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THE EVALUATION OF MULTIDIMENSIONAL INTEGRALS BY THE MONTE CARLO SEQUENTIAL STRATIFICATION TECHNIQUE

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1. INTRODUCTION

The basic aim of this paper is to describe and illustrate a new method to do numerical integration, Monte Carlo Sequential Stratification (MCSS). The MCSS procedure is the product of a synthesis of statistical sequential analysis and numerical analysis techniques. The result is, as we shall see, a method which will very efficiently estimate a wide class of large-dimensional multiple integrals.

The MCSS technique searches for an optimum estimator by the use of theoretical stopping and decision rules, which are developed and discussed in Sections 3, 4, and 5. In Sections 6-10, we derive the formulae needed for the efficient implementation of the procedure and describe the MCSS algorithm in detail. Numerical results are then presented, described, and discussed. We end with an outlook for further research in the field of sequential stratification.

The Monte Carlo method is defined as

> representing the solution of a problem as a parameter of a hypothetical population and using a random sequence of numbers to construct a sample of the population, from which statistical estimates of the parameter can be obtained. [HALJ-70]

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For more descriptions of the Monte Carlo method see [HAMJ-HAD], [SHY], [KAH], and [TOK].

In particular, the problem of evaluating by the Monte Carlo method a finite real valued integral

$$\theta = \int_R f(\underline{x})\underline{dx} < \infty \tag{1.1}$$

where R is a compact measurable subset of E^k, $\underline{x} = (x_1, x_2, \ldots, x_k)$, and $\underline{dx} = dx_1 dx_2 \ldots dx_k$, can be stated as estimating the parameter θ by a random variable τ defined on the probability space $(R, \underset{\sim}{R}, \mu)$, where $\underset{\sim}{R}$ denotes a σ-algebra of subsets of R and μ is a probability-measure on $\underset{\sim}{R}$ $(\mu(R)=1)$, such that, for $\underline{\xi}$ taking values on R according to μ,

$$E(\tau) = \int_R \tau\ (\underline{\xi})\ d\mu\ (\underline{\xi}) = \theta < \infty\ , \tag{1.2}$$

$$\mathrm{var}(\tau) = \int_R (\tau\ (\underline{\xi}) - \theta)^2\ d\mu\ (\underline{\xi}) < \infty\ . \tag{1.3}$$

By Schwartz's inequality, (1.2) and (1.3) imply that $E(|\tau|) < \infty$. This random variable, τ, is called the primary estimator for θ. If the points $\underline{\xi}_1, \underline{\xi}_2, \ldots$ are independently identically distributed as $\underline{\xi}$, then

$$\hat{\theta}_n = \hat{\theta}_n\ (\underline{\xi}_1, \underline{\xi}_2, \ldots, \underline{\xi}_n) = n^{-1} \sum_{r=1}^{n} \tau(\underline{\xi}_r) \tag{1.4}$$

is called the secondary estimator for θ. It should be noted that

$$E(\hat{\theta}_n) = \theta \quad \text{and} \quad \mathrm{var}(\hat{\theta}_n) = n^{-1}\ \mathrm{var}(\tau), \tag{1.5}$$

and that the estimator $\hat{\theta}_n$ converges with probability one, to θ, as $n \to \infty$ (see, e.g. [LOM] p. 239).

In order that the estimate should have less than a given error, ε, with more than a given probability $1-\alpha$, we require that

$$\Pr \{ |\hat{\theta}_n - \theta| \leq \varepsilon \} \geq 1-\alpha . \tag{1.6}$$

The estimator, $\hat{\theta}^*$, will be called an optimum estimator over the class, $\underset{\sim}{\Theta}$, of estimators if, for given positive constants ε and t_α,

$$L(\hat{\theta}^*) = \min \{ L(\hat{\theta}) : \hat{\theta} \in \underset{\sim}{\theta}, \sqrt{\operatorname{var}(\hat{\theta})} < \varepsilon/t_\alpha \}, \tag{1.7}$$

where $L(\hat{\theta})$ is the total amount of labor needed to calculate the estimator $\hat{\theta}$ and the minimum is taken over all estimators, $\hat{\theta}$, of θ, in the class $\underset{\sim}{\theta}$.

Before we continue describing the Monte Carlo method, let us see why we would want to use it. The need to resort to a Monte Carlo approach to estimate (1.1) arises, for example, when the dimension, k, of the integration problem is large. Consider estimating

$$\theta = \int_0^1 \int_0^1 \cdots \int_0^1 [\exp(x_1 x_2 \ldots x_{20}) - 1] \, dx_1 dx_2 \ldots dx_{20} . \tag{1.8}$$

The numerical-quadrature trapezoidal rule, where we evaluate the integrand at each corner of the twenty-dimensional hypercube, required 2^{20} or approximately one million evaluations of the

function to yield a result with more than 90% relative error. The simplest, the crude, Monte Carlo estimator, is defined to be the secondary estimator

$$\hat{\theta}_{C,n} = n^{-1} \sum_{r=1}^{n} \tau_C(\underset{\sim}{\xi}_r) \quad ; \tag{1.9}$$

where

$$\tau_C(\underset{\sim}{\xi}) = f(\underset{\sim}{\xi}) \tag{1.10}$$

is the primary estimator, and $\underset{\sim}{\xi}$ is a random point chosen from a multivariate uniform distribution over the region $U^{20} = X_{i=1}^{20}(0,1)$ and having a probability density function: $p(\underset{\sim}{\xi})=1$, $\underset{\sim}{\xi} \in U^{20}$, and $p(\underset{\sim}{\xi}) = 0$, otherwise. This estimator required 150,000 function evaluation to yield a result with about 10% relative error. (Here, $\theta = .95\text{x}10^{-6}$, $\hat{\theta} = .85\text{x}10^{-6}$, and the trapezoidal estimate was $1.72\text{x}10^{-6}$.)

