answer to the unknown problem can be calculated more accurately by adding the estimate of the difference to the known answer rather than by estimating the unknown one directly. The known answer is usually the solution of an idealization of the problem of interest.

b. The difference between problems is of interest. If the sampling is carried out in a correlated fashion, it is usually possible to estimate the differences more accurately than if the sampling were done on the problems independently and the answers subtracted.

c. A parametric study of n problems is being conducted. If the problems are done simultaneously, it may not be necessary to duplicate n times the similar portions. This will bring down the total cost, or enable the computer to do a much larger study for the same cost.

For the example to be considered, it will be assumed that the computer knows how to evaluate, analytically or otherwise,

$$\bar{v} = \iint_A v(x,y)g(x,y)dxdy \qquad (59)$$

and that $\overline{z - \alpha v}$ will be estimated by the sampling (condition a). As before, a set of quantities is defined for each j region:

$$q_j = \iint_{A_j} g(x,y)\,dxdy$$

$$g_j(x,y) = \begin{cases} \dfrac{g(x,y)}{q_j} & (x,y) \text{ in } A_j \\ 0 & (x,y) \text{ not in } A_j \end{cases}$$

$$\bar{v}_j = \iint_A v(x,y)\,g_j(x,y)\,dxdy \tag{60}$$

$$\overline{v_j^2} = \iint v^2(x,y)\,g_j(x,y)\,dxdy$$

In addition, the correlation coefficient ρ is defined by

$$\rho = \frac{\overline{(z - \bar{z})\,(v - \bar{v})}}{\sigma_1 \sigma_2} \tag{61}$$

$$= \frac{\overline{zv} - \bar{z}\,\bar{v}}{\sigma_1 \sigma_2}$$

where σ_1 is the s.d. of $z(x,y)$ for the sampling method used and σ_2 is the corresponding quantity for $v(x,y)$ It can be shown by applying Schwarz's inequality to the $\int (z - \bar{z})^2 f(x,y)\,dxdy$, $\int (v - \bar{v})^2 f(x,y)\,dxdy$, and $\int (z - \bar{z})\,(v - \bar{v}) f(x,y)\,dxdy$ that $-1 \leq \rho \leq 1$.

The correlated sampling can be carried out by the following scheme:

a. A j value is picked at random from a set of probabilities q_j^*.

b. For every value of j picked, an (x_i, y_i) is picked out of $f_j(x,y)$ and an (x_i', y_i') from $g_j(x,y)$. If it is feasible the (x', y') may be correlated with (x,y); in this case the (x_i', y_i') is picked from a $g(x', y' : x, y)$.

c. (a) and (b) are repeated until N samples are picked. An estimate of $\bar{z}$ is then calculated by

$$\hat{z}_6 = \hat{z} - a(\hat{v} - \bar{v}) \tag{62}$$

where

$$\hat{z} = \frac{1}{N} \sum_{i=1}^{N} \frac{p_{j(i)}}{q^*_{j(i)}} z(x_i, y_i)$$

$$\hat{v} = \frac{1}{N} \sum_{i=1}^{N} \frac{q_{j(i)}}{q^*_{j(i)}} v(x_i', y_i')$$

The computer should try to pick a to minimize

$$V_6 = \overline{(\hat{z}_6 - \bar{z})^2} \tag{63}$$

$$= \overline{\left[(\hat{z} - \bar{z}) - a(\hat{v} - \bar{v})\right]^2}$$

$$= \overline{(\hat{z} - \bar{z})^2} - 2a\overline{(\hat{z} - \bar{z})(\hat{v} - \bar{v})} + a^2\overline{(\hat{v} - \bar{v})^2}$$

$$= \frac{1}{N}\left[\sigma_1^2 - 2a\rho\sigma_1\sigma_2 + a^2\sigma_2^2\right]$$

where

$$\sigma_1^2 = \sum q_j^* \iint \left[z_j(x,y) \frac{p_j}{q_j^*}\right]^2 f_j(x,y)\,dx\,dy - \bar{z}^2 \tag{64}$$

$$= \sum \iint \frac{z_j^2(x,y) p_j^2}{q_j^*} f_j(x,y)\,dx\,dy - \bar{z}^2$$

$$\rho \sigma_1 \sigma_2 = \overline{zv} - \bar{z}\,\bar{v}$$

$$\overline{zv} = \sum q_j^* \iiiint \left[z(x,y) \frac{p_j}{q_j^*} \right] \left[v(x',y') \frac{q_j}{q_j^*} \right] g_j(x',y':x,y)\, f(x,y)\,dx'\,dy'\,dx\,dy$$

$$\sigma_2^2 = \sum q_j^* \iint \left[v_j(x',y') \frac{q_j}{q_j^*} \right]^2 g_j(x',y')\,dx'\,dy' - \bar{v}^2$$

$$= \sum \iint \frac{v_j^2(x',y') q_j^2}{q_j^*} g_j(x',y')\,dx'\,dy' - \bar{v}^2$$

The optimum α is determined by setting $\frac{\partial V_6}{\partial \alpha} = 0$ which makes

$$\alpha = \rho \frac{\sigma_1}{\sigma_2} \tag{65}$$

With the optimum α the variance becomes

$$V_6 = \frac{1}{N} \sigma_1^2 (1 - \rho^2) \tag{66}$$

Therefore it is seen that the higher the correlation, the smaller the variance V_6.

Unfortunately the computer usually cannot calculate α analytically. It can be estimated by substituting $\hat{z}$, $\hat{v}$, $\widehat{zv}$, and $\widehat{v^2}$ for the corresponding expected values in

$$\alpha = \rho \frac{\sigma_1}{\sigma_2} \tag{67}$$

$$= \frac{\rho \sigma_1 \sigma_2}{\sigma_2^2}$$

$$= \frac{\overline{zv} - \bar{z}\,\bar{v}}{\overline{v^2} - \bar{v}^2}$$

If the same sample that is used to estimate $\bar{z}$ and $\bar{v}$ is also used to estimate α, then the variance of $\hat{z}_6$ can no longer be simply expressed. In addition, it is conceivable that a serious bias could be introduced by such a procedure. The following alternative can be used. The sample is divided into two equal parts: $\hat{z}'$, $\hat{a}'$, and $\hat{v}'$ are calculated from the first part, $\hat{z}''$, $\hat{\alpha}''$, and $\hat{v}''$ from the second part, and the estimate is changed to

$$\hat{z}'_6 = \hat{z}' - \hat{\alpha}''(\hat{v}' - \bar{v}) \tag{68}$$

or

$$\hat{z}''_6 = \hat{z}'' - \hat{\alpha}'(\hat{v}'' - \bar{v})$$

The variance of either of the above estimates is

$$V'_6 = V''_6 = \frac{2}{N}\left[\sigma^2 - 2\overline{\hat{a}'}\rho\sigma_1\sigma_2 + \overline{\hat{a}'^2}\sigma_2^2\right] \tag{69}$$

$$\approx \frac{2}{N}\hat{\sigma}^2(1 - \hat{\rho}^2)$$

This is twice as big as the optimum variance of equation (66).

If the average of $\hat{z}'_6$ and $\hat{z}''_6$ is taken as the estimate, then the variance becomes

$$V = \frac{1}{2}V'_6 + \frac{1}{2}\left[\overline{a'(v' - \bar{v})}\right]^2 \tag{70}$$

which can be shown to be less than V''_6.

In some cases the computer will be able to calculate α_2^2 analytically, but can only estimate $\rho\sigma_1\sigma_2$. It is not necessarily desirable to use this combination, because the estimates of the two quantities are correlated,

and $\frac{\hat{zv} - \hat{z}\,\hat{v}}{\hat{v}^2 - \hat{v}^2}$ may have a smaller variance than $\frac{\hat{zv} - \hat{z}\,\hat{v}}{\bar{v}^2 - \bar{v}^2}$.

John Tukey has pointed out to the author that equation (70) is not "maximally ingenious". It suffers from the defect that the correction term $\overline{a(\hat{v} - v)^2}/2$ has not been made as small as possible. One way in which it can be made smaller is to proceed as follows:

a. Divide the samples into K parts, each with N/K samples.

b. Estimate $\hat{z}_k$, $\hat{v}_k$, $(\hat{\rho\sigma_1\sigma_2})_k$ and $(\hat{\sigma_2^2})_k$ for each part, k = 1,2,...,K.

c. Define $\hat{a'''_k}$ by

$$\hat{a'''_k} = \frac{1}{K-1} \sum_{i \neq k} \frac{(\hat{\rho\sigma_1\sigma_2})_i}{(\hat{\sigma_2^2})_i} \tag{71}$$

a'''_k is therefore independent of the other quantities with the same k subscript.

d. Let

$$\hat{z'_0}' = \frac{1}{K} \sum \left[\hat{z}_k - \hat{a'_k}'(\hat{v}_k - \bar{v}) \right] \tag{72}$$

Then

$$V'''_0 = \frac{1}{N}\left[\sigma_1^2 + 2\bar{\hat{a'''}}\rho\sigma_1\sigma_2 + \overline{\hat{a'''}^2}\sigma_2^2\right] + \frac{1}{K}\left[\frac{(\hat{\rho\sigma_1\sigma_2})_k}{(\hat{\sigma_2^2})_k}(\hat{v}_k - \bar{v})\right]^2 \tag{73}$$

and the correction term is divided by K instead of 2.

e. Because the number, N/K, of samples in each part may be small, $\frac{(\hat{\rho\sigma_1\sigma_2})_k}{(\hat{\sigma_2^2})_k}$ may be a very biased estimate of $\frac{\rho\sigma_1\sigma_2}{\sigma_2^2}$. While a bias in the estimate of a''' does not bias the estimate of $\bar{z}$ it is desirable to keep such bias's small. It can be reduced by changing the definition of $\hat{a'''_k}$ to

$$\hat{\alpha}'_k = \frac{\sum_{i=k} (\hat{\rho\sigma_1\sigma_2})_i}{\sum_{i=k} (\hat{\sigma_2^2})_i} \tag{74}$$

It is intuitively clear that the correction term will still be of the same order of magnitude if this definition of $\hat{\alpha}'_k$ is used instead of the one in (c), but that the bias will be smaller.

If the α is fixed then the computer should try to choose q_j^* to minimize the variance. Going back to equation (63) and rearranging terms

$$V_6 = \frac{1}{N}\left\{\sum_{j=1}^{J} \frac{p_j^2\overline{z_j^2} - 2\alpha p_j p_j \overline{z_j v_j} + \alpha^2 q_j \overline{v_j^2}}{q_j^*} - (\bar{z} - \alpha\bar{v})^2\right\} \tag{75}$$

The optimum q_j^* to use for any given α is given by

$$q_j^* = K\sqrt{p_j^2\overline{z_j^2} - 2\alpha p_j q_j \overline{z_j v_j} + \alpha q_j^2 \overline{v_j^2}} \tag{76}$$

where

$$K = 1/\sum\sqrt{p_j^2\overline{z_j^2} - 2\alpha p_j q_j \overline{z_j v_j} + \alpha^2 q_j^2 \overline{v_j^2}} \tag{77}$$

If this is done then

$$V_6 = \frac{1}{N}\left\{\frac{1}{K^2} - (\bar{z} - \alpha\bar{v})^2\right\} \tag{78}$$

10. Russian Roulette and Splitting (A)

Two of the techniques, Importance and Stratified Sampling, depend for their effectiveness on the computer being able to change the sampling probabilities so that a high percent of the samples are in the important A_j regions and small percent in the unimportant ones. In some problems this cannot be done easily. If, for instance, p_j were not known explicitly, but were obtained by an involved process with many stages of sampling, the computer might not know how to force the separate stages to make the final sampling of j proportional to an arbitrary set of p_j's. In this eventuality, when the sampling is such that first a j is picked and then an (x,y), the following process can be used:

a. Classify each region A_j as being of type I or II. In type I, either because the variance is small or the expense of picking (x,y) and evaluating z(x,y) is large, the computer wishes to avoid getting many samples. In type II the exact opposite is true. The numerical criteria for distinguishing the two types is developed in the argument.

b. In type I regions, where the relative contribution to the answer is somehow small, Russian Roulette[1] is used. When in such a region, a sample (x_i,y_i) is obtained only some of the time, say with probability q_j, and $z(x_i,y_i)/q_j$ recorded for the sample; otherwise, with probability $1 - q_j$, there is no sample taken

---

1 The name, of course, is derived from a well known game of chance said to be popular among Russian army men. The sampling technique itself originated at Los Alamos. John von Neumann and Stanley Ulam are responsible for both the sampling technique and its name.

and zero is recorded. If the first eventuality is realized, only one (x,y) need be picked and one z(x,y) evaluated. If the second eventuality materializes, no (x,y) need be picked. The expected value of the sampling has not been changed. The variance V_j for estimating $\bar{z}_j$, given that j has been picked, is

$$V_{7j} = \frac{\overline{z_j^2}}{q_j} - \bar{z}_j^2 \tag{79}$$

c. In type II regions, Splitting can be used. n_j values of (x,y) are picked for every j. The sample estimate is then the arithmetical average $\frac{1}{N}\sum_{i=1}^{n_j} z(x_i,y_i)$ where (x_i,y_i) is the $i^{\underline{th}}$ point picked on the sample. The variance of the above expression is

$$V_{7j} = \frac{\overline{z_j^2} - \bar{z}_j^2}{n_j} \tag{80}$$

$$= \frac{1}{n_j}\sigma_j^2$$

The variance of the whole process is given by equation (23) which takes the form

$$V_7 = \sum_1^J p_j(\bar{z}_j - \bar{z})^2 + \sum_1^J p_j V_{7j} \tag{81}$$

$$= \sum_1^J p_j(\bar{z}_j - \bar{z})^2 - \sum_I p_j \bar{z}_j^2 + \sum_I p_j \frac{\overline{z_j^2}}{q_j} + \sum_{II} p_j \frac{\sigma_j^2}{n_j}$$

$$= V_o + \sum_I p_j \frac{\overline{z_j^2}}{q_j} + \sum_{II} \frac{p_j \sigma_j^2}{n_j}$$

where

$$V_o = \sum_{II} p_j \bar{z}_j^2 - \bar{z}^2$$

The expected marginal cost of a sample is given by

$$C = C_o + \sum_{I} p_j q_j C_j + \sum_{II} p_j n_j C_j \,, \tag{82}$$

where C_o is the cost of picking j and C_j is the cost of picking (x,y) and evaluating z(x,y) in the $j^{\underline{th}}$ region.

It was shown in equation (9) that an efficient sampling scheme minimizes $H = CV_7$.[1] To find the n_j's that do this, it is convenient to assume that they are continuous variables so that the ordinary techniques of differential calculus can be used. This assumption has only a minor effect on the results.

$$\frac{\partial H}{\partial n_j} = C \frac{\partial V_7}{\partial n_j} + \frac{\partial C}{\partial n_j} V_7 = 0 \tag{83}$$

$$\frac{\partial V_7}{\partial n_j} = -\frac{V_7}{C} \frac{\partial C}{\partial n_j} \tag{84}$$

Using (81) and (82), and solving for n_j:

$$-\frac{p_j \sigma_j^2}{n_j^2} = -\frac{V_7}{C} p_j C_j$$

$$n_j = \lambda \sigma_j / \sqrt{C_j} \tag{85}$$

where $$\lambda = \sqrt{C/V_7} \tag{86}$$

---

1 CV_7 corresponds to $C_2\sigma^2$ in equation (9).

This result is intuitively pleasant (and reminiscent of equation 48). Similarly it can be shown that

$$q_j = \lambda\sqrt{\overline{z_j^2}/C_j} \tag{87}$$

If these n_j and q_j are used, V_7 is obtained by substituting (85) and (87) into (81) and (82).

$$V_7 = V_o + \frac{1}{\lambda}\left\{\sum_{I} p_j\sqrt{\overline{z_j^2}C_j} + \sum_{II} p_j\sigma_j\sqrt{C_j}\right\} \tag{88}$$

$$C = C_o + \lambda\left\{\sum_{I} p_j\sqrt{\overline{z_j^2}C_j} + \sum_{II} p_j\sigma_j\sqrt{C_j}\right\} \tag{89}$$

By dividing (89) by (88) and using $\lambda^2 = C/V_7$, λ can be evaluated:

$$\lambda^2 = \frac{C_o}{V_o} \tag{90}$$

The condition for a type I region is that $\lambda^2\overline{z_j^2}/C_j < 1$. For a type II region $\lambda^2\sigma_j^2/C_j \geq 1$. It can be shown it is best to assign the borderline cases, $\lambda^2\sigma_j^2/C_j \geq 1 \geq \lambda^2\overline{z_j^2}/C_j$, to type II. Equation (90) for λ is an implicit relation. V_o depends on the number of type II regions which in turn depends on λ. The dependence is, however, not sensitive, so it is easy to adjust the two factors. In fact, almost any iteration procedure will converge.[1]

In most problems C_j is not a sensitive function of j and can be taken equal to an average C'. Similarly there is very little error introduced if V_o is taken equal to $V_o' = \overline{(\bar{z}_j - \bar{z})^2}$ and the $\sqrt{\overline{z_j^2}}$ to σ_j. When λ is set equal to $\sqrt{\frac{C_o}{V_o}}$ and these approximate substitutions made, equations (88)

---

1 It should be pointed out to the more cautious readers, that the derivation of equations (85) and (87) can be justified even if the regions I and II are allowed to depend explicitly on λ or q_j and n_j.

and (89) become

$$V_7 = V_o' + \overline{\sigma_j} \sqrt{\frac{V_o'}{C_o} C'} \tag{91}$$

$$C = C_o + \overline{\sigma_j} \sqrt{\frac{C_o}{V_o'} C'} \tag{92}$$

In this instance, the improvement due to the change in variance cannot be calculated directly as before, because here cost of a sample is taken into account. When ordinary sampling is used, the product of the cost and the variance is

$$CV_1 \approx (C_o + C') \left[V_o' + \overline{\sigma_j^2} \right] \tag{93}$$

Using Russian Roulette and Splitting,

$$CV_7 \approx C_o V_o' + 2\overline{\sigma_j} \sqrt{C_o C' V_o'} + C' \overline{\sigma_j}^2 \tag{94}$$

Subtracting (94) from (93) and collecting terms

$$CV_1 - CV_5 \approx (C_o + C') \overline{(\sigma_j - \overline{\sigma_j})^2} + (\sqrt{C' V_o'} - \overline{\sigma_j} \sqrt{C_o})^2 \tag{95}$$

The first term on the right side of equation (95) is easily interpreted. $(C_o + C')$ is the average cost of a sample when doing straightforward sampling so the improvement is measured by comparing $\overline{(\sigma_j - \overline{\rho_j})^2}$ with V_1 (i.e., the variance of σ_j with the variance of $z(x,y)$). There is an additional improvement given by the second term which is related to the fact that even if σ_j didn't vary at all, it might still pay to sample many (x,y) values for every j picked.

11. Introduction to Section B

The seven methods just introduced in Section 4 through 10 will now be treated again in Section 13 through 19. The point of view will be somewhat different and in most cases the discussion is more complete. There will, necessarily, be some paraphrasing and repetition of the previous sections. However, the ability to set up an efficient Monte Carlo problem depends more on the intuition of the computer than on being able to evaluate the formulae given, and paraphrasing may make the ideas clearer, thus helping to create a sound intuition. For the same reason, a possibly excessive number of special cases and techniques are discussed.

As already explained, most of the discussion and formulae are unchanged if x or y are actually multidimensioned variables. In most applications it is necessary to make this extension.

In what follows, each value of x is thought of as defining a "cut" or region of the whole space. These regions take the place of the j regions of the previous section. Thus $\bar{z}(:x)$ is analogous to $\bar{z}_j$. Though the implicit multidimensionality of the variable made two dimensions superfluous until this point, now for much of the analysis which follows, two variables are necessary.

The following quantities, some of which have been defined before, are needed in the discussion:

$$f(x) = \int f(x,y)dy \quad = \text{the marginal p.d.f. of X}$$

$$g(y) = \int f(x,y)dx \quad = \text{the marginal p.d.f. of Y}$$

$$f(x:y) = f(x,y)/g(y) \quad = \text{the p.d.f. of X given that Y = y}$$

$$g(y:x) = f(x,y)/f(x) \quad = \text{the p.d.f. of Y given that X = x}$$

$$\bar{z}(:x) = \int z(x,y)g(y:x)dy \quad = \text{the expected value of } z(x,y) \text{ given that } X = x$$

$$\overline{z^2}(:x) = \int z^2(x,y)g(y:x)dx \quad = \text{the expected value of } z^2(x,y) \text{ given that } X = x$$

$$\bar{z} = \int \bar{z}(:x)f(x)dx$$

$$= \int \bar{z}(:y)g(y)dy$$

$$= \iint z(x,y)f(x,y)dxdy$$

$$\overline{z^2} = \overline{\overline{z^2}(:x)} = \int \overline{z^2}(:x)f(x)dx$$

$$= \int \overline{z^2}(:y)g(y)dy$$

$$= \iint z^2(x,y)f(x,y)dxdy$$

$$\sigma^2(:x) = \overline{z^2}(:x) - \bar{z}^2(:x)$$

$$\overline{\sigma^2(:x)} = \int \sigma^2(:x)f(x)dx$$

$$V_1 = \overline{z^2} - \bar{z}^2 = \overline{\sigma^2(:x)} + \overline{\left[\bar{z}(:x) - \bar{z}\right]^2}$$

12. Estimating $\bar{z}(:x)$ and $\overline{z^2}(:x)$

It is often desirable to estimate $\bar{z}(:x)$ and $\overline{z^2}(:x)$ by sampling. In principle this can be done by picking N values of y from g(y:x) and then estimating $\bar{z}(:x)$ and $\overline{z^2}(:x)$ in the standard way:

$$\hat{\bar{z}}(:x) = \frac{1}{N}\sum_{1}^{N} z(x,y_i) \tag{96}$$

$$\hat{\overline{z^2}}(:x) = \frac{1}{N}\sum_{1}^{N} z^2(x,y_i) \tag{97}$$

However, the computer usually wishes to estimate the whole function $\bar{z}(:x)$ and $\overline{z^2}(:x)$. It may then be too expensive to sample intensively at every value of x or there may be some evaluations of $z(x_i,y_i)$ available from previous problems in which the x_i have been picked in some random fashion. The simplest procedure in this case is to divide the x space into a number of intervals $[a_{r-1}, a_r]$ (if x is multidimensional, these are subspaces). Then by testing if $a_{r-1} < x_i \leq a_r$, each of the $z(x_i,y_i)$ can be assigned to an interval. Expected values for each interval can be estimated by:

$$\hat{z}_r = B_r \sum_{i} b_i z(x_i,y_i) \qquad a_{r-1} < x_i \leq a_r \tag{98}$$

where $B_r = 1/\sum_i b_i$

$$\hat{z}^2_r = C_r \sum_{i} c_i z(x_i,y_i) \qquad a_{r-1} < x_i \leq a_r \tag{99}$$

where $C_r = 1/\sum c_i$

The b_i and c_i can be taken equal to one if desired. If, however, the $z(x_i,y_i)$ have been produced by different processes, and

$$b_i = 1/\left[\overline{z^2(x_i,y_i)} - \bar{z}^2(x_i,y_i)\right] = 1/\sigma_i^2 \tag{100}$$

$$c_i = 1/\left[\overline{z^4(x_i,y_i)} - \overline{z^2(x_i,y_i)}^2\right] \tag{101}$$

the variance of $\hat{z}_r$ and $\hat{z}_r^2$ are minimized (see discussion on averaging different estimates in Section 18). If the intervals are taken small enough the computer can assume that

$$\bar{\hat{z}}_r \approx \bar{z}\left(: \frac{a_{r-1} + a_r}{2}\right)$$

$$\overline{\hat{z}_r^2} \approx \overline{z^2}\left(: \frac{a_{r-1} + a_r}{2}\right) \tag{102}$$

However, it is undesirable to take the intervals too small, because then there won't be enough sample values in each interval to make the estimate accurate.

There is an alternative technique which the author feels is slightly more desirable. Define

$$\begin{aligned} J(x) &= \sum_i b_i z(x_i,y_i) \qquad x_i \le x \\ K(x) &= \sum_i b_i \\ L(x) &= \sum_i c_i z^2(x_i,y_i) \qquad x_i \le x \\ M(x) &= \sum_i c_i \end{aligned} \tag{103}$$

The previous estimates can be written

$$\hat{z}_r = \frac{J(a_r) - J(a_{r-1})}{K(a_r) - K(a_{r-1})}$$

$$\hat{z}^2_r = \frac{L(a_r) - L(a_{r-1})}{M(a_r) - M(a_{r-1})} \qquad (104)$$

It is clear that if the empirically determined J(x), K(x), L(x), and M(x) are first smoothed out so that derivatives J'(x), K'(x), etc. can be calculated, estimates of $\bar{z}(:x)$ and $\overline{z^2}(:x)$ are given by:

$$\hat{\bar{z}}(:x) = \frac{dJ}{dK} = \frac{dJ}{dx} \Big/ \frac{dK}{dx}$$

$$\hat{\overline{z^2}}(:x) = \frac{dL}{dM} = \frac{dL}{dx} \Big/ \frac{dM}{dx} \qquad (105)$$

The advantages, if any, of the above technique lies in that there are no intervals to bother with, and that the smoothing operation makes every sample contribute to the estimate for any given value of x. It is also possible to use various curve fitting techniques (See Appendix IV), but these have the disadvantage of requiring that hypotheses be made about the functional nature of J(x), K(x), L(x), and M(x). Nevertheless, curve fitting techniques can be very useful if it is desirable to make the estimation of $\bar{z}(:x)$ or $\overline{z^2}(:x)$ completely automatic. If the functional form assumed for $\bar{z}(:x)$ or $\overline{z^2}(:x)$ has some validity then using it may be a very advantageous way to extract a larger amount of information from the sample than is done by the other methods suggested.