This would have been a good example to show that a Monte Carlo approach would be useful except that the midpoint rule, a classical numerical quadrature formula, only required <u>one</u> function evaluation at the point (1/2, 1/2,...,1/2) and yielded a result with about .015% relative error! In fact, by the intermediate value theorem of the calculus, there always exists at least one point $\underline{z} \in R$ such that $\text{vol}(R) \cdot f(\underline{z}) = \theta$, where vol(R) is the hypervolume of the region of integration, R.

Let us go to a slightly different example and consider estimating

$$\theta = \int_0^1 \int_0^1 \cdots \int_0^1 (\exp(x_1 x_2 \cdots x_{20}) - 1 - x_1 x_2 \cdots x_{20})\, dx_1 dx_2 \cdots dx_{20} .$$

This time the midpoint rule yielded a result with greater than 99% relative error. The trapezoidal rule, using 2^{20} evaluations of the integrand as before, yielded a result with a relative error greater than 6,000%! The crude Monte Carlo estimate with 250,000 function evaluations yielded a result with less than 50% relative error. (Here, $\theta = .14 \times 10^{-9}$, $\hat{\theta}_c = .71 \times 10^{-10}$, trapezoidal rule estimate was $.72 \times 10^{-6}$, and the midpoint rule estimate was $.5 \times 10^{-12}$).

In general, multidimension numerical quadrature formulae are of the form

$$(1.11) \quad J = \sum_{j_1=1}^{N} \sum_{j_2=1}^{N} \cdots \sum_{j_k=1}^{N} A_{j_1, j_2, \ldots j_k} f(x_{1,j_1}, x_{2,j_2} \cdots, x_{k,j_k});$$

so that, the estimator, J, requires N^k function evaluations. Thus, as the dimension, k, of the integral increases, the number of function evaluations increases exponentially; whereas, the Monte Carlo estimator (1.9) is not forced to increase with k in this manner.*

Stratified sampling consists of partitioning R into disjoint subregions, or strata, R_u, u=1,...,p, so that

$$(1.12) \qquad \theta = \Sigma_{u=1}^{p} \theta_u ,$$

where

$$\theta_u = \int_{R_u} f(\underline{x}) \underline{dx} .$$

*For a fixed accuracy the number of function evaluations is

Now each θ_u is estimated independently by a Monte Carlo estimator, $\hat{\theta}_u$. (Note, it may be possible to evaluate some of the θ_u by direct computation.) If the strata, R_u, u=1,...,p, have, a priori, been assigned, then the variance of the stratified Monte Carlo estimator, $\hat{\theta}_s = \Sigma_{u=1}^{p} \hat{\theta}_u$, will be minimized, for a fixed total number of sample points, when the number of points sampled in each stratum is directly proportional to the standard deviation of the estimator for the stratum. This is the Tschuprow-Neyman theorem, [HAM-HUW] page 209, 1. If the partition of R and the number of subregions, p, were not chosen in advance, but instead allowed to vary, then further reduction of $\text{var}(\hat{\theta}_s)$ is possible. Dalenius and Hodges [DAT-HOJ] have given strong empirical evidence that the minimization of $\text{var}(\hat{\theta})$ will be nearly achieved if

$$\text{var}(\hat{\theta}_u) = \text{constant}, \quad u=1,\ldots,p. \tag{1.13}$$

(See Hammersley and Handscomb [HAMJ-HAD] for a brief discussion of stratified sampling.)

The most recent numerical quadrature programs use adaptive integration methods; that is, the points at which the integrand will be evaluated are chosen according to the behavior of the integrand. And in many cases, these programs use an iterative scheme which successively approximates the integral until the desired accuracy is achieved. McKeeman and Tesler [MCKW-TEL] and Tavernini [TAL] have good examples of programs of this type. The difficulty, as we saw before, is that for multiple integrals

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proportional to $\text{var}(\tau)$; see [KAH] p. 89-90.

the number of function evaluations needed is N^k, where N is the number of evaluations in each direction and k is the dimensionality of the integral.

The Monte Carlo Sequential Stratification (MCSS) procedure is an adaptive iterative scheme which attempts to minimize the variance of the stratified Monte Carlo estimator. The scheme produces an approximately optimal choice of strata, in the sense of (1.7), an iterative search procedure. The algorithm also yields a confidence interval (1.6) for the estimate of θ less than or equal to the one desired. (See, Halton [HALJ-67] for a discussion of other sequential Monte Carlo schemes.)

It should be noted that all the calculations actually carried out, in this study, have used the class $\underset{\sim}{\theta}$ of estimators obtained by successive bisection of strata (see Section 6). However, the theory is presented in more general form, since the generalization to the other partitioning schemes is relatively straightforward.

2. A BRIEF DESCRIPTION OF THE MONTE CARLO SEQUENTIAL STRATIFICATION (MCSS) PROCEDURE

The MCSS scheme, for the estimation of $\theta = \int_R f(\underline{x})\underline{dx}$, consists of searching, in a given partitioning scheme, for the optimum partition of the region of integration, R, and the number of points to be sampled in each stratum of the partition. The number of points to be sampled per stratum for the estimate of the integral, and the partition of the region, are dependent upon the integrand and the desired size and significance level of the probabilistic confidence interval. A few basic definitions are in order before the exposition of the procedure.

The decision rule is used to determine whether a given stratum should be stratified. The stopping rule is used to test if more sampling in a stratum is necessary in order to reach the desired accuracy. Next, let us consider an example.

The MCSS scheme with bisection-type stratification,* applied to calculating $\int_0^1 \log x \, dx$ with an error bound of 0.1 and with a 99% confidence interval, determined the stratification points to be 0, 1/16, 1/8, 1/4, 1/2, 1. Figure 2.1a indicates the tree structure. The dotted line shows where to proceed after reaching the end of a branch. Figure 2.1b shows the corresponding strata and stratification points. (Here, $\theta = -1$. The results were: $\hat{\theta} = -.9982$, standard error = .02, and number of samples = 360.)

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*For details, see Section 6.