13. Straightforward Sampling (B)

As in Section A where first j was chosen, now first the x_i will be chosen, and then the y_i. This can be done by solving the equation

$$\int_{-\infty}^{x_i} f(x)dx = R_1 \tag{106}$$

for x_i, and then the equation

$$\int_{-\infty}^{y_i} g(y:x_i)dy = R_2 \tag{107}$$

for y_i; or any of the techniques suggested in Part I can be used. Once the sample values have been drawn,

$$\begin{aligned}
\hat{z}_1 &= \frac{1}{N}\sum_{i=1}^{N} z(x_i,y_i) \\
V_1 &= \frac{1}{N}\overline{\left[\hat{z}_1 - \bar{z}\right]^2} \qquad (108) \\
&= \overline{\left\{\left[z_1^2 - \bar{z}(:x)\right] + \left[\bar{z}(:x) - \bar{z}\right]\right\}^2} \\
&= \overline{\left[z_1^2 - \bar{z}(:x)\right]^2} + \overline{\left[\bar{z}(:x) - \bar{z}\right]^2} \\
&= \overline{\sigma^2(:x)} + \overline{\left[\bar{z}(:x) - \bar{z}\right]^2}
\end{aligned}$$

The two terms can be interpreted as being the variation of $z(x,y)$ for fixed x and the variation of $\bar{z}(:x)$ respectively.

14. Importance Sampling (B)

By dividing and multiplying by an arbitrary p.d.f., $f^*(x,y)$, $\bar{z}$ can be written

$$\bar{z} = \iint z(x,y) \frac{f(x,y)}{f^*(x,y)} f^*(x,y)dxdy \tag{109}$$

which indicates that $\bar{z}$ is also the expected value of

$$z_2 = \frac{1}{N} \sum_{i=1}^{N} z(x_i,y_i) \frac{f(x_i,y_i)}{f^*(x_i,y_i)} \tag{110}$$

where the (x_i,y_i) are picked from the p.d.f. $f^*(x,y)$. The variance is given by

$$V_2 = \iint \left[\frac{z(x,y)f(x,y)}{f^*(x,y)}\right]^2 f^*(x,y)dxdy - \bar{z}^2 \tag{111}$$

$$= \iint \frac{z^2(x,y)f^2(x,y)}{f^*(x,y)} dxdy - \bar{z}^2$$

V_2 is minimized (Appendix III) when

$$f^*(x,y) = K\,|z(x,y)|f(x,y) \tag{112}$$

where $$K = 1/\int |z(x,y)| f(x,y)dxdy$$

If $z(x,y)$ is everywhere positive and the optimum $f^*(x,y)$ is used, $V_2 = 0$ for

$$f^*(x,y) = \frac{z(x,y)f(x,y)}{\bar{z}} \tag{113}$$

and

$$\frac{z(x_i,y_i)f(x_i,y_i)}{f^*(x_i,y_i)} = \bar{z}$$

independently of what (x_i,y_i) happened to be picked. It is clear that there must be something a little fraudulent about the result, and in fact, in order to know what $f^*(x,y)$ is, the normalizing constant $\bar{z}$ must be known. It is therefore not miraculous that if the answer is known in advance, a perfect sampling scheme can be designed. The chief value of the above theorem is that it demonstrates that there are no "Conservation of Cost" laws and that if the computer is clever, wise, or lucky, he may, in choosing from the infinite number of sampling schemes available, be able to choose a very efficient one.

When $z(x,y)$ changes sign in the area of integration a perfect sampling scheme cannot be designed on the basis of importance sampling alone. If $\delta(x,y)$ is +1 or -1 according as $z(x,y)$ is positive or negative, then

$$\frac{z(x_i,y_i)f(x_i,y_i)}{f^*(x_i,y_i)} = \frac{\delta(x_i,y_i)}{K} \tag{114}$$

$$V_2 = \frac{1}{N}\left\{\iint\left[\frac{\delta(x,y)}{K}\right]^2 K|z(x,y)|f(x,y)dxdy - \bar{z}^2\right\} \tag{115}$$

$$= \frac{1}{N}\left\{\frac{1}{K}\iint|z(x,y)|f(x,y)dxdy - \bar{z}^2\right\}$$

$$= \frac{1}{N}\left\{\frac{1}{K^2} - \bar{z}^2\right\}$$

$$= \frac{1}{N}\left\{\left[\iint|z(x,y)|f(x,y)dxdy\right]^2 - \left[\iint z(x,y)f(x,y)dxdy\right]^2\right\}$$

$$= \frac{1}{N}\left\{\iint\left[|z(x,y)| - z(x,y)\right] f(x,y)dxdy\right\}\left\{\iint\left[|z(x,y)| + z(x,y)\right] f(x,y)dxdy\right\}$$

$$= \frac{4}{N}\left[\iint_{A_1}|z(x,y)|f(x,y)dxdy\right]\left[\iint_{A_2} z(x,y)f(x,y)dxdy\right]$$

where $z(x,y)$ is negative in A_1 and positive in A_2.

If, as might be the case, there is a known lower bound λ for $z(x,y)$, then there would be a perfect Importance Sampling scheme for $z(x,y) + \lambda$. Or it might occur that the positive and negative parts of $z(z,y)$ could be treated separately. But it is often not practical to consider these devices as part of pure Importance Sampling. It is still possible in principle to design a perfect sampling technique for a general $z(x,y)$ by using Correlation in addition to Importance Sampling. If, for example, it is possible to find a function $v(x,y)$, such that

$$\bar{v} = \iint v(x,y)f(x,y)dxdy \tag{116}$$

can be evaluated analytically, and such that

$$z(x,y) + v(x,y) \geq 0 \text{ for all } (x,y) \tag{117}$$

then a zero variance scheme could be designed for the integral

$$I = \iint\left[z(x,y) + v(x,y)\right] f(x,y)dxdy \tag{118}$$

and $\bar{z}$ estimated by $(\hat{I} - \bar{v})$. There is some more discussion on this point in Section 18.

The name Importance Sampling was suggested by the theoretical zero variance estimates and by the corresponding generalization to integral equations. $|z(x,y)|f(x,y)$ measures the importance of the point (x,y) and the optimum sampling p.d.f. is taken proportional to this quantity.

It might be interesting to note that if $z(x,y) \geq 0$, the optimum importance sampling for $\bar{z}$ will also reduce the variance for the estimate of the higher moments, $\overline{z^n}$. The variance of the estimate of $\overline{z^n}$ without importance sampling is

$$V = \iint z^{2n}(x,y)f(x,y)dxdy - \overline{z^n}^2 \tag{119}$$

$$= \overline{z^{2n}} - \overline{z^n}^2$$

and with optimum importance sampling it is

$$V = \iint \frac{z^{2n}(x,y)f^2(x,y)}{f^*(x,y)}\,dxdy - \overline{z^n}^2 \tag{120}$$

$$= \bar{z} \iint z^{2n-1}(x,y)f(x,y)dxdy - \overline{z^n}^2$$

$$= \bar{z}\,\overline{z^{2n-1}} - \overline{z^n}^2$$

[To show that $\bar{z}\,\overline{z^{2n-1}} \leq \overline{z^{2n}}$ it can be shown more generally that if $z(x,y) \leq 0$, $\overline{z^l}\,\overline{z^{n-l}} \leq \overline{z^n}$. Since $\phi(w) = \log \iint z^w(x,y)f(x,y)dxdy$ is a convex function of w and $\phi(0) = 0$, it follows that $\phi(u) + \phi(v) \leq \phi(u + v)$ which is the property above. Hence the variance has been reduced.]

It is, however, not true that any $f^*(x,y)$ that decreases the variance of the estimate of $\bar{z}$ also decreases the variance of the estimate of $\overline{z^n}$. In fact it is easy to exhibit counter examples.

In the general case as shown in Importance Sampling (A) (Section 5), the sampling should be taken proportional to the a priori probability of getting into a region times the square root of the average of the square of $z(x,y)$ in the region. This rule is illustrated in the different types of Importance Sampling discussed below.

Importance Sampling in the x space only.

Let $\bar{z}$ be written:

$$\bar{z} = \iint \left[z(x,y) \frac{f(x)}{f^*(x)} \right] f^*(x) g(y:x) dxdy \qquad (121)$$

and

$$\hat{z} = \frac{1}{N} \sum_{i=1}^{N} z(x_i,y_i) \frac{f(x_i)}{f^*(x_i)} \qquad (122)$$

where the (x_i,y_i) are picked out of $f^*(x,y) = f^*(x)g(y:x)$.

$$V_2 = \frac{1}{N} \left\{ \iint \left[z(x,y) \frac{f(x)}{f^*(x)} \right]^2 f^*(x) g(y:x) dxdy - \bar{z}^2 \right\} \qquad (123)$$

$$= \frac{1}{N} \left[\iint \frac{z^2(x,y) f^2(x)}{f^*(x)} g(y:x) dydx - \bar{z}^2 \right]$$

$$= \frac{1}{N} \left[\int \frac{\overline{z^2}(:x) f^2(x)}{f^*(x)} dx - \bar{z}^2 \right]$$

The minimizing $f^*(x)$ (Appendix III) is given by

$$f^*(x) = \overline{\int f(x) \sqrt{\int z^2(x,y) g(y:x) dx}} \qquad (124)$$

$$= \frac{f(x) \sqrt{\overline{z^2}(:x)}}{\sqrt{\overline{z^2}(:x)}}$$

If this f*(x) is used, the variance becomes

$$V_2 = \frac{1}{N}\left[\int \frac{\overline{z^2}(:x)f^2(x)\sqrt{\overline{z^2}(:x)}}{f(x)\sqrt{\overline{z^2}(:x)}}\,dx - \bar{z}^2\right] \tag{125}$$

$$= \frac{1}{N}\left[\sqrt{\overline{z^2}(:x)}\int \sqrt{\overline{z^2}(:x)}\;\; f(x)dx - \bar{z}^2\right]$$

$$= \frac{1}{N}\left[\left(\sqrt{\overline{z^2}(:x)}\right)^2 - \bar{z}^2\right]$$

The difference between this variance and that obtained by straightforward sampling is

$$V_1 - V_2 = \frac{1}{N}\left[\overline{z^2}(:x) - \left(\sqrt{\overline{z^2}(:x)}\right)^2\right] \tag{126}$$

and the variance is reduced by the variance of a random variable that has a probability of f(x) of being equal to $\sqrt{\overline{z^2}(:x)}$.

Sampling only from the x space is significant because it is common in practice to break the problem up into two or more stages. If this is done, optimum Importance Sampling means that the a priori probability f(x) of getting into a region x should be modified by the factor $\sqrt{\overline{z^2}(:x)}$. Only when Importance Sampling is done in the entire space is the factor $|z(x,y)|$. In that case, the word "importance" is used in its natural sense--that is, those regions are called important that make large contributions to the answer being calculated. However, the natural analogue

of $|z(x,y)|$, $|\bar{z}(:x)|$, is not the correct factor for optimum Importance Sampling in the x space alone, but rather $\sqrt{\overline{z^2}(:x)}$.

In some problems the difference between $\sqrt{\overline{z^2}(:x)}$ and $|\bar{z}(:x)|$ may not be great. $\overline{z^2}(:x) = \sigma^2(:x) + \bar{z}^2(:x)$. If $\sigma^2(:x)$ is small then

$$\sqrt{\overline{z^2}(:x)} \approx \bar{z}(:x) \tag{127}$$

In general, if the computer finds it easier to estimate $\bar{z}(:x)$ than $\overline{z^2}(:x)$, he can try to take

$$f^*(x) = \frac{f(x)\,|\bar{z}(:x)|}{\bar{z}} \tag{128}$$

If this is done, the variance becomes

$$V_2 = \frac{1}{N}\left\{\bar{z}\left[\frac{\overline{z^2}(:x)}{|\bar{z}(:x)|}\right] - \bar{z}^2\right\} \tag{129}$$

$$= \frac{1}{N}\;\bar{z}\left[\frac{\sigma^2(:x)}{|\bar{z}(:x)|}\right]$$

While V_2 in this case is ordinarily much less than V_1, it is easy to see that it can be large and in fact disasters are possible if care is not taken.

$$V_1 - V_2 = \frac{1}{N}\left\{\overline{\sigma^2(:x)\left[1 - \frac{\bar{z}}{|\bar{z}(:x)|}\right]} + \overline{\left[\bar{z}(:x) - \bar{z}\right]^2}\right\} \tag{130}$$

and the computer must then worry about a possible special treatment of regions in which $\bar{z}/|\bar{z}(:x)|$ is large.

As remarked before, the problem of estimating $\overline{z^2}(ix)$ or $\bar{z}(ix)$ is crucial in Importance Sampling (estimation by sampling is discussed in Section 12). This is not necessarily difficult. In particular, knowledge gained from any source can be exploited for this purpose. In any case, only the relative importance of different regions and not their absolute values need be known.

Importance Sampling with a parameter.

In many practical problems it is convenient to restrict the choice of $f^*(x,y)$ to a single family of p.d.f's. This may be desirable to do for either computing or theoretical convenience. If such a family is represented by $h(x,y,\alpha)$, then it is desirable to determine α so as to minimize the variance. This is equivalent to minimizing

$$\iint \left[\frac{z(x,y)f(x,y)}{h(x,y,\alpha)}\right]^2 h(x,y,\alpha)dxdy = \iint \frac{z^2(x,y)f^2(x,y)}{h(x,y,\alpha)}\,dxdy \qquad (131)$$

$h(x,y,\alpha)$ is subject to the usual conditions:

$$\iint h(x,y,\alpha)dxdy = 1$$

$$h(x,y,\alpha) \geq 0$$

If the form of $h(x,y,\alpha)$ is such that these conditions are satisifiéd for all values of α, then the optimum α is formally determined by

$$\iint \frac{z^2(x,y)f^2(x,y)}{h^2(x,y,\alpha)} \frac{\partial h(x,y,\alpha)}{\partial \alpha}\,dxdy = 0 \qquad (132)$$

If the $h(x,y,\alpha)$ is not already normalized for all α, equation (132) is replaced by the set (Appendix III).

$$\iint \frac{z^2(x,y)f^2(x,y)}{h^2(x,y,\alpha)} \frac{\partial h(x,y,\alpha)}{\partial \alpha} \, dxdy = \lambda \iint \frac{\partial h}{\partial \alpha}(x,y,\alpha)dxdy \tag{133}$$

$$\iint h(x,y,\alpha)dxdy = 1 \, . \tag{134}$$

and two unknowns, α and λ, must be determined. λ, of course, is a Lagrangian multiplier. When $h(x,y,\alpha)$ is not a function of y, the intergration on y can be performed and the quantity $\frac{z^2(x,y)f^2(x,y)}{h^2(x,y,\alpha)}$ is replaced by $\frac{\overline{z^2}(x)f^2(x)}{h^2(x,\alpha)}$.

Often the only practical method of solving equations (132) or (133) is to do a preliminary parametric study by Monte Carlo. The function to be minimized is

$$I(\alpha) = \iint \frac{z^2(x,y)f^2(x,y)}{h(x,y,\alpha)} \, dxdy \tag{135}$$

It is of course possible to evaluate (135) by Monte Carlo. It is not necessary to sample from $h(x,y,\alpha)$ when doing this evaluation because $I(\alpha)$ can be written

$$I(\alpha) = \iint \frac{z^2(x,y)f^2(x,y)}{h(x,y,\alpha)f^*(x,y)} \, f^*(x,y)dxdy \tag{136}$$

so that an estimate of $I(\alpha)$ is

$$\hat{I}(\alpha) = \frac{1}{N} \sum_{i=1}^{N} \frac{z^2(x_i,y_i)f^2(x_i,y_i)}{h(x_i,y_i,\alpha)f^*(x_i,y_i)} \tag{137}$$

where the (x_i,y_i) are picked out of $f^*(x,y)$.

The chief application of (137) is when $f^*(x,y) = h(x,y,\alpha_1)$ and we wish to evaluate $I(\alpha)$ for a series of α's, say α_1, α_2, and α_3. Then

$$I(\alpha) = \iint \frac{z^2(x,y)f^2(x,y)}{h(x,y,\alpha)h(x,y,\alpha_1)}\, h(x,y,\alpha_1)dxdy \qquad (138)$$

$$\hat{I(\alpha)} = \frac{1}{N}\sum_{i=1}^{N} \frac{1}{h(x_i,y_i,\alpha)} \left[\frac{z^2(x_i,y_i)f^2(x_i,y_i)}{h(x_i,y_i,\alpha_1)}\right] \qquad (139)$$

It is important to notice that a number of α's can be studied with the same (x_i,y_i) sample values, as only $1/h(x_i,y_i,\alpha)$ needs to be recalcuated in each case. In principle, all $I(\alpha)$ values desired could be estimated using the same importance function but it is likely that this will be good Importance Sampling only in some region of the α space, perhaps in a neighborhood of α_1.

This, of course, is an example of correlated sampling. Not only is the work per value of α reduced by the correlation, but since the computer is interested in comparing different $I(\alpha)$ the sampling is more accurate than if it had been carried out independently for each value of α. This occurs because in most problems the $I(\alpha)$ will be positively correlated and fluctuate in the same direction. It is, of course, possible to use the same technique to evaluate $\frac{\partial I(\alpha)}{\partial \alpha}$ and maybe even $\frac{\partial^2 I}{\partial \alpha^2}$ directly and use these quantities to estimate what α should be in a subsequent calculation.

In particular, if $\alpha_2 < \alpha_1$ and $\alpha_3 > \alpha_1$, $I(\alpha_j)$ for these three values might indicate how α should be changed to decrease the sampling variance. The problem might even be so programmed that this adjustment of α is done automatically by the computing machine. The author however, does not know of any case where this has been tried, and the procedure certainly has dangerous pitfalls. It seems, however, natural and intriguing enough to mention.

Use of Extra Freedom

It has been pointed out[1] that the α in $h(x,y,\alpha)$ provides extra freedom which can be exploited by giving it a p.d.f., $\rho(\alpha)$. If this is done, the α can first be picked at random from $\rho(\alpha)$, and the (x,y) selected from $h(x,y,\alpha)$. For the problem and technique of this section it would presumably be valueless to do this. Since an optimum α exists, the best $\rho(\alpha)$ is $\delta(\alpha-\alpha_o)$, where α_o is this optimum α. However, if the technique is combined with the use of expected values, it can be very helpful. This combination of Importance Sampling and Use of Expected Values is discussed here rather than in Section 17 because it seems to be more an example of the former than the latter. Also, as the ideas given here are somewhat speculative, the details are necessarily sketchy.

The point (x,y) is a function $\left[x(R_1,R_2,\alpha),\ y(R_1,R_2,\alpha)\right]$ of the uniformly distributed random numbers R_1 and R_2 and the parameter α. If α is given

---

1 Hale F. Trotter and John W. Tukey, "Conditional Monte Carlo for Normal Samples", Symposium on Monte Carlo Methods, John Wiley and Sons, 1956.

a p.d.f. $\rho(\alpha)$ then $z(x,y)\,\frac{f(x,y)}{h(x,y,\alpha)}$ can be integrated over all α to give an estimate I_i for each sample

$$I_i = \int z\left[x(R_1,R_2,\alpha),y(R_1,R_2,\alpha)\right] \frac{f\left[x(R_1,R_2,\alpha),y(R_1,R_2,\alpha)\right]}{h\left[x(R_1,R_2,\alpha),y(R_1,R_2,\alpha),\alpha\right]}\rho(\alpha)d\alpha \quad (140)$$

If this is done

$$\overline{I_i^2} = \iint \rho(\alpha)\rho(\alpha')I(\alpha,\alpha')d\alpha d\alpha' \quad (141)$$

where

$$I(\alpha,\alpha') = \iint z(x,y)z(x',y')\,\frac{f(x,y)f(x',y')}{h(x,y,\alpha)h(x',y',\alpha')}\,dR_1dR_2 \quad (142)$$

is a symmetric function of α and α', and

$$x = x(R_1,R_2,\alpha)$$

$$y = y(R_1,R_2,\alpha)$$

$$x' = x(R_1,R_2,\alpha')$$

$$y' = y(R_1,R_2,\alpha')$$

In order to minimize $\iint \rho(\alpha)\rho(\alpha')I(\alpha,\alpha')d\alpha d\alpha'$ subject to the condition that $\rho(\alpha)$ be a p.d.f. it is necessary to minimize the form

$$\iint \rho(\alpha)\rho(\alpha')I(\alpha,\alpha')d\alpha d\alpha' - 2\lambda\int\rho(\alpha)d\alpha \quad (143)$$

for those $\rho(\alpha) \geq 0$. This minimization yields the integral equation

$$\int \rho(\alpha)I(\alpha,\alpha')d\alpha = \lambda \quad (144)$$

If $I(\alpha,\alpha')$ happens to possess a resolvent kernel $H(\alpha',\beta)$ with the property

$$\int I(\alpha,\alpha')H(\alpha',\beta)d\alpha' = \delta(\alpha - \beta) \tag{145}$$

then

$$\rho(\alpha) = \frac{\int H(\alpha',\alpha)d\alpha'}{\iint H(\alpha',\alpha)d\alpha'd\alpha} \tag{146}$$

and

$$\overline{I_i^2}$$

$$= 1/\iint H(\alpha',\alpha)d\alpha'd\alpha \tag{147}$$

Integrating over $\rho(\alpha)$ can also be used to estimate a $\bar{z}'$, where $\bar{z}'$ is defined by

$$\bar{z}' = \iint_{A_1} z(x,y)f(x,y)dxdy \tag{148}$$

and A_1 is a subregion of A. To do this, a subregion of the α space, $S(R_1,R_2)$ is defined, so that when α is in $S(R_1,R_2)$, the point $\left[x(R_1,R_2,\alpha),y(R_1,R_2,\alpha)\right]$ is in A_1. Then

$$I_i' = \int_{S_i(R_1,R_2)} z\left[x(R_1,R_2,\alpha),y(R_1,R_2,\alpha)\right]\frac{f\left[x(R_1,R_2,\alpha),y(R_1,R_2,\alpha)\right]}{h\left[x(R_1,R_2,\alpha),y(R_1,R_2,\alpha),\alpha\right]}\rho(\alpha)d\alpha \tag{149}$$

is an estimate of $\bar{z}'$ independently of the form of $\rho(\alpha)$ so long as $h(x,y,\alpha)$ is not zero for any (x,y) in A_1. The optimum $\rho(\alpha)$ is defined by:

$$I'(\alpha,\alpha') = \iint D(x,y)D(x',y')z(x,y)z(x',y') \frac{f(x,y)f(x',y')}{h(x,y,\alpha)h(x',y',\alpha')} dR_1 dR_2 \quad (150)$$

where

$$D(x,y) = \begin{cases} 1 & \text{if } (x,y) \text{ is in } A_1 \\ 0 & \text{otherwise} \end{cases} \quad (151)$$

and the other quantities have obvious definitions.

If the computer wishes to estimate the conditional expected value of $z(x,y)$ given that (x,y) is in A_1, then

$$\bar{z}(:A_1) = \iint_{A_1} z(x,y)f(x,y)dxdy \Big/ \iint_{A_1} f(x,y)dxdy \quad (152)$$

$$= \bar{z}'/P(A_1)$$

where $P(A_1)$ is the probability of the point (x,y) being in A. If $P(A_1)$ is not known, it can be estimated by

$$P(A_1) = \int_{S(R_1,R_2)} \frac{f\left[x(R_1,R_2,\alpha),y(R_1,R_2,\alpha)\right]}{h\left[x(R_1,R_2,\alpha),y(R_1,R_2,\alpha),\alpha\right]} \rho(\alpha)d\alpha \quad (153)$$

15. Systematic Sampling (B)

Instead of solving the equation

$$\int_{-\infty}^{x_i} f(x)dx = R_1 \tag{154}$$

for x_i, it may be simple to select the x_i systematically by solving the equation

$$\int_{-\infty}^{x_i} f(x)dx = \frac{i-1/2}{N} \qquad i = 1, 2, \ldots, N \tag{155}$$

Used in the right places, it is almost always true that systematic sampling in x is relatively or completely cost free.

The expected value of $z(x_i,y_i)$ will not in general be appreciably changed by this process. However, the purpose of using $(i - 1/2)/N$ is to pick systematically the midpoint of the N intervals defined by

$$\int_{x_i}^{x_{i+1}} f(x)dx = \frac{1}{N} \tag{156}$$

Always picking the midpoint may introduce biases. These are eliminated if Systematic Sampling is combined with random sampling by using $(i-R_1)/N$ instead of $(i-1/2)/N$. A different R_1 is used with every i.

The y_i can be obtained by a rejection technique or by solving the usual equation

$$\int_{-\infty}^{y_i} g(y:x)dy = R_2 \tag{157}$$

If this is done, the estimate is

$$\hat{z}_3 = \frac{1}{N}\sum_{1}^{N} z(x_i,y_i) \tag{158}$$

where the x_i are determined. The expected value of $\hat{z}_3$ is given by

$$\overline{\hat{z}_3} = \frac{1}{n}\sum_{1}^{N} \bar{z}(:x_i) \tag{159}$$

There is no averaging over the x_i since they are determinate, not random, quantities. However, from equations (155) and (156)

$$\frac{1}{N} \approx f(x_i)\Delta x_i \tag{160}$$

Substituting in equation (159)

$$\overline{\hat{z}_3} \approx \sum_{1}^{N} \bar{z}(:x_i)f(x_i)\Delta x_i \tag{161}$$

$$\approx \int \bar{z}(:x)f(x)dx$$

$$= \bar{z}$$

The variance is easily calculated.

$$V_3 = \overline{(\hat{z}_3 - \overline{\hat{z}_3})^2}$$

$$= \overline{\left\{\frac{1}{N}\sum \left[z(x_i,y_i) - z(:x_i)\right]\right\}^2}$$

$$= \frac{1}{N^2}\sum \overline{\left[z(x_i,y_i) - \bar{z}(:x_i)\right]^2}$$

$$= \frac{1}{N^2} \sum \sigma^2(:x_i)$$

$$\approx \frac{1}{N} \sum \sigma^2(:x_i) f(x_i) \Delta x_i$$

$$\approx \frac{1}{N} \overline{\sigma^2(:x)} \tag{162}$$

The saving over Straightforward Sampling is simply (see equation (108))

$$V_1 - V_3 \approx \frac{1}{N} \overline{\left[\bar{z}(:x) - \bar{z}\right]^2} \tag{163}$$

The variance due to the variation of $\bar{z}(:x)$ has been eliminated.

It is possible to do Systematic Sampling in the x and y spaces simultaneously, in a sense, by also taking a set of numbers $\frac{j-1/2}{N}$, $j = 1, 2, \ldots, N$ and randomly sorting them. These numbers can then be substituted for R_2 in equation (157). Whether the sort is costly or not depends on the computing equipment being used.

If Systematic Sampling is used in both the x and y spaces, the variance is still further reduced and the improvement becomes (as shown in Appendix V)

$$V_1 - V_3 = \frac{1}{N} \left\{ \overline{\left[\bar{z}(:x) - \bar{z}\right]^2} + \overline{\left[\bar{z}(:j) - \bar{z}\right]^2} \right\} \tag{164}$$

where $\bar{z}(:j)$ is defined by

$$\int_{-\infty}^{y_j(x)} g(y:x)dy = \frac{j-1/2}{N}$$

$$\bar{z}(:j) = \int_{-\infty}^{\infty} z\left[(x_1 y_j(x)\right] f(x)dx \tag{165}$$

$\bar{z}(:j)$ is a sort of analogue in the y space to $\bar{z}(:x)$. If for any reason it is inconvenient to randomly sort the numbers $\frac{j-1/2}{N}$ and if $\overline{\left[\bar{z}(:j) - \bar{z}\right]^2}$ is greater than $\overline{\left[\bar{z}(:x) - \bar{z}\right]^2}$, then the x can be sampled at random and the y systematically. In this case the variance is only reduced by $\overline{\left[\bar{z}(:j) - \bar{z}\right]^2}$.

Equation (164) indicates that the variance V associated with the ordinary Monte Carlo calculation of an n-dimensional integral must be larger than the sum of n terms of the type $\overline{\left[\bar{z}(:i) - \bar{z}\right]^2}$, one for each dimension. If all the terms are of the same order of magnitude, then doing Systematic Sampling on any one variable will reduce the variance by less than V/n. While this implies that there will be no spectacular gains by doing Systematic Sampling, as already mentioned it is usually costless to use it.

16. Stratified Sampling (B)

In Stratified Sampling, equation (155) of Systematic Sampling is replaced by

$$\frac{1}{\bar{s}} \int_{-\infty}^{x_i} s(x)f(x)dx = \frac{i-1/2}{N} \tag{166}$$

where

$$\bar{s} = \int_{-\infty}^{\infty} s(x)f(x)dx$$

and $s(x)$ is an arbitrary positive function. Here $s(x)$ is the $f^*(x)/f(x)$ of Importance Sampling. The estimate is

$$\hat{z}_4 = \frac{1}{N} \bar{s} \sum_{i=1}^{N} \frac{z(x_i,y_i)}{s(x_i)} \tag{167}$$

where the y_i are chosen randomly. The expected value of the estimate is

$$\overline{\hat{z}_4} = \frac{1}{N} \bar{s} \sum \frac{\bar{z}(x_i)}{s(x_i)} \tag{168}$$

It is easy to see that $\overline{\hat{z}_4}$ is equal to $\bar{z}$ for

$$\frac{1}{N} \bar{s} = \int_{x_i}^{x_{i+1}} s(x)f(x)dx \tag{169}$$
$$\approx s(x_i)f(x_i)\Delta x_i$$

If this value of $\frac{1}{N} \bar{s}$ is substituted into (168)

$$\bar{\hat{z}}_4 \approx \sum \bar{z}(:x_i) f(x_i) \Delta x_i$$

$$\approx \bar{z}$$

The variance is given by

$$V_4 = \overline{(\hat{\bar{z}}_4 - \bar{\hat{z}}_4)^2} \qquad (170)$$

$$= \left\{ \frac{1}{N} \bar{s} \sum \frac{\left[z(x_i, y_i) - \bar{z}(:x_i) \right]}{s(x_i)} \right\}^2$$

$$= \frac{1}{N^2} \bar{s}^2 \sum \frac{\left[z(x_i, y_i) - \bar{z}(:x_i) \right]^2}{s^2(x_i)}$$

$$= \frac{1}{N^2} \bar{s}^2 \sum \frac{\sigma^2(:x_i)}{s^2(x_i)}$$

$$\approx \frac{1}{N} \bar{s} \sum \frac{\sigma^2(:x_i)}{s^2(x_i)} s(x_i) f(x_i) \Delta x_i$$

$$\approx \frac{1}{N} \bar{s} \int \frac{\sigma^2(:x)}{s(x)} f(x) dx$$

$$= \frac{1}{N} \left[\int s(x) f(x) dx \right] \left[\int \frac{\sigma^2(:x)}{s(x)} f(x) dx \right]$$

Ideally $s(x)$ is chosen to minimize V_4.

Varying $s(x)$

$$\delta V_4 = \frac{1}{N} \left\{ \left[\int f(x) \delta s(x) dx \right] \left[\int \frac{\sigma^2(:x)}{s(x)} f(x) dx \right] - \left[\int s(x) f(x) dx \right] \left[\int \frac{\sigma^2(:x)}{s^2(x)} f(x) \delta s(x) dx \right] \right\} \qquad (171)$$

$$= 0$$

Equating coefficients of $\delta s(x)$ and cancelling $\frac{1}{N} f(x)$,

$$\frac{\sigma^2(:x)}{s^2(x)} \int s(x) f(x) dx = \int \frac{\sigma^2(:x)}{s(x)} f(x) dx \tag{172}$$

The minimum V_4 is obtained by taking

$$s(x) = \sigma(:x) \tag{173}$$

Then

$$V_4 = \frac{1}{N} \bar{s} \int \frac{\sigma^2(:x)}{s(x)} f(x) dx \tag{174}$$

$$= \frac{1}{N} \overline{\sigma(:x)}^2$$

$$V_1 - V_4 = \frac{1}{N} \left\{ \overline{\left[\sigma(:x) - \overline{\sigma(:x)}\right]^2} + \overline{\left[\bar{z}(:x) - \bar{z}\right]^2} \right\} \tag{175}$$

In many cases it is more convenient to take $s(x)$ proportional to $|\bar{z}(:x)|$. If this is done

$$V_4 = \frac{1}{N} \bar{z} \left[\overline{\frac{\sigma^2(:x)}{|\bar{z}(:x)|}} \right] f(x) dx \tag{176}$$

As can be seen from equation (129), this variance is the same as would have been obtained if the sampling on $f^*(x)$ had been done randomly rather than systematically.

However, it is usually better to do the sampling systematically because for a general $f^*(x)$ the difference in variance between the two techniques is

$$V_2 - V_4 = \frac{1}{N}\left[\int \frac{\overline{z}^2(x)f^2(x)}{f^*(x)} - \bar{z}^2 - \int \frac{\sigma^2(x)f^2(x)}{f^*(x)}dx\right]$$

$$= \frac{1}{N}\left[\int \frac{\bar{z}^2(x)f^2(x)}{f^*(x)}dx - \bar{z}^2\right] \qquad (177)$$

$$\geq 0$$

since $V_2 - V_4$ is the variance associated with doing Importance Sampling on the integral $\int \bar{z}(x)f(x)dx$. Therefore, where it is easy to use Stratified Sampling, it is preferable to Importance Sampling.

17. Use of Expected Values (B)

If it is possible to calculate analytically

$$\bar{z}(:x) = \int z(x,y)g(y:x)dy \tag{178}$$

then this analytic calculation can be used in the sampling. $\bar{z}$ can be estimated by

$$\hat{z}_5 = \frac{1}{N}\sum \bar{z}(:x_i) \tag{179}$$

where the x_i are picked out of $f(x)$. If this is done

$$V_5 = \frac{1}{N}\overline{\left[\bar{z}(:x) - \bar{z}\right]^2} \tag{180}$$

and

$$V_1 - V_5 = \frac{1}{N}\overline{\sigma^2(:x)} \tag{181}$$

The reader should not conclude from the trivial nature of the example that the technique is not valuable. As is shown in the chapters on applications, the use of expected values is often sufficient to change what would have been a hard problem into an easy one. For a sort of corollary of this type of sampling see the example at the end of the next section.

18. Correlation (B)

Only one of the three situations mentioned in Section 9 on Correlation (A) will be discussed in detail. That is: given that

$$\bar{v} = \iint_A v(x',y')g(x',y')dx'dy' \tag{182}$$

is known, how can this knowledge be used to reduce the variance of the estimate of

$$\bar{z} = \iint_A z(x,y)f(x,y)dxdy \tag{183}$$

The first part of this section will briefly discuss some of the alternatives available to the calculation. However, exactly what role these alternatives should play depends on the specific application.

It will be assumed at first that the correlation is to be done on the x space only and that the y's in the two problems are to be picked independently. There are then at least two different ways in which this can be done:

1. To use the same random numbers in picking x and x',

   i.e., let

$$F(x_i) = G(x_i') = R_i \tag{184}$$

   We can write

$$x(R) = F^{-1}(R) \tag{185}$$

and the problem can now be put in the form

$$\bar{z} = \iiint \left\{ z\left[x(R),y\right] - \alpha_1 v\left[x'(R),y'\right] \right\} f\left[y:x(R)\right] g\left[y':x'(R)\right] dydy'dR + \alpha_1 \bar{v} \qquad (186)$$

$$= \iint \left\{ z\left[x(R),y\right] f\left[y:x(R)\right] - \alpha_1 v\left[y,x'(R)\right] g\left[y:x'(R)\right] \right\} dydR + \alpha_1 \bar{v}$$

2. to pick both x and x' from the same p.d.f. and then to use weighting factors as in importance sampling. In this case the problem is transformed to

$$\bar{z} = \iiint \left[z(x,y) \frac{f(x)}{f^*(x)} - \alpha_2 v(x,y') \frac{g(x)}{f^*(x)} \right] g(y':x) f(y:x) f^*(x) dy'dydx + \alpha_2 \bar{v} \qquad (187)$$

$$= \iint \left[z(x,y) \frac{f(y,x)}{f^*(x)} - \alpha_2 \frac{v(x,y) g(y,x)}{f^*(x)} \right] f^*(x) dydx + \alpha_2 \bar{v}$$

The α's are to be chosen to minimize the variances of the respective estimates. $f^*(x)$ can be any arbitrary p.d.f. but it is usually convenient to let it be either $f(x)$ or $g(x)$. It can, however, be chosen to minimize the variance of $\hat{z}_6$.

As in Section 9, the variance of both estimates can be written

$$V_6 = \frac{1}{N} \left(\sigma_1^2 - 2\alpha\rho\sigma_1\sigma_2 + \alpha^2\sigma_2^2 \right) \qquad (188)$$

where $\hat{z}_6$ is respectively:

1. $\hat{z}_6 = \frac{1}{N} \sum \left[z(x_i,y_i) - \alpha_1 v(x_i',y_i') + \alpha_1 \bar{v} \right]$

2. $\hat{z}_6 = \frac{1}{N} \sum \left[z(x_i,y_i) \frac{f(x_i)}{f^*(x_i)} - \alpha_2 v(x_i,y_i') \frac{g(x_i)}{f^*(x_i)} + \alpha_2 \bar{v} \right]$

In the first case

$$\sigma_1^2 = \int_{-\infty}^{\infty}\int_{0}^{1} z^2\left[x(R),y\right] f\left[y:x(R)\right] dydR - \bar{z}^2 \tag{189}$$

$$= \iint_A z^2(x,y) f(x,y) dxdy - \bar{z}^2$$

$$\sigma_2^2 = \int_{-\infty}^{\infty}\int_{0}^{1} v^2\left[x'(R),y'\right] g(y':x') dy'dR - \bar{v}^2 \tag{190}$$

$$= \iint_A v^2(x',y') g(x',y') dx'dy' - \bar{v}^2$$

$$\rho\sigma_1\sigma_2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{1} \left\{ z\left[x(R),y\right] - \bar{z} \right\} \left\{ v\left[x'(R),y'\right] - \bar{v} \right\} \tag{191}$$
$$f\left[y:x(R)\right] g\left[y':x'(R)\right] dydy'dR$$

$$= \int_0^1 \left\{ \bar{z}\left[:x(R)\right] - \bar{z} \right\} \left\{ \bar{v}\left[:x'(R)\right] - \bar{v} \right\} dR$$

and in the second case

$$\sigma_1^2 = \iint_A \left[\frac{z(x,y)f(x)}{f^*(x)}\right]^2 f(y:x) f^*(x) dxdy - \bar{z}^2 \tag{192}$$

$$= \iint_A \frac{z^2(x,y)f^2(x)}{f^*(x)} f(x,y) dxdy - \bar{z}^2$$

$$\sigma_2^2 = \iint_A \left[\frac{v(x,y)g(x)}{f^*(x)}\right]^2 g(y:x)f^*(x)dxdy - \bar{v}^2 \qquad (193)$$

$$= \iint_A \frac{v^2(x,y)g^2(x)}{f^*(x)}\, g(x,y)dxdy$$

$$\rho\sigma_1\sigma_2 = \iiint z(x,y)\frac{f(x)}{f^*(x)}\, v(x,y')\frac{g(x)}{f^*(x)} f(y:x)g(y':x)f^*(x)dxdydy' - \bar{z}\,\bar{v} \qquad (194)$$

$$= \int \frac{\bar{z}(:x)\bar{v}(:x)f(x)g(x)}{f^*(x)}\, dx - \bar{z}\,\bar{v}$$

The two types of correlation mentioned above are actually special cases of a third more general type in which x is selected from the p.d.f. $f^*(x)$ and x' from the p.d.f. $g^*(x)$; the same random numbers being used in each case and the weighting factors $f(x)/f^*(x_i)$ and $g(x_i')/g^*(x_i')$ being used with their respective functions.

It is also possible to correlate the y and pick the x independently. For the first type of correlation it is then necessary to introduce functions $y_R(x)$ and $y_R'(x)$ defined by:

$$\int_{-\infty}^{y_R} f(y:x)dy = R$$

$$0 \le R \le 1 \qquad (195)$$

$$\int_{-\infty}^{y_R'(x)} g(y:x)dy = R$$

If $R = (j-1/2)/N$ then $y_R(x)$ is identical with the $y_j(x)$ discussed in Section 15 on Systematic Sampling. The correlating is done by picking x and x' independently from $f(x)$ and $f(x')$ respectively, but always

picking the same R curve when picking y and y'. One way to do this is to pick y from the conditional p.d.f. f(y:x); identify the R curve to which this value of y belongs; and then let $y' = y'_R(x')$. If this type of correlation is done σ_1^2 and σ_2^2 are unchanged but $\rho\sigma_1\sigma_2$ becomes:

$$- \iiiint z(x,y)v(x',y')\delta\left[y' - y'_{R(y)}\right]f(x,y)g(x',y')dxdydx'dy' - \bar{z}\bar{v} \quad (196)$$

where $\delta\left[y' - y'_{R(y)}\right]$ is the Dirac delta function. Its presence in the integrand guarantees that y' falls on the same R curve as y.

In the second way of correlating y, the x and x' are still picked independently from f(x) and g(x') but y and y' are identical and picked out of a p.d.f. f*(y:x,x'). These two ways of correlating y can also be considered as a special case of a general correlation method in which y is picked out of f*(y:x,x') and y' from g*(y':x,x'), using the same random number in both picks. The usual estimate

$$\hat{z}_6 = \frac{1}{N}\sum\left[z(x_i,y_i)\frac{f(y_i,x_i)}{f^*(y_i:x_i,x'_i)} - \alpha v(x'_i,y'_i)\frac{g(y':x')}{g^*(y':x,x')}\right] + \alpha\bar{v} \quad (197)$$

is then used. By allowing the conditional p.d.f.'s f*(y:x,x') and g*(y':x,x') to depend on both x and x', the computer obtains the flexibility he needs to maximize the correlation between the two problems. It is of course possible to correlate both the x and y spaces simultaneously.

No matter how the correlating is done, the optimum α still is given by

$$\alpha = \rho\frac{\sigma_1}{\sigma_2} \quad (198)$$

The variance if this optimum α is used is

$$V_6 = \frac{1}{N} \sigma_1^2(1 - \rho^2) \tag{199}$$

and all the comments made in Section 9 about estimating α still apply.

Averaging Several Estimates

Sometimes the computer has K estimates $\hat{z}_1, \ldots, \hat{z}_K$ of $\bar{z}$. When this occurs the computer can use a weighted average

$$\hat{z} = \sum_{k=1}^{K} \alpha_k \hat{z}_k \tag{200}$$

with the condition that as an estimate of $\bar{z}$

$$\sum \alpha_k = 1 \tag{201}$$

The variance of the estimate is

$$V = \overline{\left[\sum \alpha_k (\hat{z}_k - \bar{z}) \right]^2} \tag{202}$$

$$= \sum_{k,k'} \alpha_k \alpha_{k'} \rho_{kk'} \sigma_k \sigma_{k'}$$

where $\rho_{kk'}$ is the correlation coefficient between $\hat{z}_k$ and $\hat{z}_{k'}$, and $\rho_{kk} = 1$. V is to be minimized subject to the condition that $\sum \alpha_k = 1$.

$$\frac{\partial V}{\partial \alpha_k} = 2 \sum_{k'} \alpha_{k'} \rho_{kk'} \sigma_k \sigma_{k'} \tag{203}$$

Let

$$\lambda = \sum_{k'} \alpha_{k'} \rho_{kk'} \sigma_k \sigma_{k'} \tag{204}$$

If b_{ik} is an element of the inverse of the symmetric matrix $\|\rho_{kk'}\sigma_k\sigma_{k'}\|$, then

$$\sum_k b_{ik}\rho_{kk'}\sigma_k\sigma_{k'} = \begin{cases} 1 & \text{if } i = k \\ 0 & \text{if } i \neq k \end{cases} \tag{205}$$

Equation (205) can be considered as defining the b_{ik}. If equation (204) is multiplied by b_{ik} and summed on k, then

$$\alpha_i = \lambda \sum_k b_{ik} \tag{206}$$

Hence by the condition on the α's,

$$\lambda = 1/\sum_{i,k} b_{ik} \tag{207}$$

By substituting equation (206) in (202), and using (201) and (205), it follows that the minimum value of V is given by

$$\begin{aligned} V &= \lambda \\ &= 1/\sum_{i,k} b_{ik} \end{aligned} \tag{208}$$

There are two cases of special interest:

1. The $\hat{z}_k$ are independent ($\rho_{kk'} = 0$).

$$b_{kk'} = \begin{cases} 1/\sigma_k^2 & \text{for } k = k' \\ 0 & \text{for } k \neq k' \end{cases} \tag{209}$$

$$V = \lambda$$

$$= 1/\sum_{k=1}^{K} 1/\sigma_k^2 \tag{210}$$

$$\alpha_k = \frac{1}{\sigma_k^2 \sum_{k=1}^{K} 1/\sigma_k^2} \tag{211}$$

2. There are only two z_k. Then letting $\sigma_2/\sigma_1 = \gamma$ and $\rho_{12} = \rho_{21} = \rho$,

$$V = \lambda = \frac{\sigma_1^2\sigma_2^2(1 - \rho^2)}{\sigma_1^2 - 2\rho\sigma_1\sigma_2 + \sigma_2^2} \tag{212}$$

$$= \sigma_1^2 \frac{1 - \rho^2}{1 - 2\rho\gamma + \gamma^2}$$

$$\alpha_1 = \frac{\sigma_2^2 - \rho\sigma_1\sigma_2}{\sigma_1^2 - 2\rho\sigma_1\sigma_2 + \sigma_2^2} \tag{213}$$

$$= \frac{\gamma^2 - \rho\gamma}{1 - 2\rho\gamma + \gamma^2}$$

$$\alpha_2 = \frac{\sigma_1^2 - \rho\sigma_1\sigma_2}{\sigma_1^2 - 2\rho\sigma_1\sigma_2 + \sigma_2^2} \tag{214}$$

$$= \frac{1 - \rho\gamma}{1 - 2\rho\gamma + \gamma^2}$$

If σ_2 is greater than σ_1 then the factor $\frac{1-\rho^2}{1-2\rho\gamma+\gamma^2}$ can be considered as measuring the amount by which the variance of $\hat{z}_1$ is cut down if it is weighted in an optimum fashion with another random variable which has the same expected value but a larger variance. Curves of this factor as a function of ρ and γ are given in graph number 1.

Eliminating the Variance of $\bar{z}(:x)$

If $f(x)$ is simple enough so that integrals of the type $\bar{v} = \int v(x)f(x)dx$ can be calculated, then the problem of equation (186) can be reduced to the following special case:

$$\bar{z} = \iint \left\{ z\left[x(R),y\right] - v\left[x(R)\right] \right\} g\left[y:x(R)\right] dydR + \bar{v} \qquad (215)$$

The problem is to determine $v(x)$ so that $\overline{z_6^2}$ is a minimum where

$$\overline{z_6^2} = \iint \left\{ z\left[x(R),y\right] - v\left[x(R)\right] + \bar{v} \right\}^2 g\left[y:x(R)\right] dydR \qquad (216)$$

$$= \overline{z^2} + \overline{v^2} + \bar{v}^2 - 2\int \bar{z}(:x)v(x)f(x)dx + 2\bar{v}\bar{z} - 2\bar{v}^2$$

$$= z^2 + \overline{v^2} - 2\int \bar{z}(:x)v(x)f(x)dx + 2\,\bar{v}\bar{z} - \bar{v}^2$$

If $v(x)$ makes $\overline{z_6^2}$ a minimum then to first order $\overline{z_6^2}$ will not change when $v(x)$ is replaced by $v(x) + \delta v(x)$. So

$$\delta\overline{z_6^2} = \delta\overline{v^2} - 2\delta\int \bar{z}(:x)v(x)f(x)dx + 2\bar{z}\delta\bar{v} - \delta\bar{v}^2 \qquad (217)$$

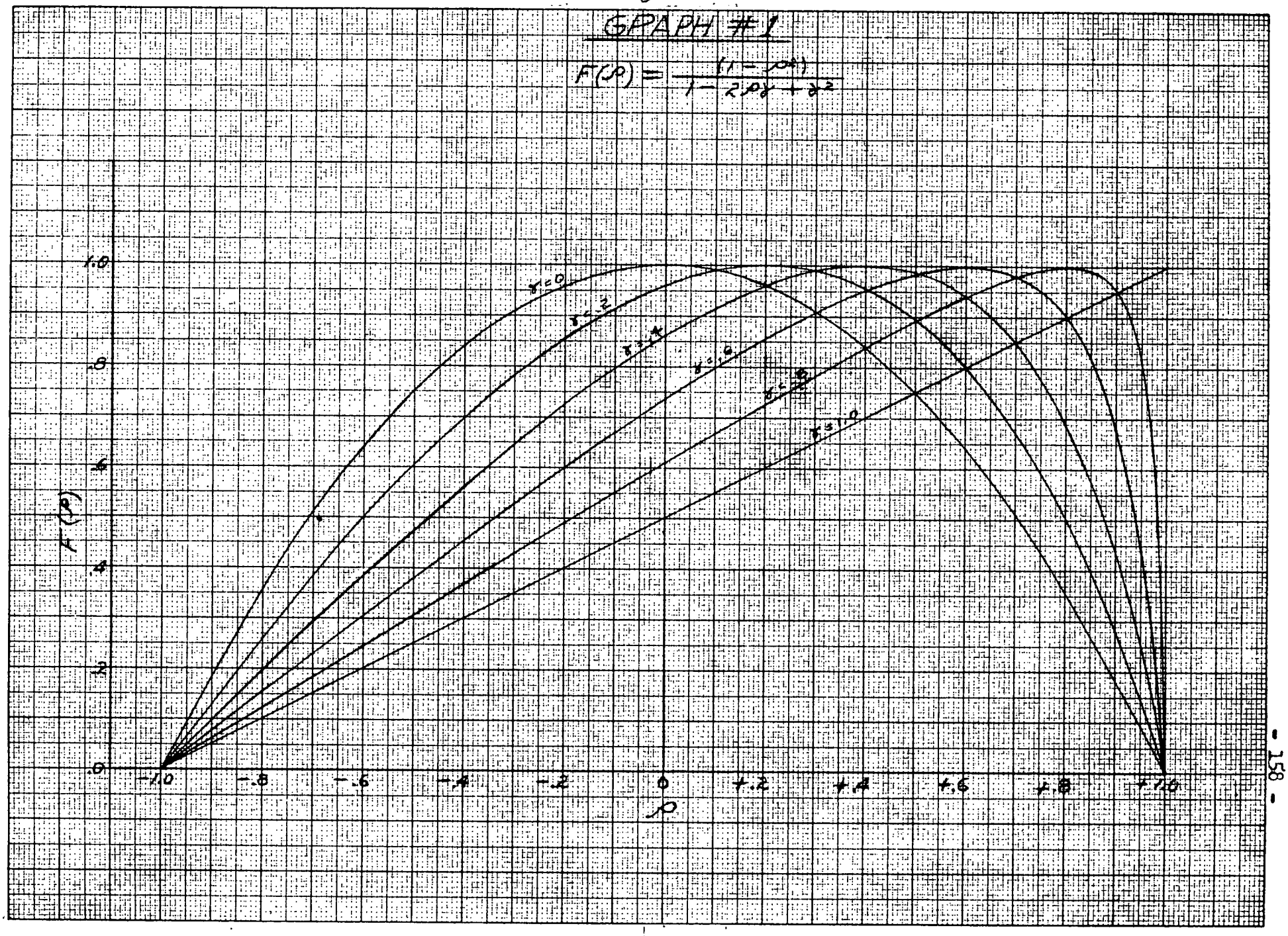
$$= 2\int v(x)\delta v(x)f(x)dx - 2\int \bar{z}(:x)\delta v(x)f(x)dx$$

$$+ 2\bar{z}\int \delta v(x)f(x)dx - 2\bar{v}\int \delta v(x)f(x)dx$$

$$= 0$$

GRAPH #1

$$F(\rho) = \frac{(1-\rho^2)}{1-2\rho\gamma+\gamma^2}$$



All the integrands can be collected together. The coefficient of $\delta v(x)$ must be zero because $\delta v(x)$ is arbitrary. This gives for the optimum $v(x)$:

$$v(x) = \bar{z}(:x) + \bar{z} - \bar{v} \tag{218}$$

Then $v(x)$ can be put equal to $\bar{z}(:x)$. If this $v(x)$ is used, $\overline{z_6^2}$ (equation 216) becomes:

$$\overline{z_6^2} = \overline{z^2} + \overline{\bar{z}^2(:x)} - \overline{2\bar{z}^2(:x)} + 2\bar{z}^2 - \bar{z}^2 \tag{219}$$

$$= \overline{z^2} - \overline{\bar{z}^2(:x)} + \bar{z}^2$$

$$V_6 = \overline{z^2} - \overline{\bar{z}^2(:x)} \tag{220}$$

$$= \overline{\left[z(x,y) - \bar{z}(:x)\right]^2}$$

$$= \overline{\sigma^2(:x)}$$

which is the same as $(V_1 - V_5)$ (equation 180)). One of the implications of the above formula is that if the computer knows $\bar{z}(:x)$ approximately, he can still take advantage of this knowledge without introducing a bias into the calculation so long as he has an exact, or at least fairly accurate knowledge, of the expected value of this approximate $\bar{z}(:x)$. In some cases (Section 6, Part III), it may be convenient to do a sort of reverse problem by:

a. First estimate $\overline{z(x,y)}$ directly by any standard technique.

b. Use the data of "a" to obtain an approximate $\bar{z}(x)$ and let $v(x)$ equal this approximate $\bar{z}(x)$.

c. Calculate accurately $\bar{v} = \int v(x)f(x)dx$ by some numerical or Monte Carlo technique.

d. Re-estimate $\bar{z}$ by using the data of "a" in

$$\hat{z}_6 \approx \frac{1}{N} \sum_{i=1}^{N} \left[z(x_i, y_i) - v(x_i) + \bar{v} \right] \qquad (221)$$

It would not be reasonable to estimate $\bar{v}$ in "c" by Monte Carlo unless the cost of picking x and evaluating $v(x)$ is much less than the cost of picking (x,y) and evaluating $z(x,y)$. The bookkeeping is very much simplified if $v(x)$ is restricted to the form $a + bx + cx^2$. In this case "c" can be used to estimate $\bar{x}$ and $\overline{x^2}$ in advance and then "a" can be used to pick reasonable values of a, b, and c. If the form, $a + bx + cx^2$, is not accurate enough, the range of x can be broken up into intervals, and a separate form used for each interval.