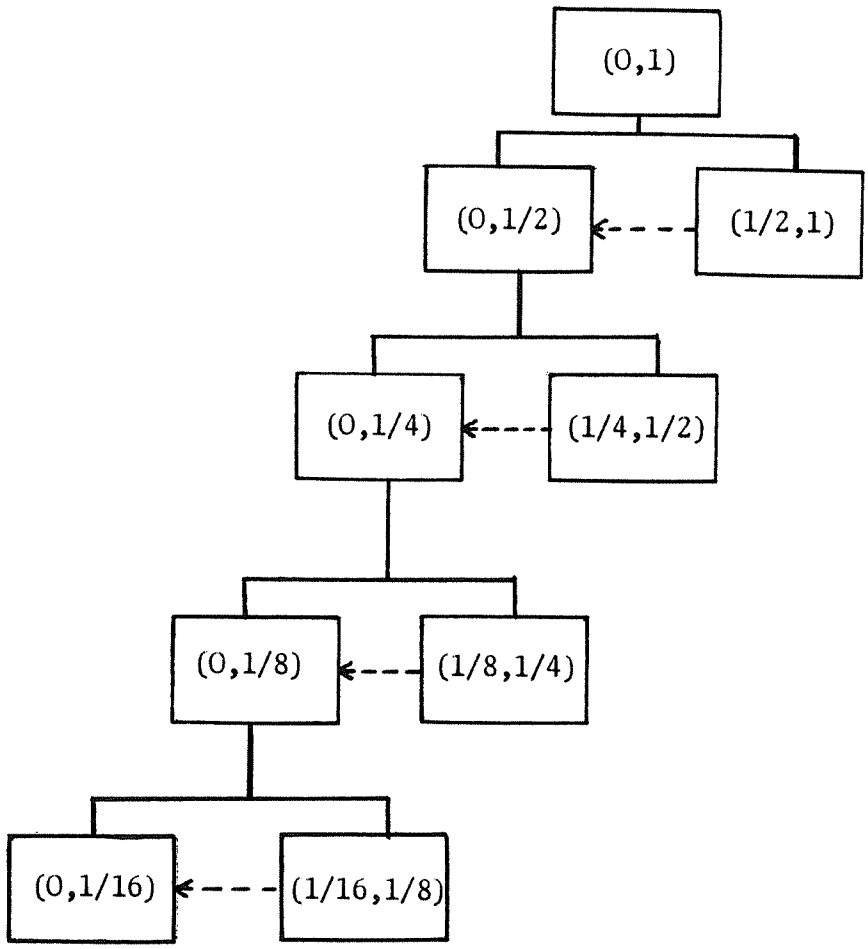


Figure 2.1a

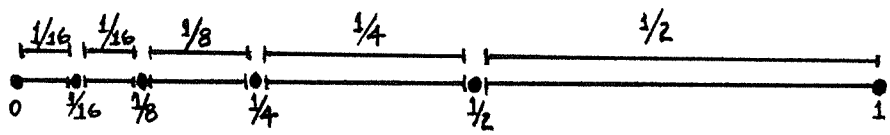


Figure 2.1b

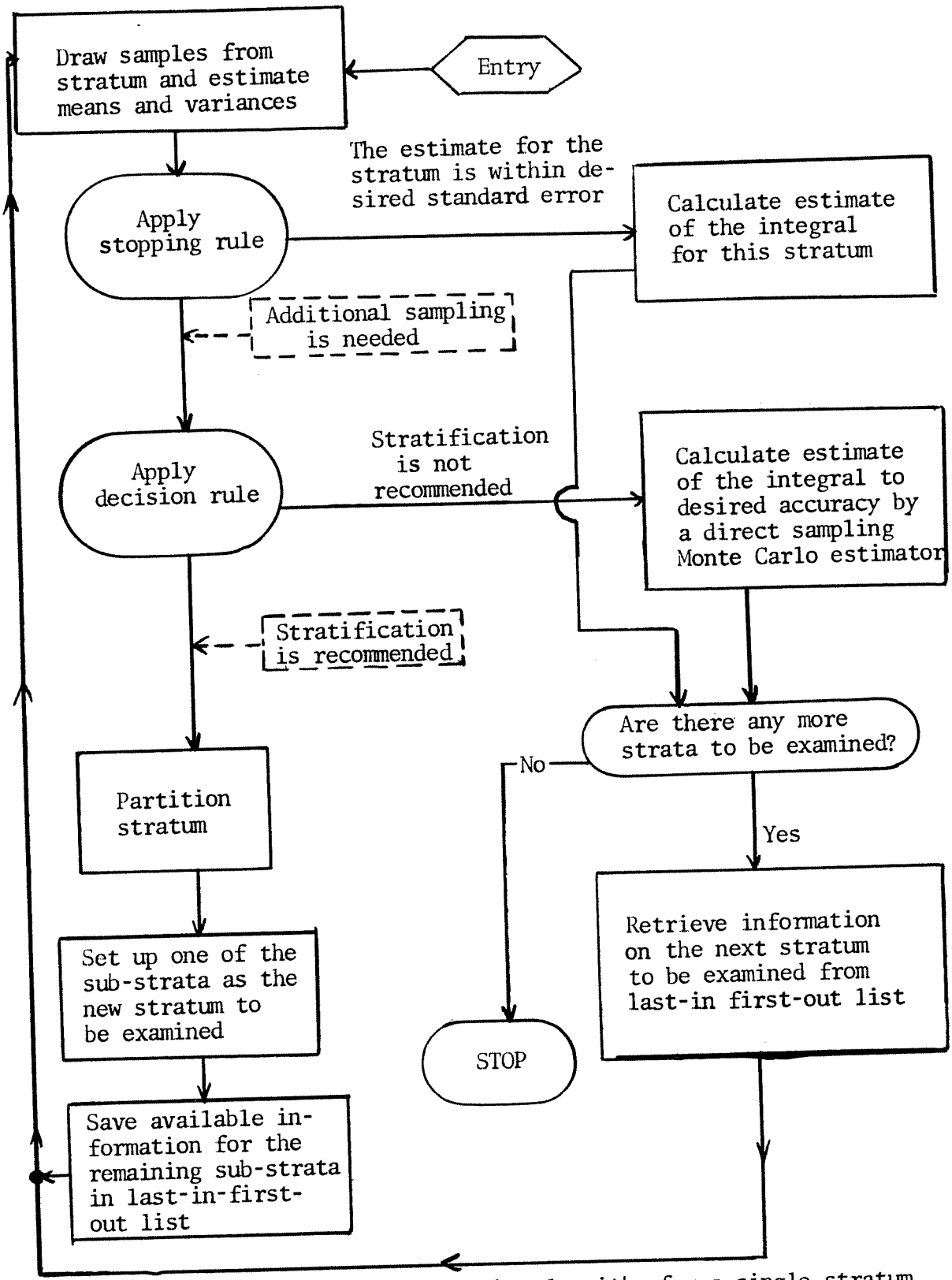


Figure 2.2: Flowchart of the algorithm for a single stratum

The following is a brief description of the MCSS algorithm. A more detailed version will be given in Section 8.

The procedure begins by drawing a sample from the entire region of integration. The stopping rule is applied. If the condition is satisfied, the search procedure stops and the estimate of the value of the integral is calculated. If not, the decision rule is applied. If the decision rule signifies that stratification is not advantageous, then sampling over the entire region is continued until the stopping rule is satisfied. If the decision rule recommends stratification, the entire region is partitioned according to a given stratification scheme (e.g., bisecting, along a randomly-chosen coordinate axis, into two strata of equal volumes.) Next the algorithm in a recursive fashion examines one of the subregions (or strata) just partitioned. The available information for the remaining strata is saved and stored in a last-in-first-out (LIFO) list. (In trial calculations, the length of this list has remained small.)