19. Russian Roulette and Splitting (B)

The continuous analogue of Section 10 is put here for the sake of completeness though the details are close enough so that the reader is referred to that section for them.

A general Russian Roulette and Splitting procedure can be described as follows:

Let the x space be divided into two regions, R_1 and R_2. Select a value of x. If it lies in R_1, Russian Roulette is done with probability

$$q(x) = \lambda U_1(x) \tag{222}$$

If it lies in R_2, n(x) independent values of y are selected for each x with

$$n(x) \simeq \lambda U_2(x) \tag{223}$$

The variance of the above process is

$$V_7 = V_o + \frac{V_o'}{\lambda} \tag{224}$$

$$V_o = \int_{R_2} \bar{z}^2(x) f(x)dx - \bar{z}^2 \tag{225}$$

$$V_o' \simeq \int_{R_1} \frac{\bar{z}^2(x)}{U_1(x)} f(x)dx + \int_{R_2} \frac{\sigma^2(x)}{U_2(x)} f(x)dx \tag{226}$$

where the "$\simeq$" sign is used in the last equation because n(x) must be integral and is therefore only approximately equal to $\lambda U_2(x)$. If C_o is the cost of picking x, $C_1(x)$, the cost of picking y and evaluating z(x,y), and C the total marginal cost of a sample; then

$$C = C_o + \lambda C_o' \tag{227}$$

$$C_o' = \int_{R_1} U_1(x)C_1(x)f(x)dx + \int_{R_2} U_2(x)C_1(x)f(x)dx \tag{228}$$

The value of λ that minimizes CV_7 is

$$\lambda^2 = \frac{C_o}{V_o} \cdot \frac{V_o'}{C_o'} \tag{229}$$

With this value of λ,

$$V_7 = V_o + \sqrt{\frac{V_o}{C_o}}\sqrt{V_o'C_o'} \tag{230}$$

$$C = C_o + \sqrt{\frac{C_o}{V_o}}\sqrt{V_o'C_o'} \tag{231}$$

$$\frac{V_7}{C} = \frac{V_o}{C_o} \tag{232}$$

V_o is an approximately fixed variance; C_o is a fixed cost. The optimum choice of λ makes the actual cost and variance proportional to the fixed cost and variance. If the computer chooses $q(x)$ and $n(x)$ in optimum fashion, then

$$U_1(x) = \sqrt{z^2(x)/C_1(x)} \tag{233}$$

$$U_2(x) = \sigma(x)/\sqrt{C_1(x)} \tag{234}$$

With this optimum choice,

$$V_o' = \int_{R_1} \sqrt{z^2(x)C_1(x)}\, f(x)dx + \int_{R_2} \sigma(x)\sqrt{C_1(x)}\, f(x)dx \tag{235}$$

$$= C_o'$$

and the ratio of the cost contributed by any x sub-region to the variance contributed by the same region is

$$\lambda^2 = \frac{C_o}{V_o} = \frac{C}{V_7} \tag{236}$$

If the sampling is optimum, the region R_1 is chosen as large as possible as determined by the equation,

$$\lambda^2 \frac{\overline{z^2(:x)}}{C_1(x)} \leq 1 \tag{237}$$

As mentioned previously, (236) and (237) are really simultaneous equations for λ and R_1.

In many cases it is inconvenient to use Splitting and the computer uses only Russian Roulette. In this situation,

$$q(x) = \lambda U(x) \qquad x \text{ in } R_1 \tag{238}$$

$$n(x) = 1 \qquad x \text{ in } R_2$$

$$V_7 = V_o + \frac{1}{\lambda} \int_{R_1} \frac{\overline{z^2(:x)}}{U(x)} f(x)dx + \int_{R_2} \sigma^2(:x) f(x)dx \tag{239}$$

where

$$V_o = \int_{R_2} \bar{z}^2(:x) f(x)dx - \bar{z}^2$$

$$C = C_o + \lambda \int_{R_1} U(x) C_1(x) f(x)dx + \int_{R_2} C_1(x) f(x)dx \tag{240}$$

The optimum λ is given by

$$\lambda^2 = \frac{C_o + \int_{R_2} C_1(x) f(x)dx}{V_o + \int_{R_2} \sigma^2(:x) f(x)dx} \cdot \frac{\int_{R_1} \frac{\overline{z^2(:x)}}{U(x)} f(x)dx}{\int_{R_1} U(x) C_1(x) f(x)dx} \tag{241}$$

$$= \frac{C_o + \int_{R_2} C_1(x)f(x)dx}{\int_{R_2} \overline{z^2}(:x)f(x)dx - \bar{z}^2} \frac{\int_{R_1} \frac{\overline{z^2}(:x)}{U(x)}f(x)dx'}{\int_{R_1} U(x)C_1(x)f(x)dx}$$

$$\frac{C}{V_7} \frac{\int_{R_1} \frac{\bar{z}^2(:x)}{U(x)}f(x)dx}{\int_{R_1} U(x)C_1(x)f(x)dx}$$

where the approximation assumes that the integral over R_2 is replaced by an integral over all space. If $U(x)$ is chosen in optimum fashion,

$$U(x) = \sqrt{\overline{z^2}(:x)/C_1(x)} \tag{242}$$

$$\lambda^2 \approx \frac{C}{V_7} \tag{243}$$

and the region R_1 for Russian Roulette can be taken as being determined by

$$\frac{\lambda^2\overline{z^2}(:x)}{C_1(x)} = \frac{C}{V_7}\frac{\overline{z^2}(:x)}{C_1(x)} \leq 1 \tag{244}$$

Application to Particle Diffusion

A special case of some interest involving three random variables (X,W,M) arises in particle diffusion problems. X is a generalized position variable which represents the position and momentum of the particle. W is a pseudo weight that is assigned to the particle, and which changes as the particle jumps from point to point. M is the final weight of the particle divided by the current weight. It is convenient to think of it the other way, as a factor which multiplies the current weight when the

random walk is terminated. The function whose expected value is desired is the final weight of the particle; so

$$z(x, w, m) = wm \tag{245}$$

where if ordinary sampling were being done the m would be independent of w. However, if the w happened to be very small one would be willing to sample m rather inaccurately if it saved some cost; if it were large one would want to sample m quite accurately even if it were expensive. This is thus a natural problem on which to use Russian Roulette and Splitting.

The regions R_1 and R_2 will be defined in the (x,w) space and the decisions of Russian Roulette or Splitting concern the number of m values that are to be picked for an (x,w) value.

In discussing particles it is convenient to change the language slightly. Instead of speaking of picking n independent values of m for each (x,w) in region R_2, the particle is said to split into n independent particles each of weight w/n. Similarly in region R_1 if the particle loses the Russian Roulette it is said to have died (or disappeared); if it wins it is assigned a new weight, w/q(x,w) and its random walk continued.

In the case of most interest the p.d.f. for (X, W, M) (after the Russian Roulette and Splitting has been done) has the special from, g(m:x)f(x,w); that is the conditional p.d.f. of m is not dependent on W. (The plausibility of the assumption is discussed below.) With this assumption,

$$\overline{z^2}(:x,w) = w^2\overline{m^2}(:x) \tag{246}$$

$$\sigma^2(:x,w) = w^2\left[\overline{m^2}(:x) - \bar{m}^2(:x)\right] \tag{247}$$

Since the cost of picking an m value is independent of w, the optimum choice of q(x,w) and n(x,w) is given by

$$q(x,w) = \lambda w \sqrt{\frac{\overline{m^2}(x)}{C_1(x)}}$$

$$n(x,w) = \lambda w \sqrt{\frac{\overline{m^2}(x) - \bar{m}^2(x)}{C_1(x)}} \qquad (248)$$

and regions R_1 and R_2 are determined as before by the appropriate inequalities. If the particle is in R_1 and happens to survive the Russian Roulette it is assigned a new weight

$$w' = \frac{w}{q(x,w)} = \frac{1}{\lambda} \sqrt{\frac{C_1(x)}{\overline{m^2}(x)}} \qquad (249)$$

If the particle is in R_2 then each of the n independent particles is given a weight.

$$w' = \frac{w}{n(x,w)}$$

$$= \frac{1}{\lambda} \sqrt{\frac{C_1(x)}{\overline{m^2}(x) - \bar{m}^2(x)}} \qquad (250)$$

In both cases, the final weight of the particle is independent of the original weight and is a function of x only. (This seems to be, in general, one of the criteria for a good sampling scheme for particle diffusion problems.) It is because the weight of the particle after collision is independent of the weight before collision that m can be taken to be independent of w.

Truncating Sample Series

Sometimes in doing a Monte Carlo problem instead of getting a single number for the estimate from a single sample, one obtains an infinite series; more precisely each sample generates a process for calculating an infinite series term by term, and it is the sums of these series which are to be averaged in obtaining the final estimate. This occurs most often in the Use of Expected Values.

The computer is then faced with the problem of terminating each of the sample series. This can be done by summing each series to a fixed number of terms or it can be done by summing until a term gets smaller than some previously assigned amount. Both of these methods are inefficient as one is then faced with either calculating a number of very small terms or truncating too soon and introducing an unknown bias into the estimate.

A much more effective method of terminating such sample series is made possible by the use of Russian Roulette. One can simply play the supplementary game of chance as soon as the terms in the series begin to get small. If a term fails to survive the supplementary game the series is terminated right then and there; if it survives, the weights of all subsequent terms are multiplied by the proper factor and the term by term summation continued until a new term becomes small. In this way the series can be terminated in a completely unbiased fashion and yet very little effort is spent computing small and insignificant numbers.

PART III

INTEGRAL EQUATIONS

PART III

TABLE OF CONTENTS

III INTEGRAL EQUATIONS[1]

Introduction and Definitions

The treatment of integral equations will follow as closely as possible the treatment of integrals in order to emphasize similarities and differences. Again there will be a certain amount of paraphrasing, but this time an attempt will be made to minimize it.

The problem is to estimate

$$\bar{z} = \iint_A z(x,y)M(x,y)dxdy \tag{1a}$$

by Monte Carlo. $M(x,y)$ is an unknown function which is determined by the integral equation

$$M(x,y) = \iint_A K(x,y:x',y')M(x',y')dx'dy' + M_o(x,y) \tag{1b}$$

$z(x,y)$, $K(x,y:x',y')$, and $M_o(x,y)$ are known. $K(x,y:x',y')$ is called the kernel of the integral equation. The above equation is known as a Fredholm equation. It arises naturally in many applications in physics, mathematics, and engineering. Associated with the Fredholm equation is another equation known as the adjoint equation.

$$S(x',y') = \iint_A S(x,y)K(x,y:x',y')dxdy + z(x',y'). \tag{2a}$$

It can be shown that

$$\bar{M}_o = \iint_A M_o(x',y')S(x',y')dx'dy' \tag{2b}$$

---

1 The reader is reminded that judicious skipping (or skimming) may be advisable. In most sections more details are given than are needed for applications.

The mathematician may find the chapter clearer if he realizes from the outset that we are here studying a Markoffian process in the three dimensional space (w,x,y). The process is specialized so that it is still Markoffian in any of the averages over w.

It should be obvious to the reader that almost anything said in this context about integral equations applies also to matrix equations.

$S(x',y')$ is now the unknown function. By multiplying Equation (1b) with $S(x,y)dxdy$ and Equation (2a) with $M(x',y')dx'dy'$ and integrating, it is easy to show that

$$\bar{z} = \overline{H}_o. \tag{3}$$

There are thus always two different sets of equations which can be used to calculate $\bar{z}$.

It is convenient to discuss the problem in terms of a random walk in which a particle jumps from one point to another, changing its weight by a factor which may depend on the initial and final positions every time it jumps. The points to which it jumps are called collision points. If it ever jumps outside a preassigned area, A, the particle is said to have been trapped or die and the random walk is terminated. It will be shown that $\bar{z}$ can be interpreted as the expected weight that jumps into a particular trap state and can be estimated a la Monte Carlo by performing N random walks and averaging the trapped weight of the N particles.[1]

Most of the applications of Monte Carlo to integral equations have actually been concerned with studying random walks. The author would, however, like to emphasize that for the purposes of this chapter their introduction is an expository device and does not limit in any way the class of integral equations which can be treated.

Before showing the connection between integral equations and random walks some definitions are needed:

$p(x,y:x',y')$ is the p.d.f. for the new non-trap position (x,y) of a particle that was at (x',y'). If $\int_A p(x,y:x',y')dxdy$ is < 1 then the particle has a non-zero probability of jumping directly to a trap state from (x',y').

---

1 See Sections on "Realization" and "Collisions Formulation" for a more detailed description of the random walk.

$p(:x',y') = 1 - \iint_A p(x,y:x',y')dxdy$ is the probability that a particle at the point (x',y') will be trapped instead of jumping to a new point in A. In some cases $p(:x',y')$ will be taken less than $1 - \iint_A p(x,y:x',y')dxdy$; in which case it is to be interpreted as the probability of jumping to a given one of several trap states.

$m(x,y:x',y')$ is the factor by which the weight of a particle is multiplied if it jumps from (x',y') to (x,y).

$m(:x,y)$ is the factor by which the weight of the particle is multiplied if it jumps to the trap state from (x,y).

$w_o(x,y)$ is the initial weight of a particle that starts at (x,y). The weight can have either sign, but in most problems it is positive.

w_i is the weight of the particle at the i'th collision.

$i = 0, 1, \ldots, I$.

$W = W = m(:x_I,y_I)w_I$ is the weight of the particle on being trapped.

$f_i(w,x,y)$ is the p.d.f. for the weight and position of a particle at the i'th collision. $\iiint_A f_i(w,x,y)dwdxdy$ is the probability that the particle has not been trapped by the i'th collision.

$P_i(x,y) = \int f_i(w,x,y)dw$ is the p.d.f. for the position of the particle at its i'th collision.

$M_i(x,y) = \int w f_i(w,x,y)dw$ is the expected weight (actually weight density) at (x,y) on the i'th collisiton. The expected weight of the particle itself is $M_i(x,y)/P_i(x,y)$.*

$Q_i(x,y) = \int w^2 f_i(w,x,y)dw$ is the expected square weight at (x,y) on the i'th collision. The expected square of the weight of the particle is $Q_i(x,y)/P_i(x,y)$.

$g_i(w:x,y)$ is the conditional probability that a particle that starts at (x,y) with weight one, is trapped in exactly i collisions with weight w.

$R_i(:x,y) = \int g_i(w:x,y)dw$ is the probability that a particle that starts at (x,y) is trapped directly after the i'th collision.

$S_i(:x,y) = \int w g_i(w:x,y)dw$ is the expected weight that is trapped after the i'th collision given that the particle starts at (x,y) with weight one. The expected weight of such a particle when it is trapped is $S_i(:x,y)/R_i(x,y)$.

$T_i(:x,y) = \int w^2 g_i(w:x,y)dw$ is the expected square weight that is trapped after the i'th collision given that the particle starts at (x,y) with weight one. The expected square of the weight of the particle when trapped is $T_i(:x,y)/R_i(:x,y)$.

$P(x,y) = \sum_0^\infty P_i(x,y)$ is the expected number of collisions that the particle makes at (x,y) before it is trapped.

---

* The somewhat stilted language is used to emphasize the difference between the notion of "expected weight of a particle," given that it is at a point and "expected weight" at the same point. The former is sometimes called the conditional expected value; the latter is equal to the former times the probability of the particle being there.

$M(x,y) = \sum_{0}^{\infty} M_n(x,y)$ is the total expected weight at (x,y), and similarly for $Q(x,y)$, $R(:x,y)$, $S(:x,y)$, and $T(:x,y)$.

Derivation of Integral Equations

The only way a particle can get to the point (x,y) in i ($i > 0$) collisions is to be at some point in A on its i-1'th collision and then jump to the point (x,y). Therefore,

$$P_i(x,y) = \iint_A p(x,y:x',y')P_{i-1}(x',y')dx'dy' \quad . \tag{4a}$$

Summing both sides from 1 to ∞

$$\sum_1^\infty P_i(x,y) = \iint_A p(x,y:x',y') \sum_1^\infty P_{i-1}(x',y')dx'dy' \tag{4b}$$

$$= \iint_A p(x,y:x',y') \sum_0^\infty P_i(x',y')dx'dy'$$

$$= \iint_A p(x,y:x',y')P(x',y')dx'dy' \quad ,$$

but $$\sum_1^\infty P_i(x,y) = \sum_0^\infty P_i(x,y) - P_o(x,y) \tag{5}$$

$$= P(x,y) - P_o(x,y) \quad ,$$

so $$P(x,y) = \iint_A p(x,y:x',y')P(x',y')dx'dy' + P_o(x,y) \quad . \tag{6}$$

Equation (6) is intuitively plausible. It states that the expected number of collisions at (x,y) is equal to the sum of the probabilities of all the ways in which a particle can have a collision at some other point and then jump to (x,y), plus the probability that the particle had its first collision at (x,y).

Similarly it can be shown that

$$M(x,y) = \iint_A m(x,y:x',y')p(x,y:x',y')M(x',y')dx'dy' + M_o(x,y) \qquad (7)$$

$$Q(x,y) = \iint_A m^2(x,y:x',y')p(x,y:x',y')Q(x',y')dx'dy' + Q_o(x,y) \qquad (8)$$

where $$M_o(x,y) = w_o(x,y)P_o(x,y) \qquad (9)$$

$$Q_o(x,y) = w_o^2(x,y)P_o(x,y) \ . \qquad (10)$$

If $m(x,y:x',y')$, $p(x,y,x',y')$, $w_o(x,y)$, and $P_o(x,y)$ are chosen so that

$$K(x,y,x',y') = m(x,y:x',y')p(x,y:x',y') \qquad (11)$$

$$w_o(x,y)P_o(x,y) = M_o(x,y) \ ,$$

then Equation (7) is identical with Equation (2). This is, of course, the identification which is intended.

The expected trapped weight is given by

$$\iint_A M(x,y)p(:x,y)m(:x,y)dxdy \ .$$

Therefore, if $m(:x,y)$ is taken to be

$$m(:x,y) = z(x,y)/p(:x,y) \ , \qquad (12)$$

the expected trapped weight is $\bar{z}$ (Equation 3) which completes the identification.

Equations can also be written for R(:x,y), S(:x,y) and T(:x,y). For example,

$$R_i(:x,y) = \iint_A R_{i-1}(:x',y')p(x',y':x,y)dx'dy' \qquad (13)$$

because the probability of being trapped in exactly i collisions is equal to the probability of jumping to somewhere else in A, times the probability of being trapped in i-1 collisions from the second point.

From Equation (13) it is easy to obtain

$$R(:x,y) = \iint_A R(:x',y')p(x',y':x,y)dx'dy' + R_o(:x,y) \qquad (14)$$

$$R_o(:x,y) = p(:x,y) .$$

This equation is also intuitively plausible. A particle can be trapped in two ways. It can first jump to some other point in A and then eventually be trapped or it can jump directly into the trap state. Equation (14) states that R(:x,y) is the sum of the probabilities of these mutually exclusive events. Because

$$R_o(:x,y) = p(:x,y) = 1 - \iint_A p(x',y':x,y)dx'dy' ,$$

it can be shown that R(:x,y) = 1 is a solution of the equation. If there were different types of trap states and $R_o(:x,y)$ were the probability of jumping directly into just one of the trap states, then $R_o(:x,y)$ would be less than

$$1 - \iint_A p(x',y':x,y)dx'dy',$$

and R(:x,y) would be less than one. In practical problems, this situation is the common one.

Equations for S(:x,y) and T(:x,y) can also be written

$$S(:x,y) = \iint_A S(:x',y')m(x',y':x,y)p(x',y':x,y)dx'dy' + S_o(:x,y) \quad (15)$$

$$S_o(:x,y) = p(:x,y)m(:x,y) \ . \quad (16)$$

$$T(:x,y) = \iint_A T(:x',y')m^2(x',y':x,y)p(x',y':x,y)dx'dy' + T_o(:x,y) \quad (17)$$

$$T_o(:x,y) = p(:x,y)m^2(:x,y) \ . \quad (18)$$

It should be noticed that Equations (14), (15), and (17) are adjoint respectively to Equations (6), (7) and (8).

Realization of Integral Equation by Monte Carlo

The $\bar{z}$ of Equation (1a) can be estimated as follows:

a. An (x,y) is picked from $P_o(x,y)$ and a weight $w_o = w_o(x,y)$ assigned to the particle.

b.* If on the i'th collision the particle is at (x_i,y_i) with weight w_i, then the computer first picks randomly between the alternatives of being trapped $\left[\text{probability } p(:x_i,y_i)\right]$ or of having another collision $\left\{\text{probability}\left[1 - p(:x_i,y_i)\right]\right\}$. If the first alternative materializes the particle is assigned a trapped weight, $W = m(:x_i,y_i)w_i$.

c.* If the particle is not trapped then an (x_{i+1},y_{i+1}) is picked from the normalized p.d.f., $\dfrac{p(x_{i+1},y_{i+1}:x_i,y_i)}{1 - p(:x_i,y_i)}$, and a weight, $w_{i+1} = m(x_{i+1},y_{i+1}:x_i,y_i)w_i$, assigned to the particle.

d. b and c are repeated until the particle is trapped. If N particle histories are traced and their weights when trapped denoted by $W_1,\ldots W_n,\ldots W_N$ respectively, then

$$\tilde{W} = \frac{1}{N} \sum_{n=1}^{N} W_n$$

is an estimate of $\bar{z}$.

---

* In many problems it is more natural to describe (b) and (c) as follows: an (x_{i+1},y_{i+1}) is picked from $p(x_{i+1},y_{i+1}:x_i,y_i)$. If (x_{i+1},y_{i+1}) is in the trap state a weight $W = m(:x_i,y_i)w_i$ is assigned to it. Otherwise the weight $w_{i+1} = m(x_{i+1},y_{i+1}:x_i,y_i)w_i$ assigned to the particle.

Because of the existence of adjoint equations, two different integrals can be written for $\bar{W}$, $\overline{W^2}$, etc. For instance,

$$\bar{z} = \bar{W} = \iint_A M(x,y)p(:x,y)m(:x,y)dxdy \tag{19}$$

$$= \iint_A P_o(x,y)w_o(x,y)S(:x,y)dxdy \ . \tag{20}$$

The first integral can be read as saying that the expected trapped weight is equal to the expected weight at any point, times the probability that the particle will be trapped, times the factor by which the weight is multiplied if the particle jumps to a trap state, all this summed over all possible points. The second integral says that the expected trapped weight is equal to a similar sum of the expected weight starting at any point times the expected factor by which the original weight is multiplied when the particle is finally trapped.

Similarly,

$$\overline{W^2} = \iint_A W(x,y)p(:x,y)m^2(:x,y)dxdy \tag{21}$$

$$= \iint_A P_o(x,y)w_o^2(x,y)T(:x,y)dxdy \tag{22}$$

Sampling from the Initial Distribution $P_o(x,y)$

Equations (19) to (22) indicate that if any of the techniques of Part II were to be applied to sampling the initial position of the particle, then the following correspondence,

$$\begin{aligned} f(x) &\longrightarrow P_o(x,y) \\ \bar{z}(:x) &\longrightarrow \bar{W}(:x,y) = w_o(x,y)S(:x,y) \\ \overline{z^2}(:x) &\longrightarrow \overline{W^2}(:x,y) = w_o^2(x,y)T(:x,y), \end{aligned} \tag{23}$$

can be used in designing the sampling. If it is desirable to use the sampling techniques only on the x coordinate of the initial position of the particle, then the analogy is given by:

$$\begin{aligned} f(x) &\longrightarrow P_o(x) = \int P_o(x,y)dy \\ \bar{z}(:x) &\longrightarrow \bar{W}(:x) = \int w_o(x,y)S(:x,y)P_o(y:x)dy \\ \overline{z^2}(:x) &\longrightarrow \overline{W^2}(:x) = \int w_o^2(x,y)T(:x,y)P_o(y:x)dy. \end{aligned} \tag{24}$$

Thus, just about all of Part II can be applied to sampling from $P_o(x)$ or $P_o(x,y)$. Because $T(:x,y)$ depends on $p(x',y':x,y)$ and will change if the transition probability is changed, the techniques and ideas of Part II must be modified before being applied to the integral equation as a whole.