The procedure for this stratum is the same as for the entire interval. The stopping rule is applied first and if necessary, the decision rule is applied. As before, if the decision is to stratify, then this stratum is partitioned, one of the subregions examined, and the information on the remaining one stored in the LIFO list. If stratification is <u>not</u> recommended the sampling continues in the entire region being examined until the stopping rule is satisfied. Afterwards, the unexamined stratum, whose location, as well as

other information,have previously been stored in the LIFO list, is explored. This process continues recursively until the entire region of integration is examined and the estimate of the integral for each stratum is calculated. The sum of all these estimates is the estimate of the integral. (See Fig. 2.2). This process is no more than an iterative search procedure. If the partition scheme is a bisection process, then we have a binary search. The decision rule indicates whether or not to branch, the stopping rule determines the amount of sampling at each node of the tree, and the LIFO list shows where the process should return to,after the end of a branch has been reached. (See Fig. 2.1)

3. THE STOPPING RULE

Let us recall, see (1.1) and (1.6), that the problem is to estimate $\theta = \int_R f(\underline{x})\underline{dx}$ to within a given error ε with a given probability of at least $1-\alpha$. Now,we can apply the central limit theorem (see, e.g. [LOM] p. 275) to the secondary estimator $\hat{\theta}_n$, defined in (1.4), to yield that

$$(3.1) \qquad \text{pr}\{|\hat{\theta}_n-\theta| \leq \varepsilon\} = (2\pi)^{-1/2} \int_{-z}^{z} \exp(-x^2/2)dx + \psi(n,\varepsilon) ;$$

where $z = \varepsilon[\text{var}(\hat{\theta}_n)]^{-1/2}$, and $|\psi(n,\varepsilon)|\sqrt{n}$ is bounded above for all sufficiently large n. Also,for a given α, there exists a $t_\alpha \geq 0$ such that

$$(3.2) \qquad (2\pi)^{-1/2} \int_{-t_\alpha}^{t_\alpha} \exp(-x^2/2)dx = 1-\alpha.$$

Hence the condition (1.6) reduces to

$$(2\pi)^{-1/2} \int_{-z}^{z} \exp(-x^2/2)dx + \psi(n,\varepsilon) > (2\pi)^{-1/2} \int_{-t_\alpha}^{t_\alpha} \exp(-x^2/2)dx,$$

which yields, with a little algebra, that

$$(3.3) \qquad (2/\pi)^{1/2} \int_{t_\alpha}^{z} \exp(-x^2/2)dx + \psi(n,\varepsilon) > 0.$$

Now, we observe that, by (1.5) as $n\to\infty$, $z=\varepsilon[\mathrm{var}(\hat{\theta}_n)]^{-1/2}$ $= \varepsilon\sqrt{n}[\mathrm{var}(\tau)]^{-1/2} \to \infty$, while t_α remains constant;so that

$$\int_{t_\alpha}^{z} \exp(-x^2/2)dx \to \int_{t_\alpha}^{\infty} \exp(-x^2/2)dx > 0 .$$

Also, as $n\to\infty$, $\psi(n,\varepsilon) \to 0$. Thus, for all sufficiently large n, (3.3) will hold; whence (1.6) will be satisfied.

In the absence of further information about $\psi(n,\varepsilon)$, it is customary (and perhaps reasonable!) to assume that (1.6) holds, that is, pr $\{|\hat{\theta}_n-\theta| \leq \varepsilon\} \geq 1-\alpha$, as soon as n is large enough for $z>t_\alpha$, or equivalently, as soon as

$$(3.4) \qquad \mathrm{var}(\tau)/n < \varepsilon^2/t_\alpha^2 .$$

In practice very often the value var(τ) is unknown. It is estimated by the estimator

$$s_n^2 = \frac{1}{n-1} \sum_{r=1}^{n} (\tau(\underline{\xi}_r) - \hat{\theta}_n)^2 \quad , \text{ for } n \geq 2 \ , \tag{3.5}$$

where $\tau(\underline{\xi}_r)$ and $\hat{\theta}_n$ are defined in (1.4). That s_n^2 is an unbiased estimator of var(τ) follows from

Lemma 3.1. For s_n^2 as defined in (3.5) and var(τ) as defined in (1.3)

$$E(s_n^2) = \text{var}(\tau) \ . \tag{3.6}$$

Proof: This is a standard result; see e.g. [WIS] p. 199. H

If we substitute the estimator for var(τ) into (3.4) we obtain

$$s_n^2/n < \varepsilon^2/t_\alpha^2 \ .$$

We are now ready to state the

Stopping Rule: Stop sampling as soon as

$$n > s_n^2 \, t_\alpha^2/\varepsilon^2 \ . \tag{3.7}$$

This is a standard sequential analysis procedure, see [ANJ], [STN], and [TOK]. That this Monte Carlo process is a finite one follows from

Theorem 3.1

$$\Pr[n<\infty] = 1.$$

Proof: (Cf. Starr [STN])

By Lemma 5.2,

(3.8) $\lim_{n\to\infty} s_n^2 = \mathrm{var}(\tau)$ with probability one .

Thus, by (3.7),

$$\Pr[n=\infty] = \Pr[n \le s_n^2\, t_\alpha^2/\varepsilon^2 \ , \ \text{for all } n \ge 2]$$

$$\le \Pr[\lim_{n\to\infty} s_n^2 = \infty]$$

Hence, by (3.8), and since $\mathrm{var}(\tau) < \infty$ by (1.3),

$$\Pr[\lim_{n\to\infty} s_n^2 = \infty] = 0.$$

Therefore,

$$\Pr[n=\infty] = 0.$$ ⊣

The Monte Carlo Sequential Stratification procedure (MCSS) uses unbiased primary estimators, τ_u, to estimate the values θ_u of the integral over the separate strata R_u. That is,

$$\theta_u = \int_{R_u} f(\underline{x})\, \underline{dx} \ , \tag{3.9}$$

where the R_u are disjoint and $\cup_{u=1}^{p} R_u = R$, yielding that

$$\theta = \sum_{u=1}^{p} \theta_u \ , \tag{3.10}$$

when p is the total number of strata.