The Collision Formulation

The whole formulation of the problem of solving integral equations by Monte Carlo can be changed slightly to make it look like the situation considered in Section A of Chapter II. The following additional definitions are needed:

$$q_i = \iint P_i(x,y)p(:x,y)dxdy$$

$$= \iint R_i(x,y)P_o(x,y)dxdy$$

$$h_i(x,y) = \frac{P_i(x,y)p(:x,y)}{q_i}$$

$$q_i h_i(w,x,y) = \underset{A_{i-1}}{\iint} \cdots \underset{A_o}{\iint} \delta\left[w - w_o \prod_{j=1}^{i} m(x_j,y_j:x_{j-1},y_{j-1})\right] P_o(x_o,y_o)$$

$$\prod_{r=1}^{i}\left[p(x_r,y_r:x_{r-1},y_{r-1})dx_{r-1}\,dy_{r-1}\right]$$

where the subscript on A indicates which (x,y) are being integrated and $\delta[\ldots]$ is the Dirac delta function.

$$h_i(w:x,y) = h_i(w,x,y)/h_i(x,y)$$

q_i is the probability that the particle is trapped on its i'th collision. $h_i(x,y)$ is the p.d.f. of the (x,y) from which the particle jumped when it was trapped. $h_i(w,x,y)$ is the similar p.d.f. for (w,x,y). The sampling problem can now be defined as follows:

1. An i value is picked from q_i
2. An (x,y) is picked from $h_i(x,y)$

3. A w is picked from $h_i(w:x,y)$

4. The function W = wm(:x,y) is calculated

The average value of the samples W's is an estimate of $\bar{z}$.

Unfortunately the q_i are not known explicitly, and the only way in which i values can be picked is to sample all the previous i values. For most problems focusing attention on the collision number rather than the position of the particle is a highly artificial and non-productive point of view. However, when the $\bar{w}_i(:x,y)$ are strongly dependent on the i and not on (x,y) then this point of view can be useful. In this report the main application of the collision formulation is in deriving formulae.

1. Straightforward Sampling

The sampling procedure described in the previous sections is not really a faithful analogue of most physical situations. In the typical particle diffusion problem there are alternative ways, besides jumping to a unique trap state or states of interest, in which the particle can terminate its random walk. Some of them correspond to uninteresting trap states, while others correspond to a special type of trap state in which the particle simply disappears. If the latter event occurs, the particle is said to have been absorbed. If it does not the particle is said to have survived the collision. In this physical situation the weight of the particle does not change as it jumps from one point to another or to the trap state; $m(x,y:x',y')$ is not a weighting factor but a survival probability, and therefore necessarily less than one. $m(:x,y)$ is the product of a survival probability and some function of the particles coordinates; for example the energy. If the survival or absorption of a particle is treated as a random event then the equations for $P(x,y)$, $Q(x,y)$, $R(:x,y)$, and $T(:x,y)$ cease to have any meaning; the equations for $M(x,y)$ and $S(:x,y)$ are unchanged in form, but $M_i(x,y)$ is now to be interpreted as the probability of being at (x,y) at the i'th collision, and [if $m(:x,y)$ is a probability of survival] $S_i(x,y)$ is the probability of the particle being trapped directly after its i'th collision if it starts from (x,y).

Under this interpretation the particle has a weight of one if it gets to the trap state and is defined as having a weight of zero if it fails. If primes are used to distinguish the physical random

walk from the previous one, and P' is the probability of getting to the trap state, then

$$\begin{aligned} \bar{z} &= \overline{W'} \\ &= P' \cdot 1 + (1-P') \cdot 0 \\ &= P' \\ \overline{z^2} &= \overline{W'^2} \\ &= P' \cdot 1^2 + (1-P') \cdot 0^2 \\ &= P' \end{aligned} \tag{25}$$

and the variance is

$$\begin{aligned} V_1' &= P' - P'^2 \\ &= \bar{z} - \bar{z}^2 \, . \end{aligned} \tag{26}$$

In the previous formulation the variance was given by:

$$V_1 = \iint Q(x,y) m^2(x,y) p(:x,y) dxdy - \bar{z}^2 \, . \tag{27}$$

$$V_1' - V_1 = \iint \left[M(x,y) m(:x,y) - Q(x,y) m^2(:x,y) \right] p(:x,y) dxdy \, . \tag{28}$$

It is easy to see that $V_1' - V_1 \geq 0$. $m^2(:x,y)$ is less than $m(:x,y)$ because $m(:x,y)$ is less than one. Similarly, from the fact that $m^2(x',y':x,y) \leq m(x',y':x,y)$, it can be deduced that $Q(x,y) \leq M(x,y)$, so $Qm^2 \leq Mm$ and $V_1 \leq V_1'$.

The formulation with weighting factors corresponds to replacing the random survival of the physical random walk with a weight that is the expected value of the survival probability. This is an example of the application of the use of expected values and therefore it is not surprising that there is a reduction in the variance. There is also

an increase in the expected cost of a single history, for if the particle were occasionally allowed to terminate its walk before jumping into the trap state then the average history would involve fewer collisions and be less work to compute. The section on Russian Roulette discusses the inter-play of these two factors in more detail.

2. Importance Sampling

The problem is to select the six functions $p(:x,y)$, $p(x',y':x,y)$, $P_o(x,y)$, $m(:x,y)$, $m(x',y':x,y)$, and $w_o(x,y)$ so that the weight of a particle when trapped is an estimate of $\bar{z}$, and so that $\overline{W^2}$ is a minimum. The condition on $\bar{W}$ is satisfied if

$$m(:x,y) = z(x,y)/p(:x,y) \tag{29a}$$

$$m(x',y':x,y) = K(x',y':x,y)/p(x',y':x,y) \tag{29b}$$

$$w_o(x,y) = M_o(x,y)/P_o(x,y) \ , \tag{29c}$$

and only the three p.d.f.'s are arbitrary.

Under these circumstances the equations for $M(x,y)$ and $S(:x,y)$ are given by (1b) and (2b). The equations for $Q(x,y)$ and $T(:x,y)$ are obtained by substituting Equation (29) into Equations (8) and (17) respectively:

$$Q(x,y) = \iint_A \frac{K^2(x,y:x',y')}{p(x,y:x',y')} Q(x',y')dx'dy' + \frac{M_o^2(x,y)}{P_o(x,y)} \tag{30a}$$

$$T(:x,y) = \iint_A T(:x',y') \frac{K^2(x',y':x,y)}{p(x',y':x,y)} dx'dy' + \frac{z^2(x,y)}{p(:x,y)} \ , \tag{30b}$$

and from Equations (21) and (22)

$$\overline{W^2} = \iint_A Q(x,y) \frac{z^2(x,y)}{p(:x,y)} dxdy \tag{31a}$$

$$= \iint_A T(:x,y) \frac{M_o^2(x,y)}{P_o(x,y)} dxdy \tag{31b}$$

Because $\overline{W^2} - \bar{W}^2 \geq 0$, the minimum value of $\overline{W^2}$ is $\bar{W}^2$. If this value is achieved then the variance is zero and the sampling is perfect; a sample of one gives the correct answer. If $K(x,y:x,y)$, $M_o(x,y)$, and $z(x,y)$ are all positive, a zero variance random walk can be obtained and is given by the following choice of the three p.d.f.'s:

$$p(:x,y) = z(x,y)/S(:x,y) \tag{32a}$$

$$p(x',y':x,y) = S(:x',y')K(x',y':x,y)/S(:x,y) \tag{32b}$$

$$P_o(x,y) = S(:x,y)M_o(x,y)/\bar{z}. \tag{32c}$$

By using Equation (2b) for $S(:x,y)$ it can be shown that the $p(:x,y)$ and $p(x',y':x,y)$ given above satisfy $p(:x,y) + \iint p(x',y':x,y)dx'dy' = 1$. Similarly Equations (1a) and (3) guarantee that $\iint P_o(x,y)dxdy = 1$.

Substituting into the equations for $Q(x,y)$ and $T(:x,y)$:

$$Q(x,y) = \iint \frac{K(x,y:x',y')S(:x',y')}{S(:x,y)} Q(x',y')dx'dy' + \frac{M_o(x,y)}{S(:x,y)} \bar{z} \tag{33a}$$

$$T(:x,y) = \iint T(:x',y') \frac{K(x',y':x,y)S(:x,y)}{S(:x',y')} dx'dy' + z(x,y)S(:x,y) \tag{33b}$$

Solutions of these equations are given by

$$Q(x,y) = \bar{z}M(x,y)/S(:x,y)$$

$$T(:x,y) = S^2(:x,y) ,$$

for as can be verified by substitution, Equations (33a) and (33b) then reduce to Equations (1b) and (2b) respectively. Either of the above solutions when substituted into Equation (31) give

$$\overline{W^2} = \bar{z}^2 \tag{34}$$
$$= \bar{W}^2 .$$

Even though a great deal more than just the answer, $\bar{z}$, must be known before a zero variance sampling technique can be designed, the result does indicate that the variance can be cut down if it is possible to exploit some previous knowledge about the problem.

It is interesting to examine some of the details of the zero variance estimate. Any particular particle history can be represented by a set of numbers. $(w_o,x_o,y_o;w_1,x_1,y_1;\cdots w_i,x_i,y_i;w_I,x_I,y_I)$ where the (x_i,y_i) are the successive positions of the particle and the w_i are the weights at the i'th collision. The sample estimate is

$$W = m(:x_I,y_I)w_I. \tag{35}$$

If the optimum importance sampling is used,

$$w_o = M_o(x_o,y_o)/P_o(x_o,y_o) \tag{36}$$

$$= \bar{z}/S(:x_o,y_o).$$

$$w_i = m(x_i,y_i:x_{i-1},y_{i-1})w_{i-1} \tag{37}$$

$$= \frac{K(x_i,y_i:x_{i-1},y_{i-1})}{p(x_i,y_i:x_{i-1},y_{i-1})} w_{i-1}$$

$$= \frac{S(:x_{i-1},y_{i-1})}{S(:x_i,y_i)} w_{i-1}$$

$$= \frac{S(:x_{i-1},y_{i-1})}{S(:x_i,y_i)} \cdot \frac{S(:x_{i-2},y_{i-2})}{S(:x_{i-1},y_{i-1})} \cdots \frac{\bar{z}}{S(:x_o,y_o)}$$

$$= \bar{z}/S(:x_i,y_i) .$$

Because of the successive cancellations, the weight w_i does not depend on the history of the particle but only on its position. It will turn out in the section on Russian Roulette that there are other ways besides importance sampling in which this condition occurs.

$$m(:x_I,y_I) = z(x_I,y_I)/p(:x_I,y_I) \tag{38}$$

$$= S(:x_I,y_I) ,$$

$$W = w_I m(:x_I,y_I) \tag{39}$$

$$= \frac{\bar{z}}{S(:x_I,y_I)} S(:x_I,y_I)$$

$$= \bar{z} .$$

It is customary in engineering practice to refer to $S(:x,y)$ as the importance or influence function. As can be seen from Equation (32), the sampling is taken proportional to this function. Normally $S(:x,y)$ is not known and an approximate importance function, $I(x,y)$, must be used. The sampling p.d.f.'s then becomes

$$p(:x,y) = z(x,y)/C(x,y) \tag{40}$$

$$p(x',y':x,y) = I(x',y')K(x',y':x,y)/C(x,y)$$

$$P_o(x,y) = I(x,y)M_o(x,y)/C_o ,$$

where
$$C(x,y) = \iint_A I(x',y')K(x',y':x,y)dx'dy' + z(x,y) \tag{41}$$

and
$$C_o = \iint_A I(x,y)M_o(x,y)dxdy \tag{41b}$$

are required for normalization purposes.

The equations for Q(:x,y) and T(:x,y) now become

$$I(x,y)Q(x,y) = \iint_A K(x,y:x',y')C(x',y')Q(x',y')dx'dy' + C_o M_o(x,y) \qquad (42a)$$

$$\frac{T(:x,y)}{C(x,y)} = \iint_A \frac{T(:x',y')}{I(x',y')} K(x',y':x,y)dx'dy' + z(x,y) . \qquad (42b)$$

If the substitutions

$$Q(x,y) = C_o M^*(x,y)/I(x,y) \qquad (43a)$$

$$T(:x,y) = C(x,y)S^*(:x,y) \qquad (43b)$$

are made, Equations (42a) and (42b) become:

$$M^*(x,y) = \iint K(x,y:x',y') \frac{C(x',y')}{I(x',y')} M^*(x',y')dx'dy' + M_o(x,y) \qquad (44a)$$

$$S^*(:x,y) = \iint S^*(:x',y')K(x',y':x,y) \frac{C(x,y)}{I(x,y)} dx'dy' + z(x,y) . \qquad (44b)$$

If the optimum sampling had been used, $M^*(x,y)$ would be equal to $M(x,y)$ and $S^*(:x,y)$ would equal $S(:x,y)$. They are not equal to the desired functions because in effect, there is an extra multiplying factor, $C(x,y)/I(x,y)$.

For this approximate importance sampling, using (31a) and (40)

$$\overline{W^2} = \iint_A Q(x,y)z(x,y)C(x,y)dxdy \qquad (45a)$$

$$= C_o \iint_A M^*(x,y)z(x,y) \frac{C(x,y)}{I(x,y)} dxdy$$

$$= C_o \overline{z^*} ,$$

or using (31b) and (40)

$$\overline{W^2} = C_o \iint T(:x,y) \frac{M_o(x,y)}{I(x,y)} \, dxdy \qquad (45b)$$

$$= C_o \iint S^*(:x,y) M_o(x,y) \frac{C(x,y)}{I(x,y)} \, dxdy$$

$$= C_o \overline{z^*} \, .$$

$\overline{z^*}$ is the ordinary expected weight of trapped particles when the weighting factors of the random walk have the additional factor $C(x,y)/I(x,y)$. The variance is

$$V_2 = C_o \overline{z^*} - \bar{z}^2 \, . \qquad (46)$$

The formula $C_o \overline{z^*}$ for $\overline{W^2}$ is exactly what would have been expected. If a random walk uses the p.d.f.'s of Equation (40) and the weighting of (29) then

$$w_i = \frac{C_o}{I(x_o,y_o)} \cdot \frac{C(x_o,y_o)}{I(x_1,y_1)} \cdots \frac{C(x_{i-1},y_{i-1})}{I(x_i,y_i)} \qquad (47)$$

$$W = m(:x_I,y_I) w_I \qquad (48)$$

$$= \frac{C_o}{I(x_o,y_o)} \cdot \frac{C(x_o,y_o)}{I(x_1,y_1)} \cdots \frac{C(x_{I-1},y_{I-1})}{I(x_I,y_I)} C(x_I,y_I)$$

For the z* random walk with the same p.d.f.'s

$$w_i^* = \frac{C_o}{I(x_o,y_o)} \cdot \frac{C(x_o,y_o)C(x_o,y_o)}{I(x_o,y_o)I(x_1,y_1)} \cdots \frac{C(x_{i-1},y_{i-1})C(x_{i-1},y_{i-1})}{I(x_{i-1},y_{i-1})I(x_i,y_i)} \qquad (49)$$

$$= w_i^2 \frac{I(x_i,y_i)}{C_o}$$

$$w^* = m^*(:x_I,y_I)w_I^* \tag{50}$$

$$= m(:x_I,y_I)\frac{C(x_I,y_I)}{I(x_I,y_I)}w_I^*$$

$$= \frac{C^2(x_I,y_I)}{I(x_I,y_I)}w_I^*$$

$$= C^2(x_I,y_I)w_i^2/C_o$$

$$= W^2/C_o$$

Therefore $C_o W^* = W^2$ (51a)

$$\overline{C_o W^*} = \overline{W^2} \tag{51b}$$

$$= C_o\overline{z^*} .$$

The equation does, however, indicate how the variance can be estimated for an importance function $I'(x,y)$, when an $I(x,y)$ is actually used in the calculation. The weight w_i is multiplied by the factor

$$m' = \frac{C'(x_o,y_o)}{I'(x_o,y_o)}\,\frac{C'(x_1,y_1)}{I'(x_1,y_1)}\cdots\frac{C'(x_{i-1},y_{i-1})}{I'(x_{i-1},y_{i-1})} \tag{52a}$$

and the trapped weight W by the additional factor $C'(x_I,y_I)/I'(x_I,y_I)$

$$W' = W\frac{C'(x_o,y_o)}{I'(x_o,y_o)}\cdot\frac{C'(x_1,y_1)}{I'(x_1,y_1)}\cdots\frac{C'(x_I,y_I)}{I'(x_I,y_I)} \tag{52b}$$

The sampling variance, if $I'(x,y)$ had been used instead of $I(x,y)$ is

$$V_2' = C_o'\overline{W'} - \bar{z}^2 . \qquad (53)$$

Estimating the Importance $I(x,y)$

Method I.

Usually the most convenient method for obtaining good importance functions is to try to calculate $S(:x,y)$ by some approximate analytic, numerical, or experimental procedure. It is somewhat easier to do this than might be thought because only relative values of the function are needed. If there is a consistent bias in the approximate calculation, even if it is large, it may cancel itself out for the purposes of sampling. In many cases the computer has sufficient intuition about the problem to be able to guess a reasonable $I(x,y)$ with very little work.

Method II.

The sampling is set up so that the p.d.f.'s have parameters in them. The parameters can then be varied until the estimated value of $\overline{W^2}$ is sufficiently small. While $\bar{W}$ does not change when the parameters are varied, the author has found that there is usually sufficient positive correlation between $\tilde{V} = \tilde{W^2} - \tilde{W}^2$ and $\tilde{W}^2$, that $\tilde{V}/\tilde{W}^2$ is a better guide than just $\tilde{V}$.

Method III.

Method II can be used in a little more sophisticated manner if the results of Equations (53), (54), and (55) are applied. It is usually relatively cheap to carry along with the sampling for the

answer, some additional machinery which will enable the computer to estimate what the variance would have been if a different importance function had been used. As soon as information about the sampling characteristics of different importance functions is obtained, it can be fed back into the problem.

Method IV

It is perfectly feasible to interchange the roles of the normal and adjoint equations. Sampling can then be done on the adjoint equation and S(:x,y) estimated. This estimated S(:x,y) can then be used to improve the sampling that estimates M(:x,y) and vice versa. If necessary the iteration procedure could be carried through many times. As far as the author knows Method IV has never been used in a systematic fashion. The first three have.

Importance Sampling Only In The x Space

It is sometimes desirable to separate the x and y spaces and do Importance Sampling only on the former. The simplest thing to do is to take I(x) proportional to an approximate $\bar{S}(:x)$ where $\bar{S}(:x)$ is a

suitable average of $S(:x,y)$. This corresponds to the sampling proportional to $\bar{z}(:x)$ in the second chapter and like that sampling is by no means optimal. However, the description of the optimum sampling for the x space only is extremely non-intuitive and while a short discussion is included here for the sake of completeness, the equations that determine this optimum sampling in the x space do not seem very useful.

The Greens function $\bar{K}(x'',y'':x',y')$ is defined by the equation

$$\bar{K}(x'',y'':x',y') = \iint_A \bar{K}(x'',y'':x,y)K(x,y:x',y') \frac{C(x',y')}{I(x',y')}\,dxdy + \delta(x''-x')\delta(y''-y'). \tag{54a}$$

By multiplying Equation (44a) by $\bar{K}(x'',y'':x,y)$ and integrating over (x,y), the equation

$$M^*(x'',y'') = \frac{I(x'',y'')}{C(x'',y'')} \iint \bar{K}(x'',y'':x,y)M_o(x,y)dxdy \tag{54b}$$

is obtained. By substituting Equations (41b) and (54b) into (45a) an expression for $\overline{W^2}$

$$\overline{W^2} = \iint I(x,y)M_o(x,y)dxdy \iint_A \iint_A z(x,y)\bar{K}(x,y:x',y')M_o(x',y')dxdydx'dy' \tag{55}$$

can be written in terms of $I(x,y)$ where $\bar{K}(x,y:x',y')$ depends implicitly on $I(x,y)$ through Equation (54a). This dependence is very complex, even when $I(x,y)$ is specialized to be a function of x only. Therefore, when the condition that makes $\overline{W^2}$ a minimum is derived, the equations are relatively intractable and non-suggestive.

3. Systematic Sampling

The most important application of systematic sampling is to the sampling of initial points. This subject is discussed in the section on sampling $P_o(x,y)$ and also in Section 6 on correlation. The discussion which follows concerns the much less important but still interesting subject of the systematic sampling of the transition probabilities.

A surface $x_j(x,y)$ can be defined by the equations:

$$p(x':x,y) = \int p(x',y':x,y)dy' \tag{56}$$

$$\int_{}^{x_j} p(x':x,y)dx' = \frac{j - 1/2}{N} \tag{57}$$

If systematic sampling is used when picking values of x_i then the x_i values will fall on one of these N surfaces $x_j(x_{i-1},y_{i-1})$. However, since some of the N particle histories will have terminated before reaching the i'th collision it is not true that each one of the surfaces will have an x_i value on it.

The reduction in variance due to systematic sampling can be calculated exactly as in Section 15 of the previous chapter. A random variable U_i is defined which is equal to the weight W of the trapped particle given that the particle had at least i-1 collisions before being trapped. Then

$$\bar{U}_i(:w_{i-1},x_{i-1},y_{i-1},x_i,y_i) = w_{i-1}m(x_i,y_i:x_{i-1},y_{i-1})S(:x_i,y_i) \text{ if } (x_i,y_i) \text{ in A} \tag{58}$$

$$= w_{i-1}m(:x_{i-1},y_{i-1}) \text{ if } (x_i,y_i) \text{ in trap state}$$

$$\overline{U_i^2}(:w_{i-1},x_{i-1},y_{i-1},x_i,y_i) = w_{i-1}^2 m^2(x_i,y_i:x_{i-1},y_{i-1})T(:x_i,y_i) \text{ if } (x_i,y_i) \text{ in A}$$

$$= w_{i-1}^2 m^2(:x_{i-1},y_{i-1}) \text{ if } (x_i,y_i) \text{ in trap state} \tag{59}$$

The p.d.f. for $(w_{i-1},x_{i-1},y_{i-1},x_i,y_i)$

is $f_{i-1}(w_{i-1},x_{i-1},y_{i-1})p(x_i,y_i:x_{i-1},y_{i-1})/P_{i-1}$

where $$P_{i-1} = \iiint f_{i-1}(w,x,y)dwdxdy \tag{60}$$

$$= \iint P_{i-1}(x,y)dxdy$$

is the probability that a particle will have an i-1st collision. $\bar{U}_i$ and $\overline{U_i^2}$ can be calculated by integrating this p.d.f. against the conditional expected values defined in Equations (58) and (59). It is also necessary to define the expected value,

$$\bar{U}_i(:j), \text{ of } \bar{U}_i(:w_{i-1},x_{i-1},y_{i-1},x_i,y_i)$$

on the equiprobability surface $x_j(x_{i-1},y_{i-1})$. While the surface is defined independently of the collision number, $\bar{U}_i(:j)$ depends on it because the p.d.f. is a function of i.

$$\bar{U}_i(:j) = \int_{-\infty}^{\infty} dy_i \iint_A dx_{i-1}dy_{i-1} \int_0^{\infty} dw_{i-1} \bar{U}\left[:w_{i-1},x_{i-1},y_{i-1},x_j(x_{i-1},y_{i-1}),y_i\right] \tag{61}$$

$$\frac{f_{i-1}(w_{i-1},x_{i-1},y_{i-1})}{P_{i-1}} p\left[x_j(x_{i-1},y_{i-1}),y_i:x_{i-1},y_{i-1}\right]$$

$$= \int_{-\infty}^{\infty} dy_i \iint_A dx_{i-1} dy_{i-1} S'\left[:x_j(x_{i-1},y_{i-1})\right] K'\left[x_j(x_{i-1},y_{i-1}),y_i:x_{i-1},y_{i-1}\right]$$

$$M_{i-1}(x_{i-1},y_{i-1})$$

where $S'K'$ is defined as equal to SK if (x_j,y_i) is in A and is equal to $m(:x_{i-1},y_{i-1})p(:x_{i-1},y_{i-1})$ if (x_j,y_i) is in the trap state.

If N_1 particles had an i-1st collision and ordinary sampling was used then the variance of the estimate of $N_1 \bar{U}_i$ would be $N_1(\overline{U_i^2} - \bar{U}_i^2)$. By a trivial modification of the technique of 3B it can be shown that this variance is approximately reduced by an amount $N_1\overline{\left[\bar{U}_i(:j) - \bar{U}_i\right]^2}$. Therefore the variance of the original sampling problem is reduced by $P_{i-1}\overline{\left[\bar{U}_i(:j) - \bar{U}_i\right]^2}$.

If systematic sampling is used on y_i then a surface $y_k(x_{i-1},y_{i-1},x_i)$ is defined by

$$p(y_i:x_{i-1},y_{i-1},x_i) = p(x_i,y_i:x_{i-1},y_{i-1})/p(x_i:x_{i-1},y_{i-1}) \tag{62}$$

$$\int_{}^{y_k(x_{i-1},y_{i-1},x_i)} p(y_i:x_{i-1},y_{i-1},x_i)dy_i = \frac{k - 1/2}{N} \qquad k = 1, 2,\ldots, N \tag{63}$$

and the expected value of $\bar{U}(:w_{i-1},x_{i-1},y_{i-1},x_i,y_i)$ on this surface by

$$\bar{U}_i(:k) = \int_{-\infty}^{\infty} dx_i \iint_A dx_{i-1} dy_{i-1} S'\left[:x_i,y_k(x_{i-1},y_{i-1},x_i)\right] K'\left[x_i,y_k(x_{i-1},y_{i-1},x_i):\right.$$

$$\left. x_{i-1},y_{i-1}\right] M_{i-1}(x_{i-1},y_{i-1} \tag{64}$$

The reduction in variance is $P_{i-1}\overline{\left[\bar{U}_i(:k) - \bar{U}_i\right]^2}$. If systematic sampling is used at several points in the particles history then the reductions are approximately additive.