The secondary estimators of θ_u are:

$$\hat{\theta}_u = \frac{1}{n_u} \sum_{u=1}^{n_u} \tau_u(\underline{\xi}_r) \ , \quad \text{for } u=1,\ldots,p \ , \tag{3.11}$$

where n_u is the total number of samples drawn in the region R_u, and the $\underset{\sim}{\xi}_r$ are sampled independently from $(R_u, \underset{\sim}{R}_u, \mu_u)$. We have that

$$\hat{\theta}_S = \sum_{u=1}^{p} \hat{\theta}_u \tag{3.12}$$

as the stratified sampling estimator of θ.

That $\hat{\theta}_S$ is an unbiased estimator of θ follows from

Lemma 3.2. Let $\hat{\theta}_u$ and $\hat{\theta}_S$ be defined in (3.11) and (3.12) respectively then

$$E(\hat{\theta}_S) = \theta \ .$$

Proof:

$$E(\hat{\theta}_S) = E(\sum_{u=1}^{p} \hat{\theta}_u) = \sum_{u=1}^{p} E(\hat{\theta}_u).$$

Denoting $\tau_u(\underset{\sim}{\xi}_r)$ by τ_{ur}, we have that

$$E(\hat{\theta}_S) = \sum_{u=1}^{p} E(\frac{1}{n_u} \sum_{r=1}^{n_u} \tau_{ur}) = \sum_{u=1}^{p} \frac{1}{n_u} \sum_{r=1}^{n_u} E(\tau_{ur})$$

$$= \sum_{u=1}^{p} \frac{1}{n_u} n_u \theta_u \ , \quad \text{since } \tau_u \text{ is an unbiased estimator of } \theta_u \ ,$$

$$= \sum_{u=1}^{p} \theta_u = \theta \ , \quad \text{by (3.10)} \ . \qquad \text{H}$$

This Lemma and the next one are standard results in the theory of stratified sampling (see, e.g. [COW]). Their proofs are included for completeness.

Lemma 3.3.

If $\hat{\theta}_S$ defined as in (3.12), then

$$\mathrm{var}(\hat{\theta}_S) = \sum_{u=1}^{p} \mathrm{var}(\hat{\theta}_u) \text{ , where } \mathrm{var}(\hat{\theta}_u) = \frac{1}{n_u} \mathrm{var}(\tau_u) \text{ .}$$

Proof:

$$\mathrm{var}(\hat{\theta}_S) = \mathrm{var}\Big(\sum_{u=1}^{p} \hat{\theta}_u \Big) \text{ , } \qquad \text{by (3.12),}$$

$$= \sum_{u=1}^{p} \mathrm{var}(\hat{\theta}_u) \text{ , } \qquad \text{by the Bienaymé equality [LOM, p. 334],}$$

$$= \sum_{u=1}^{p} \mathrm{var}\Big(\frac{1}{n_u} \sum_{r=1}^{n_u} \tau_{ur} \Big) \text{ , } \qquad \text{by (3.11)}$$

$$= \sum_{u=1}^{p} \frac{1}{n_u^2} \sum_{r=1}^{n_u} \mathrm{var}(\tau_{ur}) \text{ , } \qquad \text{by the Bienaymé equality,}$$

$$= \sum_{u=1}^{p} \frac{1}{n_u} \mathrm{var}(\tau_u) \text{ , } \qquad \tau_{ur}\text{'s independent random variables.}$$

In order to satisfy the condition $z > t_\alpha$ (see (3.1),(3.2)) we must have, by Lemma 3.3, that

$$\mathrm{var}(\hat{\theta}_S) = \sum_{u=1}^{p} \mathrm{var}(\hat{\theta}_u) < \frac{\varepsilon^2}{t_\alpha^2} \text{ .} \tag{3.13}$$

Let

$$T = \varepsilon^2/t_\alpha^2 \,, \tag{3.14}$$

and define

$$T_u = \alpha_u T, \text{ for } u=1,2,\ldots,p, \tag{3.15}$$

where $\sum_{u=1}^{p} \alpha_u = 1$, and the α_u are constants .

Then, if

$$\text{var}(\hat{\theta}_u) \leq T_u \,, \text{ for } u=1,2,\ldots,p, \tag{3.16}$$

we have that

$$\sum_{u=1}^{p} \text{var}(\hat{\theta}_u) = \text{var}(\hat{\theta}_S) \leq \sum_{u=1}^{p} T_u = T \sum_{u=1}^{p} \alpha_u = T \,;$$

that is, if conditions (3.16) hold, then condition (3.13) holds. As before, in practice the value of $\text{var}(\tau_u)$ is unknown, but it is estimated by the unbiased estimator

$$s^2_{u,n_u} = \frac{1}{n_u - 1} \sum_{r=1}^{n_u} (\tau_u(\underline{\xi}_r) - \hat{\theta}_u)^2 \,, \quad n_u \geq 2 \tag{3.17}$$

(Remark: $\lim_{n_u \to \infty} s^2_{u,n_u} = \text{var}\, \tau_u$ with probability one, by the strong law of large numbers; see Lemma 5.2.) On using (1.5) and (3.11)

in (3.16) and substituting s^2_{u,n_u} for $\mathrm{var}(\tau_u)$, we get the

MCSS Stopping Rule

As soon as

$$n_u > \frac{s^2_{u,n_u}}{T_u}, \tag{3.18}$$

we stop sampling in the uth stratum; that is, n_u is the minimum integer such that (3.18) holds.

Remarks:

1) The stopping rule is illustrated in figure 4.3. Cases I and II represent typical statistical sample values of $s^2_{u,n_u}/T_u$ against $n_u = \nu, 2\nu, \ldots$, for a given positive integer ν; $n_{u,\mathrm{stop}}$ is the stopping value of n_u, in each case, according to (3.18) (the first point from the left falling below the line $s^2_{u,n_u}/T_u = n_u$).

2) Because s^2_{u,n_u} only approximates $\mathrm{var}(\tau_u)$, the MCSS rules (3.18) and (4.28) may, in fact, give a wrong decision. To reduce the chance of making a wrong decision, we used a "second stopping rule". This will be discussed in Section 5.

4. THE DECISION RULE

Let R_o be any stratum contained in R, and partition R_o into p disjoint substrata, R_u, u=1,...,p. The following theorem states how many samples should be taken in each substratum to achieve the minimum variance of the estimator.

Theorem 4.1 (Tschuprow-Neyman).

Let $n_1, n_2, \ldots, n_p$, be positive real number whose sum n_S is fixed, where p is any integer such that $p \geq 2$, then

$$(4.1) \qquad \min_{n_1,\ldots,n_p} \sum_{u=1}^{p} \frac{1}{n_u} \operatorname{var}(\tau_u) ,$$

subject to

$$(4.2) \qquad n_S = \sum_{u=1}^{p} n_u ,$$

is attained when the n_u are equal to

$$(4.3) \qquad n_u^* = [\operatorname{var}(\tau_u)]^{1/2} \, n_S / \sum_{v=1}^{p} [\operatorname{var}(\tau_v)]^{1/2}$$

for u=1,...,p. This yields that

$$(4.4) \qquad \min \sum_{u=1}^{p} \frac{1}{n_u} \operatorname{var}(\tau_u) = \frac{1}{n_S} \Big(\sum_{u=1}^{p} [\operatorname{var}(\tau_u)]^{1/2} \Big)^2 .$$

Although this theorem and its proof are given in [HAM-HUW]

p. 132, II, it is included here for completeness.

Proof:

Let

$$\sigma_u = [\mathrm{var}(\tau_u)]^{1/2} \quad \text{, for } u=1,2,\ldots,p \text{ .} \tag{4.5}$$

Using the Lagrangian multiplier, λ, we get the equations

$$\frac{\partial}{\partial n_v}\left[\sum_{u=1}^{p} \frac{\sigma_u^2}{n_i}\right] + \lambda \frac{\partial}{\partial n_v}\left(\sum_{u=1}^{p} n_u\right) = 0 \text{ ,} \tag{4.6}$$

for $v=1,2,\ldots,p$.

Differentiating (4.6), we get that

$$-\frac{\sigma_v^2}{n_v^2} + \lambda = 0, \quad \text{for } v=1,\ldots,p; \tag{4.7}$$

so that the optimal values of n_v, denoted by n_v^*, are

$$n_v^* = \frac{\sigma_v}{\sqrt{\lambda}} \quad \text{, for } v=1,\ldots,p \text{ .} \tag{4.8}$$

Using (4.2), we get that

$$\sum_{u=1}^{p} \frac{\sigma_u}{\sqrt{\lambda}} = n_S \text{ ,} \tag{4.9}$$

whence

$$(4.10) \qquad \sqrt{\lambda} = \frac{1}{n_S} \sum_{u=1}^{p} \sigma_u .$$

Combining (4.8) and (4.10), we get that

$$(4.11) \qquad n_v^* = \sigma_v \, n_S / \left(\sum_{u=1}^{p} \sigma_u \right) ,$$

$v=1,\ldots,p,$

as desired.

Upon substituting (4.11) into (4.1), we obtain (4.4).