4. Stratified Sampling

As in systematic sampling the important application is to the initial positions of the particles. This subject is discussed in the section on sampling $P_o(x,y)$ and also in Section 6 on correlation. The application to the transition probabilities seems completely negligible and will not be discussed.

5. Use of Expected Values

Type I

Let H denote the set of numbers, $(w_o,x_o,y_o; w_1,x_1,y_1; \ldots; w_I,x_I,y_I)$, that constitute a history. The estimate W is a simple function of H:

$$W = m(:x_I,y_I)w_I \tag{73}$$

There are many other functions of H that can be used to estimate $\bar{z}$. Because most of them can be intuitively justified by replacing a random variable by its expected value, they are discussed in this section. The estimate in Equation (73) will be referred to by the symbol L_1 and will be called a Type I estimate. A few other functions of H that can be used will now be discussed.

Type II

Instead of recording the weight of the particle after it jumps into the trap state, the computer calculates the weight that every collision is expected to put into the trap state by:

$$L_2 = \sum_{i=0}^{I} w_i p(:x_i,y_i)m(:x_i,y_i) \tag{74}$$

The expected value of any term of L_2 can be obtained by calculating the expected value of the weight given that the particle is at (x,y), and then averaging over all (x,y).

The former is given by

$$\bar{w}_i(:x,y) = M_i(x,y)/P_i(x,y), \tag{75}$$

the latter by

$$\overline{w_i p(:x_i,y_i) m(:x_i,y_i)} = \iint \overline{w_i}(:x,y) p(:x,y) m(:x,y) P_i(x,y) dxdy \qquad (76)$$

$$= \iint M_i(x,y) p(:x,y) m(:x,y) dxdy \ .$$

If each term is replaced by its expected value the sum must be taken to infinity instead of just to I and

$$\bar{L}_2 = \sum_{i=0}^{\infty} \iint M_i(x,y) p(:x,y) m(:x,y) dxdy \qquad (77)$$

$$= \iint M(x,y) p(:x,y) m(:x,y) dxdy$$

$$= \bar{z} \ .$$

The expected value of L_2^2 can also be calculated

$$L_2^2 = \sum_{\substack{i=0 \to I \\ j=0 \to I}} w_j p(:x_j,y_j) m(:x_j,y_j) w_i p(:x_i,y_i) m(:x_i,y_i) \qquad (78)$$

$$= \sum_{i=0}^{I} w_i^2 p^2(:x_i,y_i) m^2(:x_i,y_i) + 2 \sum_{i=0}^{I-1} \sum_{j=i+1}^{I} w_j p(:x_j,y_j) m(:x_j,y_j) w_i p(:x_i,y_i) m(:x_i,y_i)$$

The expected value of the i'th term in the first sum is

$$\overline{w_i^2 p^2(:x_i,y_i) m^2(:x_i,y_i)} = \iint \overline{w_i^2}(:x,y) p^2(:x,y) m^2(x,y) P_i(x,y) dxdy \qquad (79)$$

$$= \iint Q_i(x,y) p^2(:x,y) m^2(:x,y) dxdy$$

since $\overline{w_i^2}(:x,y) = Q_i(x,y)/P_i(x,y)$. (80)

If the (w_j,x_j,y_j) were independent of (w_i,x_i,y_i), the second sum would drop out of the calculation of the variance. Because there is a positive correlation between the two sets of random variables the variance is increased. It is convenient at this point to make some additional definitions.

$$p_i(x',y':x,y) = \iint_A p_{i-r}(x,y:x'',y'')p_r(x'',y'':x',y')dx''dy'' \quad 1 \leq r \leq i-1 \tag{81}$$

$$p_1(x,y:x',y') = p(x,y:x',y')$$

$$K_i(x,y:x',y') = \iint_A K_{i-r}(x,y:x'',y'')K_r(x'',y'':x',y')dx''dy'' \quad 1 \leq r \leq i-1 \tag{82}$$

$$K_1(x,y:x',y') = m(x,y:x',y')p(x,y:x',y')$$

$$= K(x,y:x',y')$$

$$m_i(x',y':x,y) = K_i(x',y':x,y)/p_i(x',y':x,y) . \tag{83}$$

$p_i(x,y:x',y')$ is the probability that a particle which starts at (x,y) is at (x',y') on its i'th collision. $K_i(x',y':x,y)$ is the expected weight at (x',y') after i collisions, given that the particle starts at (x,y) with weight one. $m_i(x',y':x,y)$ is the expected factor by which the original weight of the particle is multiplied if the particle goes from (x,y) to (x',y') in i collisions.

The expected value of w_j in the second sum of Equation (78) is

$$\overline{w_j}(:x_j,y_j,w_i,x_i,y_i) = w_i m_{j-i}(x_j,y_j:x_i,y_i) . \tag{84}$$

The expected value of $m_{j-i}(x_j,y_j:x_i,y_i)p(:x_j,y_j)m(:x_j,y_j)$ for given (x_i,y_i) is

$$\iint_A m_{j-i}(x_j,y_j:x_i,y_i)p(:x_j,y_j)m(:x_j,y_j)p_{j-i}(x_j,y_j:x_i,y_i)dx_jdy_j \tag{85}$$

$$= \iint_A K_{j-i}(x,y:x_i,y_i)p(:x,y)m(:x,y)dxdy$$

$$= S_{j-i}(:x_i,y_i) .$$

The expected value of the (i,j)'th term of the second sum in Equation (78) is

$$\iint_A S_{j-i}(x,y)\overline{w_i^2}(:x,y)p(:x,y)m(:x,y)P_i(x,y)dxdy \tag{86}$$

$$= \iint_A S_{j-i}(x,y)p(:x,y)m(:x,y)Q_i(:x,y)dxdy$$

The sum from j=i+1 to ∞ replaces the $S_{j-i}(:x,y)$ by $\left[S(:x,y) - S_o(:x,y)\right]$. The sum from i=0 to ∞ replaces $Q_i(x,y)$ by $Q(x,y)$ in both Equations (79) and (86). Making these changes and substituting $S_o(x,y) = p(:x,y)m(:x,y)$, the expected value of $\overline{L_2^2}$ becomes

$$\overline{L_2^2} = \iint Q(x,y)p^2(:x,y)m^2(:x,y)dxdy + 2\iint_A S(:x,y)Q(x,y)p(:x,y)m(:x,y)dxdy \tag{87}$$

$$- 2\iint Q(x,y)p^2(:x,y)m^2(:x,y)dxdy$$

$$= \iint Q(x,y)p(:x,y)m(:x,y)\left[2S(:x,y) - p(:x,y)m(:x,y)\right]dxdy$$

$$\overline{L_1^2} - \overline{L_2^2} = \iint Q(x,y)p(:x,y)m(:x,y)\left[m(:x,y) + p(:x,y)m(:x,y) - 2S(:x,y)\right]dxdy. \tag{88}$$

The method is useful when the appropriately weighted average

$$\overline{m(:x,y)\left[1 + p(:x,y)\right]} - 2S(:x,y) > 0 \ . \tag{89}$$

In some problems $\overline{S(:x,y)}$ is of the order $\alpha\overline{m(:x,y)R(:x,y)}$. Using this rough estimate roughly gives

$$\overline{p(:x,y)} \lesssim 1 - 2\alpha\overline{R(:x,y)} \tag{90}$$

for the condition that is necessary for $\overline{L_2^2}$ to be less than $\overline{L_1^2}$. The implication is that the estimate is useful when $p(:x,y)$ or $R(:x,y)$ is small. This is in contrast to a type I estimate which works best when $p(:x,y)$ or a suitable average of $R(:x,y)$ is large.

The method is particularly advantageous when estimates of the function $M(x,y)$ are desired. The usual estimate of $M(x,y)$ is given directly by the history, H, and can be written

$$\tilde{M}'(x,y) = \sum_{i=0}^{I} w_i \delta(x - x_i)\delta(y - y_i). \tag{91}$$

If the results for a number of histories are averaged and smoothed out in the manner discussed in the section on estimating $\bar{z}(:x)$ and $\overline{z^2}(:x)$, then something like a Type I estimate of $M(x,y)$ is obtained. The corresponding Type II estimate would be

$$\tilde{M}(x,y) = \sum_{i=0}^{I} w_i K(x,y:x_i,y_i) + M_o(x,y). \tag{92}$$

Equation (92) has a familiar look. It corresponds to improving an approximate solution, $M'(x,y)$, of an integral equation by iteration. $\tilde{M}'(x,y)$ is substituted into the right side of Equation (1b) and integrated. An iterative procedure of this type is especially

effective when there is a large separation between the first two eigenvalues of $K(x',y':x,y)$. In the present statistical situation, iteration may be useful even if the condition on the eigenvalues is not satisfied, because every sample is allowed a better chance to contribute effectively to the answer. The expected value and variance of the estimate can be calculated in a straightforward manner;

$$\bar{\tilde{M}}(x,y) = \sum_{i=0}^{\infty} \iint_A \bar{w}_i(:x',y')K(x,y:x',y')P_i(x',y')dx'dy' + M_o(x,y) \qquad (93)$$

$$= \sum_{i=0}^{\infty} \iint K(x,y:x',y')M_i(x',y')dx'dy' + M_o(x,y)$$

$$= \iint K(x,y:x',y')M(x',y')dx'dy' + M_o(x,y)$$

$$= M(x,y)$$

$$\bar{\tilde{M}}^2(x,y) = \sum_{i=0}^{\infty} \iint_A \overline{w_i^2}(:x',y')K^2(x,y:x',y')P_i(x',y')dx'dy' \qquad (94)$$

$$+ 2\sum_{i=0}^{\infty} \iint_A \overline{w_i^2}(:x',y')K(x,y:x',y')P_i(x',y')dx'dy' \sum_{j=i+1}^{\infty} \iint$$

$$K(x,y:x'',y'')m_{j-1}(x'',y'':x',y')p_{j-1}(x'',y'',x',y')dx''dy''$$

$$+ 2M_o(x,y)\sum_{i=0}^{\infty} \iint \bar{w}_i(:x',y')K(x,y:x',y')\ P_i(x',y')dx'dy'$$

$$+ M_o^2(x,y)$$

$$= \iint_A K^2(x,y:x',y')Q(x',y')dx'dy'$$

$$+ 2 \sum_{i=0}^{\infty} \iint_A K(x,y:x',y')Q_i(x',y')dx'dy' \sum_{j=i+1}^{\infty} K_{j-i=1}(x,y:x',y')$$

$$+ 2M_o(x,y)\left[M(x,y) - M_o(x,y)\right] + M_o^2(x,y)$$

$$= \iint_A K^2(x,y:x',y')Q(x',y')dx'dy' + 2 \iint_A K(x,y:x',y')Q(x',y')$$

$$\left[M(x,y:x',y') - K(x,y:x',y')\right]dy'dy'$$

$$+ 2M_o(x,y)M(x,y) - M_o^2(x,y)$$

$$= \iint_A K(x,y:x',y')Q(x',y')\left[2M(x,y:x',y') - K(x,y:x',y')\right]dx'dy'$$

$$+ 2M_o(x,y)M(x,y) - M_o^2(x,y)$$

where

$$M(x,y:x',y') = \sum_{i=1}^{\infty} K_i(x,y:x',y') \tag{95}$$

is the expected total weight at (x,y) if the particle starts at (x',y'). The variance of the estimate is

$$NV = \bar{\bar{M}}^2 - M^2 \tag{96}$$

$$= \iint_A K(x,y:x',y')Q(x',y')\left[2M(x,y:x',y') - K(x,y:x',y')\right]dx'dy'$$

$$-\left[M(x,y) - M_o(x,y)\right]^2$$

The expression could have been obtained directly from Equation (87), essentially by substituting $K(x,y:x',y')$ for $p(:x',y')m(:x',y')$.

It seems difficult to make any general comments about Equation (96) without making further assumptions on $K(x',y':x,y)$; therefore they will be deferred to the chapters on applications.

It is sometimes inconvenient to compute $p(:x_i,y_i)m(:x_i,y_i)$ or $K(x,y:x_i,y_i)$ for use in Equations (74) and (92) respectively. In particle diffusion problems particularly the expressions may become simpler if the collisions are "mixed." For example, if x_{i+1} is used with y_i the first estimate is changed to something of the form

$$L_2 = \sum_{i=0}^{I} w_i p(:x_{i+1},y_i)m(:x_i,y_i,x_{i+1})m(x_{i+1}:x_i,y_i) \tag{97}$$

The detailed discussions of these estimates are also deferred to the chapters on applications.

Type III

The Type I estimate can usually be obtained very cheaply even if one of the other estimates are being used. It might therefore be conjectured that it would be efficient to use an appropriate average of Type I and any other estimate. For example

$$L_3 = \alpha_1 L_1 + \alpha_2 L_2 \tag{98}$$

$$\alpha_1+\alpha_2 = 1$$

is an estimate of $\bar{z}$ with a variance of

$$\sigma_3^2 = \alpha_1^2 \sigma_1^2 + 2\,\alpha_1\alpha_2 \rho\sigma_1\sigma_2 + \alpha_2^2 \sigma_2^2 \tag{99}$$

It is shown in Section 6B of the previous chapter that σ_3^2 is a minimum if $a_1 = \dfrac{\sigma_1^2 - \rho\sigma_1\sigma_2}{\sigma_1^2 - 2\rho\sigma_1\sigma_2 + \sigma_2^2}$. The variance then becomes

$$\sigma_3^2 = \frac{\sigma_1^2\sigma_2^2(1-\rho^2)}{\sigma_1^2 - 2\rho\sigma_1\sigma_2 + \sigma_2^2} \tag{100}$$

Whether it is advantageous to use this estimate depends rather sensitively on ρ and $\gamma = \sigma_2/\sigma_1$ [and on the computer's ability to estimate a]. It is particularly advantageous if ρ is negative. The exact dependence on ρ and γ is given in Graph 1 of Chapter II. ρ is given by the standard formula.

$$\rho\sigma_1\sigma_2 = \overline{L_1L_2} - \bar{L}_1\bar{L}_2 \tag{101}$$

$$= \overline{L_1L_2} - \bar{z}^2$$

$$\overline{L_1L_2} = \sum_{I=0}^{\infty}\sum_{i=i}^{\infty} \overline{w_I m(:x_I,y_I) w_i m(:x_i,y_i) p(:x_i,y_i)} \tag{102}$$

The expected value of any term in the above sum is easily calculated:

$$\overline{w_I m(:x_I,y_I) w_i m(:x_i,y_i) p(:x_i,y_i)} = \overline{\overline{w_I}(:x_I,y_I,w_i,x_i,y_i) m(:x_I,y_I) w_i m(:x_i,y_i) p(:x_i,y_i)} \tag{103}$$

$$= \overline{m_{I-i}(x_I,y_I:x_i,y_i) m(:x_I,y_I) w_i^2 m(:x_i,y_i) p(:x_i,y_i)}$$

$$= \iiiint m_{I-i}(x_I,y_I:x_i,y_i) m(:x_I,y_I) p(:x_I,y_I) \overline{w^2}(:x_i,y_i)$$

$$m(:x_i,y_i) p(:x_i,y_i) p_{I-i}(x_I,y_I:x_i,y_i)$$

$$P_i(x_i,y_i)\,dx_i\,dy_i\,dx_I\,dy_I$$

$$= \iiiint K_{I-i}(x_I,y_I:x_i,y_i)m(:x_I,y_I)p(:x_I,y_I)$$

$$m(:x_i,y_i)p(:x_i,y_i)Q_i(x_i,y_i)dx_i dy_i dx_I dx_I$$

$$= \iint S_{I-i}(:x_i,y_i)m(:x_i,y_i)p(:x_i,y_i)Q_i(x_i,y_i)dx_i dy_i$$

Summing from I=i to ∞ gives

$$\overline{L_1 L_2} = \sum_{i=0}^{\infty} \iint S(:x_i,y_i)m(:x_i,y_i)p(:x_i,y_i)Q_i(x_i,y_i)dx_i dy_i \qquad (104)$$

$$= \iint S(x,y)m(:x,y)p(:x,y)Q(x,y)dxdy$$

$$= \iint S(x,y)z(x,y)Q(x,y)dxdy$$

$$\overline{L}_1\overline{L}_2 = \bar{z}^2$$

$$= \left[\iint S(x,y)M_o(x,y)dxdy\right]^2 \qquad (105a)$$

$$= \left[\iint z(x,y)M(x,y)dxdy\right]^2 \qquad (105b)$$

$$= \left[\iint S(x,y)M_o(x,y)dxdy\right]\left[\iint z(x,y)M(x,y)dxdy\right] \qquad (105c)$$

There will be some discussion of the application of these formulae in Chapter VII.

Type IV

Sometimes the transition functions are of such a nature that it is possible to write (x_i,y_i,w_i) as a simple function of (x_o,y_o,w_o). For example, if a history $(w_o,x_o,y_o;w_1,x_1,y_1;\ ..\ ;w_I,x_I,y_I)$ has been calculated, then an equally good history can be obtained by picking

a y_o' from $P_o(y:x_o)$, calculating $w_o' = w_o(x_o,y_o')$ and then getting a new history $H' = \left[w_o',x_o,y_o';w_1',x_1'(x_o,y_o),\ y_1'(x_c,y_o')\ \ldots\ ;w_I',x_I'(H,y_o'),y_I'(H,y_o')\right]$. The functions $x_i'\left[H,y_o'\right]$ and $y_i'\left[H,y_o'\right]$ are the x_i and y_i that would have been obtained if the history had started with (w_o',x_o,y_o') instead of (w_o,x_c,y_o) and the same random numbers used. The w_i' are calculated by

$$w_i' = \frac{w_o'}{w_o}\, m(x_i',y_i':x_o,y_o')\ \ldots\ m(x_i',y_i':x_{i-1},y_{i-1}) \tag{106}$$

In most of the situations in which the technique is useful Equation (106) reduces to

$$w_i' = \frac{w_o'}{w_o}\, w_i \tag{107}$$

When the calculation of x_i',y_i', and w_i' is comparatively easy an estimate, L_4, can be obtained by picking several y_o's for each H and averaging their estimates. This reversed splitting technique, in which the "same" final history is joined on to different initial points, is useful when there is a marked dependence on initial conditions. It is especially cheap to do this when the new history can be produced by **translations** or **reflections**, or rotations.

The history H' may want to terminate sooner or later than H does; a corresponding adjustment must be made by adding or dropping (w_i',x_i',y_i') sets.

If the functions $x_i'(H,y_o)$ and $y_i'(H,y_o)$ are sufficiently simple, it is possible to get a very useful estimate by integrating a Type I estimate over all possible y_o'. Let B_i be a subspace of y_o' such that all $(x_j',y_j'),j \leq i$, are in A but (x_{i+1}',y_{i+1}') is in the trap state.

Then, using the Type I estimate for H' and integrating over all y_o in B_i

$$L_4 = \sum_{i=0}^{\infty} \int_{B_i} w_i' m(:x_i', y_i') P(y_o : x_o) dy_o \tag{108}$$

In most problems the B_i go to zero at some finite i. Whether or not this happens, it is always possible to use a Russian Roulette procedure to keep down the number of terms (Section 7). Type IV estimates are important not only because they cut down the variance, but because the computer, using the same histories, can study simultaneously different A regions or different initial conditions. This last often results in a very large saving of computing time.

Some typical situations in which an integration over initial values can be useful occur when Y is: a position variable in plane slab problems; an energy variable when the diffusion process is independent of the energy; an angle variable where it is possible to take advantage of some symmetry condition; an angle variable for a problem in which, by revolving the history, a target area can be hit with a high degree of probability; etc.

Type V

Integration over initial conditions can be combined with a Type II estimate. The B_i must then be defined as the subspace of y_o such that all $\left[x_j'(H,y_o), y_j'(H,y_o)\right]$ are in A for $j \leq i$. The estimate is

$$L_5 = \sum_{i=0}^{\infty} \int_{B_i} w_i' p(:x_i', y_i') m(:x_i', y_i') P_o(y_o : x) dy_o \tag{109}$$

A disadvantage of this technique over Type IV is the necessity for calculating $p(:x,y)$. In some problems this calculation is more tractable if L_5 is used with a "mixed" collision. L_5 is useful for the same sorts of situations as L_4. It is obvious that L_4 and L_5 could also be defined in terms of an integration over x_o instead of y_o or it is conceivable that both integrations could be done simultaneously.

Type VI

If the kernel $K(x',y':x,y)$ has the form

$$K(x',y':x,y) = k(y':x,y,x')k'(x':x) \tag{110}$$

it is possible to treat the $k(x':x)$ as the kernel of a simpler integral equation

$$M(x') = \int k'(x':x)M(x) + M_o(x) \tag{111}$$

$$M_o(x) = \int M_o(x,y)dy$$

and a set of histories in x calculated. Each history in x space can then be used in calculating a history in y space. For example, the angle and energy histories of a particle diffusing through a homogeneous medium are independent of the space histories and a library of energy - angle histories can be calculated in advance. This library can then be used to calculate space histories for different problems, or a Russian Roulette and splitting technique can be used and many space histories calculated for a single angle-energy history. In the early days of Monte Carlo when computing was done on I.B.M.

punched card machinery or by hand, this procedure was sometimes followed. It does not seem to be efficient for the high speed computers.

In some problems it is possible to write down the kernel $k_i(y_i':x_o,x_1,\ldots x_i,y_o)$ for the expected weight at y_i given y_o and the history in x space. If it is possible to calculate integrals with $k_i(y_i':x_o,x_1,\ldots,x_i,y_o)$ as part of the integrand then a potentially useful Type VI estimate can be made. For example if (x_i,y_i') is in the trap state and (x_o,y_o) is in A then

$$L_6 = \sum_{i=1}^{\infty} \iint m(:x_i,y_i')k_i(y_i':x_o,x_1,\ldots x_i,y_o)M_o(y_o:x_o)dy_i'dy_o \qquad (112)$$

is an estimate of $\bar{z}$. The most important case where L_6 can be calculated is when Y is a random variable associated with survival or absorption, and x is all the other variables of the problems. L_6 is then evaluated in a trivial fashion to be the product of the survival probabilities of each separate collision. It is actually possible to evaluate L_6 analytically in other cases, but the author does not know of any in which the formulae are not too cumbersome to be useful*. As always an equation similar to (112) could be written for a Type II estimate instead of a Type I.

---

* Martin Berger of the National Bureau of Standards has informed me that he is planning to use an L_6 type estimate in treating the diffusion of γ rays in finite plane slabs where the x space is the angle-energy history and the y space the distance into the slab.

6. Correlation

As in Section 18 of Part II there are two fundamentally different ways of correlating problems. The first, and possibly the most important, is to use the same $P_o(x,y)$ and $p(x',y':x,y)$ and to let the weights and/or weighting factors be different for the different problems. Specifically if two problems are determined by the functions:

a. $M_o(x,y), K(x',y':x,y)$, and $z(x,y)$

b. $M'_o(x,y), K'(x',y':x,y)$, and $z'(x,y)$

respectively, the computer can use any convenient $P_o(x,y)$, $p(x',y':x,y)$, and $p(:x,y)$ to compute the partial history $(x_o,y_o,x_1,y_1,\ldots,x_I,y_I)$. The w_i's and W's for the two problems can then be obtained from the weights and weighting factors:

a. $$w_o(x,y) = M_o(x,y)/P_o(x,y) \qquad (113)$$

$$m(x',y':x,y) = K(x',y':x,y)/p(x',y':x,y)$$

$$m(:x,y) = z(x,y)/p(:x,y)$$

b. $$w'_o(x,y) = M'_o(x,y)/P_o(x,y) \qquad (114)$$

$$m'(x',y':x,y) = K'(x',y':x,y)/p(x',y':x,y)$$

$$m'(:x,y) = z'(x,y)/p(:x,y)$$

As discussed in Part II, the strength of the correlation is measured by $\rho\sigma\sigma' = \overline{WW'} - \overline{W}\,\overline{W'}$. $\overline{WW'}$ can be calculated as the expected value of a random walk. If $S''(:x,y)$ and $M''(x,y)$ are defined by the

equations

$$S^n(:x,y) = \iint_A S^n(:x',y')m(x',y':x,y)m'(x',y':x,y)p(x',y':x,y)dx'dy'$$

$$+ p(:x,y)m(:x,y)m'(:x,y) \qquad (114a)$$

$$= \iint_A \frac{S^n(:x',y')K(x',y':x,y)K'(x',y':x,y)}{p(x',y':x,y)}dx'dy' + \frac{z(x,y)z'(x,y)}{p(:x,y)}$$

and

$$M^n(x,y) = \iint_A m(x,y:x',y')m'(x,y:x',y')p(x,y:x',y')M^n(x',y')dx'dy'$$

$$+ P_o(x,y)w_o(x,y)w'_o(x,y) \qquad (114b)$$

$$= \iint_A \frac{K(x,y:x',y')K'(x,y:x',y')M^n(x',y')}{p(x,y:x',y')}\,dx'dy' + \frac{M_o(x,y)M'_o(x,y)}{P_o(x,y)}$$

then

$$\overline{WW'} = \iint_A S^n(:x,y)\,\frac{M_o(x,y)M'_o(x,y)}{P_o(x,y)}\,dxdy \qquad (115)$$

$$= \iint_A M^n(:x,y)\,\frac{z(x,y)z'(x,y)}{p(:x,y)}\,dxdy$$

The other important method of correlation is to use the same random numbers at a corresponding point in the two calculations. It is then usually somewhat more than twice as costly to do the two problems than to do one of them. By contrast, carrying along an extra weighting factor usually increases the cost by an almost negligible amount. The implication is that the variance, if the second method of correlation is used, should be less than half of what it would be if the first were used. If, as defined in Section 3,

$x_j(x_{i-1},y_{i-1})$ and $x'_j(x'_{i-1},y'_{i-1})$ are equiprobability surfaces for the two problems, then using the second type of correlated sampling on the x space is equivalent to picking the same j surface in the two problems. In this case the expected value of WW' is given by

$$\overline{WW'} = \sum_{r=0}^{i-2} \overline{W}_r \sum_{r=0}^{i-2} \overline{W}'_r + \int\int\int\int S(:x_i,y_i)S'(x'_i,y'_i)\delta\left[x'_i - x'_{j(x_i)}\right] K(x_i,y_i:x_{i-1},y_{i-1}) \tag{116}$$

$$K'(x'_i,y'_i:x'_{i-1},y'_{i-1})M_{i-1}(x_{i-1},y_{i-1})M'(x'_{i-1},y'_{i-1})dx_{i-1} \cdots dy'_i$$

where $\delta\left[x'_i - x'_{j(x_i)}\right]$ guarantees that x'_i and x_i are on the same j surfaces and the convention has been made that $SK = m(x:_{i-1},y_{i-1})p(:x_{i-1},y_{i-1})$ and $S'K' = m(:x'_{i-1},y'_{i-1})p(:x'_{i-1},y'_{i-1})$ when (x_j,y_j) is in the trap state. Neither of the expressions in Equations (115) or (116) is particularly revealing. The reader will probably get more out of considering the examples at the end of this section and in Appendix V than by studying the above equations.