In order to see that (4.4) is actually the minimum value for (4.1), we observe that

$$\sum_{u=1}^{p} \frac{\sigma_u^2}{n_u} - \frac{1}{n_S} \left(\sum_{u=1}^{p} \sigma_u \right)^2 =$$

$$\sum_{u=1}^{p} \left(\frac{1}{n_u} - \frac{1}{n_S} \right) \sigma_u^2 - \frac{1}{n_S} \sum_{\substack{u,v \\ (u \neq v)}} \sigma_u \sigma_v =$$

$$\sum_{u=1}^{p} \frac{n_S - n_u}{n_S n_u} \sigma_u^2 - \frac{2}{n_S} \sum_{\substack{u,v \\ (u>v)}} \sigma_u \sigma_v =$$

$$\frac{1}{n_S} \left[\sum_{u=1}^{p} \left(\sum_{v \neq u} n_v \right) \sigma_u^2 / n_u - 2 \sum_{\substack{u,v \\ (u>v)}} \sigma_u \sigma_v \right] =$$

$$\frac{1}{n_S}\Big[\sum_{\substack{u,v\\(u>v)}}\Big(\frac{n_v\sigma_u^2}{n_u}+\frac{n_u\sigma_v^2}{n_v}-2\sigma_u\sigma_v\Big)\Big]=$$

$$\frac{1}{n_S}\sum_{\substack{u,v\\(u>v)}}\frac{(n_u\sigma_v-n_v\sigma_u)^2}{n_u n_v}\geq 0. \qquad \text{H}$$

This theorem states that for any given region, R_o, and partition of it, $R_1,\ldots,R_p$, the minimum variance for the stratified sampling estimator, $\hat{\theta}_S$, is attained when the number of observations in the u-th substratum, n_u, is chosen according to (4.3), for u=1,...,p. The exact minimum is not usually attainable, because the values of n_u^* from (4.3) are not always integers. In practice,we use the value of n_u^* gotten by rounding n_u^* to the nearest integer.

We again let $\sigma_u = [\mathrm{var}(\tau_u)]^{1/2}$, for u=0,1,...,p, where u corresponds to the region R_u. The variance obtained when we draw a sample of n_u points directly from a region R_u is $\mathrm{var}(\hat{\theta}_u)=\sigma_u^2/n_u$, for u=0,1,...,p, where $R_o = U_{u=1}^{p} R_u$ and the R_u are disjoint. Similarly, when we draw a sample of n_o points directly from the region R_o we have that

$$\mathrm{var}(\hat{\theta}_o) = \frac{\sigma_o^2}{n_o}. \qquad (4.12)$$

This will be called the <u>direct sampling</u> (the non-stratified) <u>variance</u> for the region R_o.

If we stratify R_o into disjoint strata, $R_1,\ldots,R_p$, and take n_u^* points in each stratum, then, by Lemma 3.3, $\mathrm{var}(\hat{\theta}_S) = \sum_{u=1}^{p} \sigma_u^2/n_u^*$. Let $n_S = \sum_{u=1}^{p} n_u^*$, $\sigma_S^2 = (\sum_{u=1}^{p} \sigma_u)^2$, and the n_u^* be defined as in (4.3) of Theorem 4.1; then

$$\mathrm{var}(\hat{\theta}_S) = \frac{\sigma_S^2}{n_S} \quad . \tag{4.13}$$

This is the optimum stratified sampling variance.

If the tolerance, T, is defined as in (3.14), if ℓ_o and ℓ_S are defined to be the amount of labor per point to calculate $\hat{\theta}_o$ and $\hat{\theta}_S$, respectively,* and if w_o and w_S are defined to be the total amount of work required to calculate $\hat{\theta}_o$ and $\hat{\theta}_S$ to within a tolerance T, respectively, then

$$\left.\begin{aligned} w_o &= n_o \ell_o = \frac{\sigma_o^2}{T} \ell_o \\ \text{and} \qquad & \\ w_S &= n_S \ell_S = \frac{\sigma_S^2}{T} \ell_S \end{aligned}\right\} \tag{4.14}$$

Therefore, from the definitions, it will require less work to stratify R_o than to sample from it directly if $w_S < w_o$. Moreover, we shall see in the section on the labor ratio that $\ell_S/\ell_o > 1$. Hence, $w_S < w_o$ implies that $n_S\ell_S < n_o\ell_o$, $1 < \ell_S/\ell_o < n_o/n_S$. So that we get

*See the footnote on page 41.

(4.15) $$n_S < n_o \ .$$

Now, by virtue of (4.14) we can state our

Theoretical MCSS Decision Rule. Stratify the region R_o if

(4.16) $$\sigma_o^2 > L\,\sigma_S^2 \ ,$$

where the labor ratio $L = \ell_S/\ell_o$,

$$\sigma_S^2 = \Big(\sum_{u=1}^{p} [\mathrm{var}(\tau_u)]^{1/2}\Big)^2 \ ,$$

and

$$\sigma_o^2 = \mathrm{var}(\tau_o) \ .$$

Otherwise, sample from R_o directly.

To illustrate more clearly the meaning of the decision rule we examine a specific stratification scheme. The scheme consists of partitioning a given stratum, R_o, into two substrata, R_1 and R_2, such that their hypervolumes are equal, that is we have $\int_{R_1} \underline{dx} = \int_{R_2} \underline{dx}$. This is essentially the multidimensional equivalent of the bisection process.

For this special case the decision rule (4.16) becomes, stratification is recommended if

(4.17) $$\sigma_o^2 > L(\sigma_1 + \sigma_2)^2, \text{ where } L = \ell_S/\ell_o \ .$$

Returning to the general, non-optimal case of Lemma 3.3 with $p = 2$, we have $\mathrm{var}(\hat{\theta}_s) = \sigma_1^2/n_1 + \sigma_2^2/n_2$.