Parametric Study of $M_o(x,y)$

In many important uses of correlation by weighting, the effect of correlation, while beneficial, is secondary. The reduction in cost is the primary reason for using it. For example it may be desirable to study what happens when different $M_o(x,y)$ are used and everything else is left unchanged. This situation could arise when $M_o(x,y)$ is one of the design parameters being studied, or more likely different $M_o(x,y)$ correspond to different idealizations of

the physical problem. It is almost no extra work to calculate three or four problems simultaneously by using the same histories with different $w_o(x_o,y_o)$. It is convenient in this case to stratify the initial distribution of (x,y) according to some $P_o^*(x,y)$ and to let $w_o(x,y) = 1$. The Monte Carlo calculation can then be used to estimate S(:x,y) and T(:x,y). The estimated S(:x,y) and T(:x,y) can be integrated against $M_o(x,y)$ and $M_o^2(x,y)/P_o(x,y)$ to get estimates of $\bar{z}$ and $\overline{z^2}$ respectively for any $M_o(x,y)$ and $P_o(x,y)$. If it is inconvenient to estimate S(:x,y) and T(:x,y), then labeling each history with the subscript n, the (x_{on},y_{on},W_n) can be recorded and the estimates

$$\tilde{z} = \frac{1}{N}\sum_{n=1}^{N} W_n \frac{M_o(x_{on},y_{on})}{P^*(x_{on},y_{on})} \tag{117}$$

$$\tilde{z^2} = \frac{1}{N}\sum_{n=1}^{N} W_n^2 \frac{M_o^2(x_{on},y_{on})}{P(x_{on},y_{on})P^*(x_{on},y_{on})} \tag{118}$$

used.

Parametric Study of K(x',y':x,y)

$$\text{Let } K(x',y':x,y) = k_o(x',y':x,y) + \sum_{1}^{J} \varepsilon_j k_j(x',y':x,y) \tag{119a}$$

$$z(x,y) = z_o(x,y) + \sum_{1}^{J} \varepsilon_j z_j(x,y) \tag{119b}$$

where the ε_j are small. If the transition probabilities are p(x',y':x,y) and p(:x,y) then

$$W = w_o(x_o,y_o)\,\frac{z(x_I,y_I)}{p(:x_I,y_I)}\prod_{i=0}^{I-1}\frac{K(x_{i+1},y_{i+1}:x_i,y_i)}{p(x_{i+1},y_{i+1},x_i,y_i)} \tag{120}$$

$$\approx W_o + w_o(x_o,y_o)\sum_1^J \varepsilon_j\gamma_j$$

where

$$W_o = w_o(x_o,y_o)\,\frac{z_o(x_I,y_I)}{p(:x_I,y_I)}\prod_{i=0}^{I-1}\frac{k_o(x_{i+1},y_{i+1}:x_i,y_i)}{p(x_{i+1},y_{i+1}:x_i,y_i)} \tag{121a}$$

$$\gamma_j = \frac{z_o(x_I,y_I)}{p(:x_I,y_I)}\sum_{i=0}^{I-1}\frac{k_j(x_{i+1},y_{i+1}:x_i,y_i)}{p(x_{i+1},y_{i+1}:x_i,y_i)}\prod_{r=0}^{I-1}{}'\frac{k_o(x_{r+1},y_{r+1}:x_r,y_r)}{p(x_{r+1},y_{r+1}:x_r,y_r)} \tag{121b}$$

$$+\frac{z_j(x_I,y_I)}{p(:x_I,y_I)}\prod_{i=0}^{I-1}\frac{k_o(x_{i+1},y_{i+1}:x_i,y_i)}{p(x_{i+1},y_{i+1}:x_i,y_i)}$$

and the symbol $\prod_{r=0}^{I-1}{}'$ means that the term r=i is left out of the product. In an actual computation the γ_j can be computed by a simple iterative scheme and not by the rather formidable looking formula in the above equations. To first order in ε_j.

$$\bar{z} = \bar{W}_o + \sum_{j=1}^{J}\varepsilon_j\overline{\gamma_j w_o(x_o,y_o)} \tag{122}$$

If the Monte Carlo calculation is used to estimate $\bar{W}_o$ and $\overline{\gamma_j w_o(x_o,y_o)}$ then the computer can use these estimates to study how $\bar{z}$ varies as a function of ε_j in the region around $\varepsilon_j = 0$. A much more interesting problem is to assume that $\bar{z}$ is known and the ε_j unknown. An example of such a problem would be when the results of bulk scattering experiments are known and the computer wants to use these results to improve the knowledge of the differential scattering cross sections.

In this situation the results of K different problems must be given with $K \geq J$. Each of the K problems then determines an equation like (122). By using a least squares technique it is possible to obtain J simultaneous equations which can be solved for the ε_j. It is not known as a practical matter under what conditions the process can be carried through accurately. The question is currently being studied in connection with the problems discussed in Chapter VI, and it is hoped that some results will be available soon.

Miscellaneous Examples

Comparing Different Strategies at Draw Poker

Let us assume that the computer wishes to compare two different drawing strategies. A simple way to achieve correlation would be to use identically shuffled decks and play out the two types of strategies. This would not be very satisfactory though, because the two decks would get out of step as soon as the number of cards drawn in the two strategies differed. The obvious solution to the difficulty is to discard the extra cards. This has the happy result that a zero difference results whenever the two strategies are the same and the Monte Carlo is being used to estimate directly only the frequency and importance of the situations in which there is a difference between the two strategies.

Comparing Different Bombing Strategies*

If a strategic or tactical bombing campaign is studied by Monte Carlo it is customary to introduce some or all of the following random

---

*

elements.

1. Number of planes that abort
2. Number of planes shot down by area defense on the way in
3. Number of planes that stray through navigational errors
4. Number of planes shot down by local defense
5. Weather conditions over target
6. Place where bombs land
7. Damage done
8. Good or bad reconnaissance
9. Number of planes shot down by area defense on the way out
10. Number of planes that don't get back for a miscellany of minor reasons

Because some of the probabilities concerned depend on the number of planes, the above problem is non-linear. This does not prevent the use of any of the techniques suggested.

If the computer wishes to compare different bombing strategies it is often effective to use correlation to cut down the sample size required to get significant information. If the correlation is done by using the same random numbers, there will be different numbers of planes aborting, shot down, etc. The computer cannot use a single list of random numbers in sequence in the two problems, for they would soon get out of step. He can either throw away the excess random numbers or what is sometimes better, save them for use on later strikes. For example, if a larger number of targets were attacked on the first strike of strategy one, the extra random numbers that were used to determine the weather on these excess targets can

be saved. If in a later strike an excess number of targets is attacked under strategy two, the saved random numbers can then be used on these targets. Correlation can thus be achieved by using the same random numbers whenever the two strategies give rise to the same type of contingencies - even if they are on different strikes with different planes and targets.

If the different strategies are such that a definite type of event is all-important to the comparison then correlation by weighting may be better than using the same random numbers. For example, if the effect of different types of defensive armament are being studied, the same kill probabilities could be used for the enemy fighters in the sampling, and weighting factors carried along to account for the differences. The correlation may be higher if this is done, because exactly the same number of bombers are shot down each time, so all of the subsequent history is the same. If the correlating were done by using the same random numbers, different numbers of planes would be shot down and the actual progress of the two strategic campaigns would be quite different. It would still be possible to obtain correlation by using the same random numbers for the same types of contingencies, but it is unlikely that the correlation would be as high.

Another case where weighting might be preferable to using the same random numbers would be when two different reconnaissance devices were being compared. The possible weather situations can then be classified according to the following criteria:

1. Both devices work

2. One works and the other does not

3. Neither works

Only situation 2 makes a difference between the two devices so that in the sampling only it should be allowed to occur. If 1 and 3 occur, the sample would give zero for the estimate, so they need not be calculated, only the percent, P, of time they occur is needed. This is automatically calculated by the weighting factors. If instead of being an all or nothing situation the devices have different probabilities of working as the weather changes, then the appropriate modification must be made in the sampling. If the same random numbers were used to do the correlating then (1-P) of the time the sample would be wasted.

Polarization*

In tracing γ rays through a medium it simplifies the problem greatly to assume that the γ rays are unpolarized. This assumption can be checked by doing two correlated problems, one using the exact laws and the other the approximate one that is obtained when it is assumed that the particles are unpolarized. If weighting factors are used to do the correlating they would fluctuate wildly because the differential scattering laws are quite different in the two cases. The actual effect of polarization turns out to be quite small in most problems of interest. This is shown very effectively if the correlating is done by using the same random numbers. It then turns out, in most situations, that even though quite different azimuthal angles are picked

* The above technique has also been used independently by Lewis V. Spencer of the National Bureau of Standards.

in the two problems every time a γ ray scatters, the answer is not affected very sharply.

$\underline{K(x',y':x,y) = k(y':x,y,x')k'(x':x)}$.

When the kernel of the integral equation is as in Equation (110) and the computer finds it very easy to treat Equation (111) either analytically or by some numerical technique, then the technique at the end of Section 18 of Part II [Eliminating the Variance of $\bar{z}(:x)$] can be used in the manner described there to cut down the variance.

7. RUSSIAN ROULETTE AND SPLITTING

In Section 2 on Importance Sampling there was a fairly complete discussion on the cirteria to use in choosing transition probabilities for a Monte Carlo calculation. In many probabilistic problems, however, the set of transition probabilities and weighting functions given directly by the physical situation are often computationally much simpler to sample from than the ones that the computer would choose if the principles of importance sampling were followed. It is possible to use a non optimum (in the sense of importance sampling) set of transition probabilities and still spend most the computing time on "important regions" by using Russian Roulette and Splitting.

The discussion which follows, assumes that a Type I estimate is being used. If some other type is used an appropriate modification of the formulae and results must be made.

The variance of a Russian Roulette and Splitting sampling procedure was calculated in Part II by representing the variance of the straightforward sampling procedure in a form such as

$$\int \sigma^2(:x) f(x)dx + \int \left[\bar{z}(:x) - \bar{z}\right]^2 f(x)dx$$

and then noticing that the first term is modified in a very simple fashion if Russian Roulette or Splitting is used and that the second term is not affected by the modification. The

same technique will be used in this section.

If $W(:x,y,w)$ is the conditional random trapped weight given that the particle starts at (x,y) with weight w and no Russian Roulette or Splitting is used, then

$$\bar{W}(:x,y,w) = wS(:x,y) \tag{130a}$$

$$\overline{W^2}(:x,y,w) = w^2T(:x,y) \ . \tag{130b}$$

The variance $V(:x,y,w)$ of $W(:x,y,w)$ is given by the usual expression

$$V(:x,y,w) = \overline{\left[W(:x,y,w) - \bar{W}(:x,y,w)\right]^2} \tag{131}$$

$$= w^2\left[T(:x,y) - S^2(:x,y)\right]$$

Define w' as the weight of the particle after collision.

$$w' = wm(x',y':x,y) \tag{132}$$

Then using Equation (30b) for $T(:x,y)$ an integral equation can be written for $V(:x,y,w)$

$$V(:x,y,w) = \iint_A w'^2T(:x',y')p(x',y':x,y)dx'dy' \tag{133a}$$
$$+ w^2m^2(:x,y)p(:x,y) - w^2S^2(:x,y)$$

$$= \iint_A V(:x',y',w')p(x',y':x,y)dx'dy' \tag{133b}$$
$$+ \iint_A w'^2S^2(:x',y')p(x',y':x,y)dx'dy'$$
$$+ w^2m^2(:x,y)p(:x,y) - w^2S^2(:x,y)$$

$$= \iint_A V(:x',y',w')p(x',y':x,y)dx'dy' \tag{133c}$$
$$+ \iint\left[w'S(:x',y') - wS(:x,y)\right]^2p(x',y':x,y)dx'dy'$$
$$+ w^2\left[m(:x,y) - S(:x,y)\right]^2p(:x,y)$$

The variance of the sampling procedure is given by

$$V = \iint_A V\left[:x,y,w_o(x,y)\right] P_o(x,y)dxdy + \iint_A \left[w_o(x,y)S(:x,y) - \bar{z}\right]^2 P_o(x,y)dxdy \quad (134)$$

As already indicated only the first term is affected by the introduction of Russian Roulette and Splitting. It is convenient at this point to introduce a few definitions:

a. $W^*(:x,y,w)$ is a conditional random variable that is the sum of the random trapped weights of the particles produced by a parent particle that starts from (x,y) with weight w. Because the expected value of the trapped weight is not changed by the use of Russian Roulette or Splitting,

$$\overline{W^*}(:x,y,w) = \bar{W}(:x,y,w) \quad (135)$$
$$= wS(:x,y) .$$

The expected values of $W^{*2}(:x,y,w)$ is changed.

Let

$$T^*(:x,y,w) = \overline{W^{*2}}(:x,y,w) \quad (136a)$$

$$V^*(:x,y,w) = T^*(:x,y,w) - w^2S^2(:x,y,w) . \quad (136b)$$

b. R_1' is a subarea of A. The initial (x,y) point is picked out of $P_o(x,y)$. If it happens to be in R_1', a Russian Roulette procedure with a probability $q_o(x,y)$ of survival is used. If the particle survives it is assigned a weight

$$w_{o1} = w_o(x,y)/q_o(x,y) . \quad (137)$$

The variance associated with this event is given by

$$\left[T^*(:x,y,w_o')q_o(x,y) - w_o^2(x,y)S^2(:x,y)\right] \quad (138)$$

c. $R_2' = A - R_1'$ is the rest of A. If the initial (x,y) point is in R_2', the particle is split into $n_o(x,y)$ independent particles, each of weight

$$w_{o2} = w_o(x,y)/n_o(x,y) \quad (139)$$

The variance associated with this event is

$$V^*(:x,y,w_{o2})n_o(x,y) \quad (140)$$

d. $R_1(x,y,w)$ is a subarea of A that depends on the particle position and weight. If the particle jumps to a point (x',y') in $R_1(x,y,w)$ then a Russian Roulette procedure with probability $q(x',y':x,y,w)$ is used before the next collision point is chosen. If the particle survives the Russian Roulette it is given a weight

$$w_1' = wm(x',y':x,y)/q(x',y':x,y,w) \quad (141)$$
$$= w'/q(x',y':x,y,w)$$

The variance introduced by an event of this type is

$$\left[T^*(:x',y',w_1')q(x',y':x,y,w) - w'^2S^2(:x',y')\right] \quad (142)$$

e. $R_2(x,y,w) = A - R_1(x,y,w)$ is the rest of A. If (x',y') is in $R_2(x,y,w)$, then the particle is split into n(x',y':x,y,w) independent particles. Each of these particles is given a weight

$$w_2' = wm(x',y':x,y)/n(x',y':x,y,w) \quad . \quad (143)$$
$$= w'/n(x',y':x,y,w)$$

$n(x',y':x,y,w)$ must be an integer, but in the very rough derivation which follows it will be considered as being a continuous variable. The variance introduced by the $n(x',y':x,y,w)$ independent particles is

$$n(x',y':x,y,w)V^*(:x',y',w_2') \tag{144}$$

Using 'a' to 'e' the modification of Equation (133b) appropriate to Russian Roulette and Splitting can now be written

$$V^*(:x,y,w) = \iint_{R_1}\left[T^*(:x',y',w_1')q(x',y':x,y,w) - w'^2S^2(:x',y')\right]p(x',y':x,y)dx'dy' \tag{145a}$$

$$+ \iint_{R_2} V^*(:x',y',w_2')n(x',y':x,y,w)p(x',y':x,y)dx'dy'$$

$$+ \iint_{A} w'^2S^2(:x',y')p(x',y':x,y)dx'dy'$$

$$w^2m^2(:x,y)p(:x,y) - w^2S^2(:x,y)$$

$$= \iint_{R_1} V^*(:x',y';w_1')q(x',y':x,y,w)p(x',y':x,y)dx'dy' \tag{145b}$$

$$\iint_{R_2} V^*(:x',y',w_2')n(x',y':x,y,w)p(x',y':x,y)dx'dy'$$

$$w^2A(x,y,R_1) + w^2B(x,y)$$

$$w^2A(x,y,R_1) = \iint_{R_1}\left[w_1'^2S^2(:x',y')q(x',y':x,y,w) - w'^2S^2(:x',y')\right]p(x',y':x,y)dx'dy' \tag{146a}$$

$$= \iint_{R_1} w'^2S^2(:x',y')\left[\frac{1}{q(x',y':x,y,w)} - 1\right]p(x',y':x,y)dx'dy'$$

$$= w^2\iint_{R_1} S^2(:x',y')m^2(x',y':x,y)\left[\frac{1}{q(x',y':x,y,w)} - 1\right]p(x',y':x,y)dx'dy'$$

$$B(x,y) = \iint S^2(:x',y')m^2(x',y':x,y)p(x',y':x,y)dx'dy' \quad (146b)$$

$$+ m^2(:x,y)p(:x,y) - S^2(:x,y)$$

Equation (134) becomes

$$V_7 = \iint_{R_1} V(:x,y,w_{o1})q_o(x,y)P_o(x,y)dxdy \quad (147)$$

$$\iint_{R_2} V(:x,y,w_{o2})n_o(x,y)P_o(x,y)dxdy$$

$$+ \iint_A \left[w_o(x,y)S(:x,y) - \bar{z}\right]^2 P_o(x,y)dxdy.$$

$B(x,y)$ is independent of the choice of $q(x',y':x,y,w)$, $n(x',y':x,y,w)$, and the regions R_1 and R_2. If the computer chooses

$$p(x',y':x,y) = S(:x',y')K(x',y':x,y)/S(:x,y) \quad (148)$$

$$p(:x,y) = z(x,y)/S(:x,y)$$

$$m(x',y':x,y) = S(:x,y)/S(:x',y')$$

$$m(:x,y) = S(:x,y)$$

then it is easy to show [by using Equation (15)] that $B(x,y)$ is zero.

If in addition the region R_1 is chosen to be zero so that no Russian Roulette is used, then $A(x,y,R_1)$ is zero and therefore also $V^*(:x,y,w)$. Since the above choice weighting functions and transition probabilities corresponds to optimum or zero variance importance sampling it is not completely surprising that the splitting process should still be zero variance.

It was shown in Section 19 of Part II that the Russian Roulette or Splitting should be done in such a manner that the weights w_1' or w_2' assigned to the final particle or particles are independent of w', but unique (different) functions of the position. In the discussion which follows it will be assumed that the computer has decided to carry out a scheme in which the particle or particles will always end up with a weight always equal to some function, $1/\lambda U(x,y)$. Since this final weight does not depend on whether the particle has just gone through the ordeal of Russian Roulette or merely split, the scheme will not be optimum, but it will be close enough for all practical purposes. The scheme is as follows:

a. The region R_1' is determined by

$$w_o(x,y) < 1/\lambda U(x,y) \tag{149a}$$

and the probability of survival

$$q_o(x,y) = \lambda U(x,y) w_o(x,y) \tag{149b}$$

$$w_{o1} = w_o(x,y)/q_o(x,y)$$
$$= 1/\lambda U(x,y) \tag{149c}$$

b. In the complementary region R_2'

$$w_o(x,y) \geq 1/\lambda U(x,y) \tag{150a}$$

$$n_o(x,y) = \lambda U(x,y) w_o(x,y) \tag{150b}$$

$$w_{o2} = w_o(x,y)/n_o(x,y)$$
$$= 1/\lambda U(x,y) \tag{150c}$$

c. The region $R_1(x,y)$ no longer depends explicitly on the weight since $w = 1/\lambda U(x,y)$ is a function of (x,y).

The region is determined by the inequality

$$\frac{m(x',y':x,y)}{U(x,y)} \leq \frac{1}{U(x',y')} \qquad (151a)$$

and

$$q(x',y':x,y) = \frac{U(x',y')}{U(x,y)}\, m(x',y':x,y)$$

d. In the complementary region $R_2(x,y)$,

$$\frac{m(x',y':x,y)}{U(x,y)} \geq \frac{1}{U(x',y')} \qquad (152a)$$

$$n(x',y':x,y) = \frac{U(x',y')}{U(x,y)}\, m(x',y':x,y) \qquad (152b)$$

It is clear that rules 'a' to 'd' will result in the particle always having a weight equal to the desired $1/\lambda U(x,y)$. Under these circumstances Equations (145b) and (147) become

$$V^*\left[:x,y,\frac{1}{\lambda U(x,y)}\right] = \iint_{R_1} V^*\left[:x',y',\frac{1}{\lambda U(x',y')}\right]\frac{U(x',y')}{U(x,y)}\, m(x',y':x,y)p(x',y':x,y)dx'dy'$$

$$+ \iint_{R_2} V^*\left[:x',y',\frac{1}{\lambda U(x',y')}\right]\frac{U(x',y')}{U(x,y)}\, m(x',y':x,y)\, p(x',y':x,y)dx'dy'$$

$$+ \frac{A(x,y,R_2)}{\lambda^2 U^2(x,y)} + \frac{B(x,y)}{\lambda^2 U^2(x,y)} \qquad (153)$$

$$V_7 = \iint_{R_1} V^*\left[:x,y,\frac{1}{\lambda U(x,y)}\right]\lambda U(x,y)w_o(x,y)P_o(x,y)dxdy \qquad (154)$$

$$+ \iint_{R_2} V^*\left[:x,y,\frac{1}{\lambda U(x,y)}\right]\lambda U(x,y)w_o(x,y)P_o(x,y)dxdy$$

$$+ \iint_{A}\left[w_o(x,y)S(:x,y) - \bar{z}\right]^2 P_o(x,y)dxdy\ .$$

By combining the regions R_1 and R_2, defining

$$V^*(:x,y) = \lambda^2 V^*\left[:x,y,\frac{1}{\lambda U(x,y)}\right] \tag{155}$$

and making standard substitutions the equations

$$V^*(:x,y) = \iint_A V^*(:x',y')\,\frac{U(x',y')}{U(x,y)}\,K(x',y':x,y)\,dx'dy' \tag{156}$$

$$+\,\frac{A(x,y,R_2)}{U^2(x,y)} + \frac{B(x,y)}{U^2(x,y)}$$

$$V_7 = \frac{1}{\lambda}\iint_A V^*(:x,y)U(x,y)M_o(x,y)\,dxdy\,, \tag{157}$$

$$+\iint_A \left[w_o(x,y)S(:x,y) - \bar{z}\right]^2 P_o(x,y)\,dxdy\,.$$

are derived. If the correspondence

$$S(x,y) \longrightarrow V^*(:x,y)U(x,y) \tag{158a}$$

$$z(x,y) \longrightarrow \frac{A(x,y,R_2)}{U(x,y)} + \frac{B(x,y)}{U(x,y)} \tag{158b}$$

$$M_o(x,y) \longrightarrow M_o(x,y) \tag{158c}$$

is made, then Equation (156) is the same as Equation (2b) and the first integral in (157) is the same as (?a). Therefore by using the equivalent of Equation (3), (157) can be written

$$V_7 = \frac{1}{\lambda}\iint_A \frac{A(x,y,R_2)}{U(x,y)}\,M(x,y)\,dxdy \tag{159}$$

$$+\,\frac{1}{\lambda}\iint_A \frac{B(x,y)}{U(x,y)}\,M(x,y)\,dxdy$$

$$+\iint_A \left[w_o(x,y)S(:x,y) - \bar{z}\right]^2 P_o(x,y)\,dxdy$$

In addition to the variance V_7 of the sampling procedure, the cost C must be considered. Let:

C_o be the expected marginal cost of starting a history.

$C_1(x,y)$ be the expected cost of tracing a history that starts with weight $1/\lambda U(x,y)$.

$C_2(x,y)$ be the expected cost of terminating history that jumps to the trap state from (x,y).

$C_3(x,y)$ is the cost of computing a new collision point starting from (x,y).

The expected marginal cost of a sample is given by

$$C = \iint_{R_1'} C_1(x,y) q_o(x,y) P_o(x,y)\,dxdy + \iint_{R_2'} C_1(x,y) n_o(x,y) P_o(x,y)\,dxdy + C_o \quad (160a)$$

$$= \lambda \iint_A C_1(x,y) U(x,y) w_o(x,y) P_o(x,y)\,dxdy + C_o$$

$$= \lambda \iint_A C_4(x,y) U(x,y) M_o(x,y)\,dxdy + C_o \quad (160b)$$

$C_1(x,y)$ is determined by the integral equation

$$C_1(x,y) = \iint_{R_1} C_1(x',y') q(x',y':x,y) p(x',y':x,y)\,dx'dy' \quad (161a)$$

$$+ \iint_{R_2} C_1(x',y') n(x',y':x,y) p(x',y':x,y)\,dx'dy'$$

$$+ \left[1 - p(:x,y)\right] C_3(x,y) + p(:x,y) C_2(x,y)$$

$$= \iint_A C_1(x',y') \frac{U(x',y')}{U(x,y)} m(x',y':x,y) p(x',y':x,y)\,dx'dy' + D(x,y)$$

$$= \iint_A C_1(x',y') \frac{U(x',y')}{U(x,y)} K(x',y':x,y)\,dx'dy' + D(x,y) \quad (161b)$$

where

$$D(x,y) = C_3(x,y) + p_3(x,y)\left[C_2(x,y) - C_3(x,y)\right] \quad (161c)$$

In the same way that Equation (159) was derived, Equation (160b) and (161b) imply that

$$C = \lambda \iint_A U(x,y)D(x,y)M(x,y)dxdy + C_o \quad (162)$$

Equation (159) and (162) are essentially the same as Equations (224) and (227) of Part II. They are a little more complicated because $A(x,y,R_1)$ in Equation (159) is a function of $U(x,y)$. Using Equations (146a) and (151b), $A(x,y,R_1)$ can be written

$$A(x,y,R_1) = U(x,y)\iint_{R_1(x,y)} \frac{S^2(:x',y')K(x',y':x,y)}{U(x',y')}\,dx'dy' \quad (163)$$

$$- \iint_{R_1(x,y)} S^2(:x',y')m^2(x',y':x,y)p(x',y':x,y)dx'dy'$$

Therefore V_7 can be written:

$$V_7 = \frac{1}{\lambda}\iint_A M(x,y)dxdy \iint_{R_1(x,y)} \frac{S^2(:x',y')K(x',y':x,y)}{U(x',y')}\,dx'dy' \quad (164)$$

$$- \frac{1}{\lambda}\iint_A \frac{M(x,y)}{U(x,y)}dxdy \iint_{R_1(x,y)} S^2(:x',y')m^2(x',y':x,y)$$
$$p(x',y':x,y)dx'dy'$$

$$+ \frac{1}{\lambda}\iint_A \frac{B(x,y)}{U(x,y)}M(x,y)dxdy$$

$$+ \iint_A \left[w_o(x,y)S(:x,y) - \bar{z}\right]^2 P_o(x,y)dxdy$$

By interchanging the order of integration, the first term can be written:

$$\frac{1}{\lambda}\iint_A \frac{S^2(x,y)}{U(x,y)}dxdy \iint_{R_2(x,y)} K(x,y:x',y')M(x',y')dx'dy'$$

V_7 can then be written in the form

$$V_7 = \frac{1}{\lambda} V_o' + V_o \,, \qquad (165)$$

where

$$V_o' = \iint_A \frac{V(x,y)}{U(x,y)} M(x,y)dxdy \qquad (166a)$$

$$V_o = \iint_A \left[w_o(x,y) - \bar{z}\right]^2 P_o(x,y)dxdy \qquad (166b)$$

$$V(x,y) = \frac{S^2(x,y)}{M(x,y)} \iint_{R_2(x,y)} K(x,y:x',y')M(x',y')dx'dy' \qquad (166c)$$

$$- \iint_{R_1(x,y)} S^2(x',y')m^2(x',y':x,y)p(x',y':x,y)dx'dy'$$

$$+ B(x,y)$$

C can be written [Equation (162)]

$$C = \lambda C_o' + C_o \qquad (167)$$

where

$$C_o' = \iint U(x,y)D(x,y)M(x,y)dxdy \qquad (167a)$$

$$C_o = C_o \,. \qquad (167b)$$

To minimize CV_7 with respect to λ, let

$$\lambda^2 = \frac{V_o'}{C_o'}\frac{C_o}{V_o} \qquad (168)$$

This value of λ makes

$$V_7 = V_o + \sqrt{\frac{V_o}{C_o} C_o'V_o'} \tag{169a}$$

$$C = C_o + \sqrt{\frac{C_o}{V_o} C_o'V_o'} \tag{169b}$$

$$\frac{V_7}{C} = \frac{V_o}{C_o} \tag{169c}$$

$$CV_7 = \left(\sqrt{V_oC_o} + \sqrt{C_o'V_o'}\right)^2. \tag{169d}$$

To minimize CV_7 with respect to $U(x,y)$ it is sufficient to minimize $C_o'V_o'$. This minimum is obtained by taking

$$U(x,y) = \sqrt{\frac{V(x,y)}{D(x,y)}} \tag{170}$$

where $D(x,y)$ is the expected cost of calculating a single collision from the point (x,y) and $V(x,y)$ is approximately [the first two terms of Equation (166c) have a tendency to cancel] $B(x,y)$. $B(x,y)$ can be written [Equation (146b)]

$$B(x,y) = \iint_A \left[S(:x',y')m(x',y':x,y) - S(:x,y)\right]^2 p(x',y':x,y)dx'dy' + \left[m(:x,y) - S(:x,y)\right]^2 p(:x,y). \tag{171}$$

$B(x,y)$ is therefore the variance of a random variable which has an expected value $S(:x,y)$, a discrete probability $p(:x,y)$ of taking on the value $m(:x,y)$, and a p.d.f. $p(x',y':x,y)$ for taking on values $S(:x',y')$.

* * *

This concludes the exposition of the more formal part of the theory of Monte Carlo techniques.

APPENDIX I

Generation of Psuedo-Random Numbers

It was shown in Part I that if one wishes to produce random numbers according to any distribution, this can be done by choosing numbers from another distribution and then performing certain arithmetical transformations on these numbers. Therefore, when one talks about using random numbers, he need only talk about using a certain basic set of random numbers and getting the other kinds of random numbers from this basic set by a transformation. By general convention and convenience, the random numbers defined as being uniformly distributed between zero and one comprise the basic set.

To call a set of numbers random is not so much to make a statement about the properties of the numbers themselves but a statement about their history. It implies that the numbers were produced by some sort of stochastic process. Therefore, when one talks about random numbers one is really talking about stochastic processes. There are many processes which can be used to produce numbers, such as gambling devices of any kind, physical processes such as radio-active decay or "shot noise", etc. However, while it is perfectly possible to adapt such a device to a high speed machine (and in fact this has been done in at least one case) it is actually inconvenient to use such devices, both because of the minor technical fact that it is difficult to tell when it is in working order and the much more important reason that one wishes to reproduce a calculation to see if it is correct. In order to do this one has to know what random numbers entered into the calculation.

It is, of course, conceivable that if one was using a random device one could simply print all the numbers that are used and then reuse them in the check calculations or as an alternative one could prepare the numbers in advance. This is,

of course, not convenient or practical because of the limited memory and input-output capacity of modern machines. However, there are extensive card tables and several books of random numbers available, and The RAND Corporation has put out a book with a million such numbers so that if desired one can use this alternative.

What is really desired is for the machine to compute in a perfectly deterministic fashion a set of numbers which are operationally indistinguishable from numbers which result from the random process. By "operationally indistinguishable" we mean indistinguishable by an reasonable[1] statistical test. (These tests are discussed in the references.) Such numbers have been called "psuedo-random numbers" and there are a number of methods for getting them. In this Appendix we will discuss only one. The reason we restrict our attention to this one is that it seems to be almost completely satisfactory for our purpose and while other methods can have some minor advantages in certain situations, we know of no case where the advantage is really important.

The following is the method of congruences. Let S_o be any odd integer between 1 and n. Let $S_i \equiv k\, S_{i-1} \pmod{n}$. The choice of k and n depends on the machine used. n is usually equal to the capacity of a single register in the machine, a power of 2 or 10, according to whether the machine is binary or decimal. If the multiplication kS_{i-1} is done with double precision, then it is the n least significant digits of the product which form the next random integer. $R_i = S_i/n$ are the psuedo-random numbers in the interval (0,1).

One usually chooses k to be the largest integer, which will conveniently fit in one storage register, and which will realize the maximum possible period length of the sequence. It is chosen large mainly to avoid local correlation between the

---

1 By "reasonable" we mean "good enough for our purposes"[2].

2 By "good enough", . . .

numbers produced. When the congruence is modulo 2^{β}, this period is at most $2^{\beta-2}$. If $\beta \geq 3$, $k = 5^{d}$ for any odd d will achieve this greatest length. If the congruence is modulo 10^{β}, then the maximum period is $5 \cdot 10^{\beta-2}$. If $\beta \geq 5$ and $k = 3^{d}$, where d is prime to 10, the maximum will be obtained. There are other multipliers which will also do, but for these purposes, they seem to be equivalent.

References

1. D. H. Lehmer, Mathematical Methods on Large Scale Computing Units, Harvard University Computation Laboratory, Annals 26 (1951), P. 141-146.
2. John von Neumann, Various Techniques Used in Connection With Random Digits, National Bureau of Standard Symposium, NBS Applied Mathematics Series 12, June 1951.
3. Mario Juncosa, Random Number Generation on the BRL High-Speed Computing Machines, Ballistic Research Laboratories Report No. 855, May 1953.
4. Olga Taussky and John Todd, Generation and Testing of Psuedo-Random Numbers, Symposium on Monte Carlo, John Wiley and Sons, 1956.
5. The RAND Corporation, A Million Random Digits, The Free Press, 1955.

APPENDIX III

Constrained Maximum[1] of a Function

I. Consider the problem of finding the maximum of a function $f(x_i,\ldots,x_n)$ subject to the inequalities

$$a_i \leq x_i \leq b_i \tag{1}$$

The above inequalities define a region in the $(x_1,\ldots,x_n)$ space. If any of the x_i happen to be equal to a_i or b_i, we will say that independent variable is at a boundary, otherwise, we will refer to the independent variable as being interior.

It is well known that at the maximum point the following equations have to be satisfied:

$$\frac{\partial f}{\partial x_i} = 0 \text{ if } a_i < x_i < b_i \qquad (x_i \text{ interior})$$

$$\left.\begin{aligned} \frac{\partial f}{\partial x_i} &\geq 0 \text{ if } x_i = b_i \\ \frac{\partial f}{\partial x_i} &\leq 0 \text{ if } x_i = a_i \end{aligned}\right\} \qquad (x_i \text{ at a boundary}) \tag{2}$$

The above equations are intuitively obvious. They state that at a maximum point you can't increase f by changing the value of any x_i by a small amount either because f is stationary with respect to that x_i or because the x_i is at a boundary. (It is of course possible that equation (2) will be satisfied and yet we will not have a maximum. We will defer discussing that possibility for a moment.)

---

1 The changes that have to be made for a minimum will be obvious to the reader.

In actual practice about the only way to solve a maximization problem like the above is to do it iteratively. An iterative procedure that works well in a large number of cases (when there are no intervals with $\frac{\partial^2 f}{\partial x_i} \neq 0$) is to consider first the system of equations

$$\frac{\partial f}{\partial x_i} = 0 \text{ for all } x_i \tag{3}$$

After this system is solved one checks to see if any x_i violate the limits

$$a_i \leq x_i \leq b_i \tag{4}$$

If they do, one then moves these x_i to their limiting values and solves the reduced system of equations

$$\frac{\partial f}{\partial x_i} = 0 \tag{5}$$

for all the other independent variables. One then checks again to see which new x_i violate their limits and also if the previously placed x_i should be left at the boundaries, and repeats the process until convergence.

II. Let us now consider a slightly more complicated maximization problem. That is, let us consider the problem of calculating the maximum of $f(x_1,\ldots,x_n)$ subject to the new condition

$$g(x_1,\ldots,x_n) = K \tag{6}$$

as well as the old conditions

$$a_i \leq x_i \leq b_i \tag{7}$$

$g(x_1,\ldots,x_n) = K$ defines a surface in the old volume. The point $(x_1,\ldots,x_n)$ must lie on this surface. It is easy to see, in this case, that at the maximum whenever one

of the independent points is interior, that is

$$a_i < x_i < b_i \tag{8}$$

that

$$\frac{\frac{\partial f}{\partial x_i}}{\frac{\partial g}{\partial x_i}} = \lambda \text{ , a constant for all interior } x_i \tag{9}$$

That is, the rate of change of f with respect to any interior x_i when divided by the rate of change of g with respect to that same x_i is a constant. The reason for this is clear. If this ratio differed for any two interior independent variables then we could for instance increase the x_i for which the ratio was large and decrease the x_i value for the ratio which was small. By this means we could increase the value of f without changing the value of g. By the same line of reasoning then it must also be true that for any x_i that are at a boundary

$$\begin{aligned} &\frac{\frac{\partial f}{\partial x_i}}{\frac{\partial g}{\partial x_i}} \geq \lambda \qquad \text{for } x_i = b_i \\ &\frac{\frac{\partial f}{\partial x_i}}{\frac{\partial g}{\partial x_i}} \leq \lambda \qquad \text{for } x_i = a_i \end{aligned} \tag{10}$$

It is customary to write equations (9) and (10) in the form

$$\begin{aligned} &\frac{\partial f}{\partial x_i} = \lambda \frac{\partial g}{\partial x_i} && a_i < x_i < b_i \\ &\frac{\partial f}{\partial x_i} \geq \lambda \frac{\partial g}{\partial x_i} && x_i = b_i \\ &\frac{\partial f}{\partial x_i} \leq \lambda \frac{\partial g}{\partial x_i} && x_i = a_i \end{aligned} \tag{11}$$

The above equations can be solved by the same sort of iterative procedure as suggested for the first maximization problem. One first chooses some value of λ and finds the $(x_1,\ldots,x_n)$ that satisfy equations (11). One then substitutes this $(x_1,\ldots,x_n)$ in $g(x_1,\ldots,x_n)$ (equation (6)) to find K. In this way one can find K as a function of λ. One can then find by inverse interpolation the λ that makes $g(x_1,\ldots,x_n)$ equal to the desired value of K.

III. Let us consider a third maximization problem: to choose $f(x)$ to maximize

$$I = \int_A^B L\left[f(x),x\right]dx \tag{12}$$

subject to the conditions

$$\int_A^B M\left[f(x),x\right]dx = K \tag{13}$$

$$a(x) \leq f(x) \leq b(x)$$

It is clear that if we divide the interval (A,B) into n subintervals and write

$$I \approx \sum_{i=1}^{n} L\left[f(x_i),x_i\right]\Delta x_i$$

$$\sum_{i=1}^{n} M\left[f(x_i),x_i\right]\Delta x_i \approx K \tag{14}$$

$$a(x_i) \leq f(x_i) \leq b(x_i)$$

that there is a formal similarity with Case II with

$$\begin{aligned} f(x_i) &\longrightarrow x_i \\ I &\longrightarrow f(x_1,\ldots,x_n) \\ \sum_{i=1}^{n} M\left[f(x_i),x_i\right]\Delta x_i &\longrightarrow g(x_1,\ldots,x_n) \\ a(x_i) &\longrightarrow a_i \\ b(x_i) &\longrightarrow b_i \end{aligned} \tag{15}$$

so that I will be a maximum when

$$\begin{aligned} \frac{\partial L}{\partial f} &= \lambda \frac{\partial M}{\partial f} \quad \text{when } a(x) < f(x) < b(x) \\ \frac{\partial L}{\partial f} &\geq \lambda \frac{\partial M}{\partial f} \quad \text{when } f(x) = b(x) \\ \frac{\partial L}{\partial f} &\leq \lambda \frac{\partial M}{\partial f} \quad \text{when } f(x) = a(x) \end{aligned} \tag{16}$$

and the iterative method of finding the solution is identical to Case II.

We should mention that in many cases in the text where we had

$$\begin{aligned} I &= \int \frac{g(x)}{f(x)}\, dx \\ \int f(x)dx &= K = 1 \end{aligned} \tag{17}$$

that equations (16) become

$$\begin{aligned} \frac{g(x)}{f^2 x} &= -\lambda \\ f(x) &= \frac{\sqrt{g(x)}}{\sqrt{-\lambda}} \\ &= \frac{\sqrt{g(x)}}{\int \sqrt{g(x)}dx} \end{aligned} \tag{18}$$

L. J. Savage pointed out to me that one can get the same result by using Schwarz's Inequality which states

$$\int \alpha^2(x)dx \int \beta^2(x)dx \geq \left[\int \alpha(x)\beta(x)bx \right]^2 \tag{19}$$

with equality if and only $\alpha(x) \propto \beta(x)$. We can simply take $\alpha^2(x) = g(x)/f(x)$ and $\beta^2(x) = f(x)$.

APPENDIX V

The Variance Associated With Double Systematic Sampling

In discussing double systematic sampling, it is advantageous to define two new functions $y_j(x)$ and $\bar{z}(:j)$ by

$$\int_{-\infty}^{y_j(x)} g(y:x)dy = \frac{j-1/2}{N} \qquad j = 1, 2, \ldots, N \tag{1}$$

$$\bar{z}(:j) = \int z\left[x, y_j(x)\right] f(x)dx \tag{2}$$

For any x, the probability that $y < y_j(x)$ is $\frac{j-1/2}{N}$; $y_j(x)$ is therefore a curve of equiprobability. $\bar{z}(;j)$ is the expected value of $z(x,y)$ along this curve. The more or less horizontal strip defined by $y_{j-1/2}(x) < y \leq y_{j+1/2}(x)$ will be called the $j^{\underline{th}}$ row, the vertical strip defined by $x_{i-1/2} < x \leq x_{i+1/2}$ is called the $i^{\underline{th}}$ column. The region of integration is divided into N^2 subareas by the intersections of the columns and rows. The points picked in double systematic sampling lie approximately in the center of N of these subareas on the intersections of the curves $y_j(x)$ and the vertical lines defined by $x = x_i$. One and only one of the selected subareas lies in each column and row.

It is instructive to consider the variance of this sampling scheme when it is used to evaluate a triple rather than double integral. It will therefore be assumed that there are three independent random variables (W,X,Y) and that the quantity to be estimates is

$$\bar{z} = \iiint z(w,x,y)f(w,x,y)dwdxdy \tag{3}$$

The conditional p.d.f. for W is

$$h(w:x,y) = f(w,x,y)/f(x,y) \tag{4}$$

The standard definitions

$$\bar{z}(:x,y) = \int z(w,x,y)h(w:x,y)dw \tag{5}$$

$$\overline{z^2}(:x,y) = \int z^2(w,x,y)h(w:x,y)dw \tag{6}$$

$$\sigma^2(:x,y) = \overline{z^2}(:x,y) - \bar{z}^2(:x,y) \tag{7}$$

are also needed. If $\sigma^2(:x,y) = 0$, w is a deterministic function of (x,y) and the results for the triple integral reduce to the double integral.

If the (x_i,y_i) are picked without replacement as described, but the w_i are selected randomly from $h(w:x_i,y_i)$ then the variance is

$$V_3 = \overline{(z_3 - \bar{z})^2} \tag{8}$$

$$= \overline{\left\{ \frac{1}{N}\sum \left[z(w_i,x_i,y_i) - \bar{z}\right] \right\}^2}$$

$$= \frac{1}{N^2}\sum \overline{\left[z(w_i,x_i,y_i) - \bar{z}\right]^2} + \frac{1}{N^2}\sum_{i\neq j} \overline{\left[z(w_i,x_i,y_i) - \bar{z}\right]\left[z(w_j,x_j,y_j) - \bar{z}\right]}$$

$$= \frac{1}{N} V_1 + \frac{1}{N}(N-1)\overline{\left[z(w,x,y) - \bar{z}\right]\left[z(w',x',y') - \bar{z}\right]}$$

where the primes indicate that (x',y') is not in the same row or column as (x,y). w and w' are, of course, picked independently from their respective p.d.f's.

The second term is the difference in variance due to double systematic sampling. Denoting this difference by S:

$$S = \overline{\left[z(w,x,y) - \bar{z}\right]\left[z(w',x',y') - \bar{z}\right]} \tag{9}$$

$$= \overline{\left\{\left[z(w,x,y) - \bar{z}(:x,y)\right] + \left[\bar{z}(:x,y) - \bar{z}\right]\right\}\left\{\left[z(w',x',y') - \bar{z}(:x',y')\right] + \left[\bar{z}(:x',y') - \bar{z}\right]\right\}}$$

$$= \overline{\left[\bar{z}(:x,y) - \bar{z}\right]\left[\bar{z}(:x',y') - \bar{z}\right]}$$

because it is the only term in the sum of four products which is not 0. Before the expected value can be calculated, it is necessary to write down the joint p.d.f. for (x,y,x',y').

$$j(x,y,x',y') = j(x',y':x,y)f(x,y) \tag{10}$$

Since (x',y') has the same p.d.f. as (x,y) except that it is not allowed to fall in the same row or column as (x,y), $j(x',y':x,y)$ must be either zero or proportional to $f(x',y')$. If the point (x,y) falls in the $i^{\underline{th}}$ column and the $j^{\underline{th}}$ row, then the area $A_1(x,y)$ from which (x',y') is excluded is defined by

$$\begin{aligned} x_{i-1/2} < x' &\leq x_{i+1/2} \\ y_{j-1/2}(x') < y' &\leq y_{j+1/2}(x') \end{aligned} \tag{11}$$

where i and j are to be considered as functions of (x,y). Therefore

$$j(x',y':x,y) = \begin{cases} 0 & (x',y') \text{ in } A_1(x,y) \\ \dfrac{f(x',y')}{1 - \iint\limits_{A_1(x,y)} f(x',y')dx'dy'} & (x',y') \text{ in } \left[A - A_1(x,y)\right] \end{cases} \tag{12}$$

The normalizing factor, $1 - \iint\limits_{A_1(x,y)} f(x',y')dx'dy'$, is approximately equal to $1 - 2/N$ for (using equations (155), (164) and 174)) the integral on $A_1(x,y)$ can be done

$$\iint\limits_{A_1(x,y)} f(x',y')dx'dy' \approx \int_{-\infty}^{\infty} f(x')dx' \int_{y_{j-1/2}(x')}^{y_{j+1/2}(x')} g(y':x')dy' + \int_{x_{i-1/2}}^{x_{i+1/2}} f(x')dx' \int_{-\infty}^{\infty} g(y':x')dy' \tag{13}$$

$$\approx \frac{1}{N} \int_{-\infty}^{\infty} f(x')dx' + \int_{x_{i-1/2}}^{x_{i+1/2}} f(x')dx'$$

$$\approx \frac{2}{N}$$

S can now be calculated:

$$S = \iint_{A} \left[\bar{z}(:x,y) - \bar{z}\right] f(x,y) \iint_{A-A_1(x,y)} \left[\bar{z}(:x',y') - \bar{z}\right] \frac{f(x',y')}{1 - 2/N} \, dx'dy'dxdy \qquad (14)$$

where

$$\iint_{A-A_1(x,y)} \left[\bar{z}(:x',y') - \bar{z}\right] f(x',y') dx'dy' =$$

$$\iint_{A} \left[\bar{z}(:x',y') - \bar{z}\right] f(x',y') dx'dy' - \iint_{A_1} \left[\bar{z}(:x',y') - \bar{z}\right] f(x',y') dx'dy'$$

$$\approx 0 - \int_{-\infty}^{\infty} f(x')dx' \int_{y_{j-1/2}(x')}^{y_{j+1/2}(x')} \left[\bar{z}(:x',y') - \bar{z}\right] g(y':x')dy' - \int_{x_{i-1/2}}^{x_{i+1/2}} f(x')dx' \int_{-\infty}^{\infty} \left[\bar{z}(:x',y') - \bar{z}\right] g(y':x')dy'$$

$$\approx -\frac{1}{N} \int_{-\infty}^{\infty} f(x')dx' \left\{\bar{z}\left[:x',y_j(x)\right] - \bar{z}\right\} - \int_{x_{i-1/2}}^{x_{i+1/2}} f(x')dx' \left[\bar{z}(:x') - \bar{z}\right]$$

$$\approx -\frac{1}{N}\left[\bar{z}(:j) - \bar{z}\right] - \frac{1}{N}\left[\bar{z}(:x_i) - \bar{z}\right] \qquad (15)$$

Substituting the result in equation (14),

$$(1 - \frac{2}{N})S = -\frac{1}{N}\iint_A \left[\bar{z}(:x,y) - \bar{\bar{z}}\right]\left[\bar{z}(:j) - \bar{\bar{z}}\right]f(x,y)dxdy - \frac{1}{N}\iint_A \left[\bar{z}(:x,y) - \bar{\bar{z}}\right]\left[\bar{z}(:x) - \bar{\bar{z}}\right] f(x,y)dxdy \quad (16)$$

$$= -\frac{1}{N}\int_{-\infty}^{\infty} f(x)dx \sum_{j=1}^{N} \int_{y_{j-1/2}(x)}^{y_{j+1/2}(x)} \left[\bar{z}(:x,y) - \bar{\bar{z}}\right]\left[\bar{z}(:j) - \bar{\bar{z}}\right]g(y:x)dy - \frac{1}{N}\int_{-\infty}^{\infty} \left[\bar{z}(:x) - \bar{\bar{z}}\right]^2 f(x)dx$$

$$= -\frac{1}{N}\int f(x)dx \frac{1}{N}\sum_{j=1}^{N} \left\{\bar{z}\left[x, y_j(x)\right] - \bar{\bar{z}}\right\}\left[\bar{z}(:j) - \bar{\bar{z}}\right] - \frac{1}{N}\overline{\left[\bar{z}(:x) - \bar{\bar{z}}\right]^2}$$

$$= -\frac{1}{N^2}\sum_{j=1}^{N}\left[\bar{z}(:j) - \bar{\bar{z}}\right]^2 - \frac{1}{N}\overline{\left[\bar{z}(:x) - \bar{\bar{z}}\right]^2}$$

$$= -\frac{1}{N}\overline{\left[\bar{z}(:j) - \bar{\bar{z}}\right]^2} - \frac{1}{N}\overline{\left[\bar{z}(:x) - \bar{\bar{z}}\right]^2}$$

Neglecting terms in $\frac{1}{N^2}$, it follows that

$$V_1 - V_3 = \frac{1}{N}\left\{\overline{\left[\bar{z}(:j) - \bar{\bar{z}}\right]^2} + \overline{\left[\bar{z}(:x) - \bar{\bar{z}}\right]^2}\right\} \quad (17)$$

and the variance is reduced by the sum of the fluctuations due to the variation of $\bar{z}(:j)$ and $\bar{z}(:x)$.

I-VIII AND
1-250

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK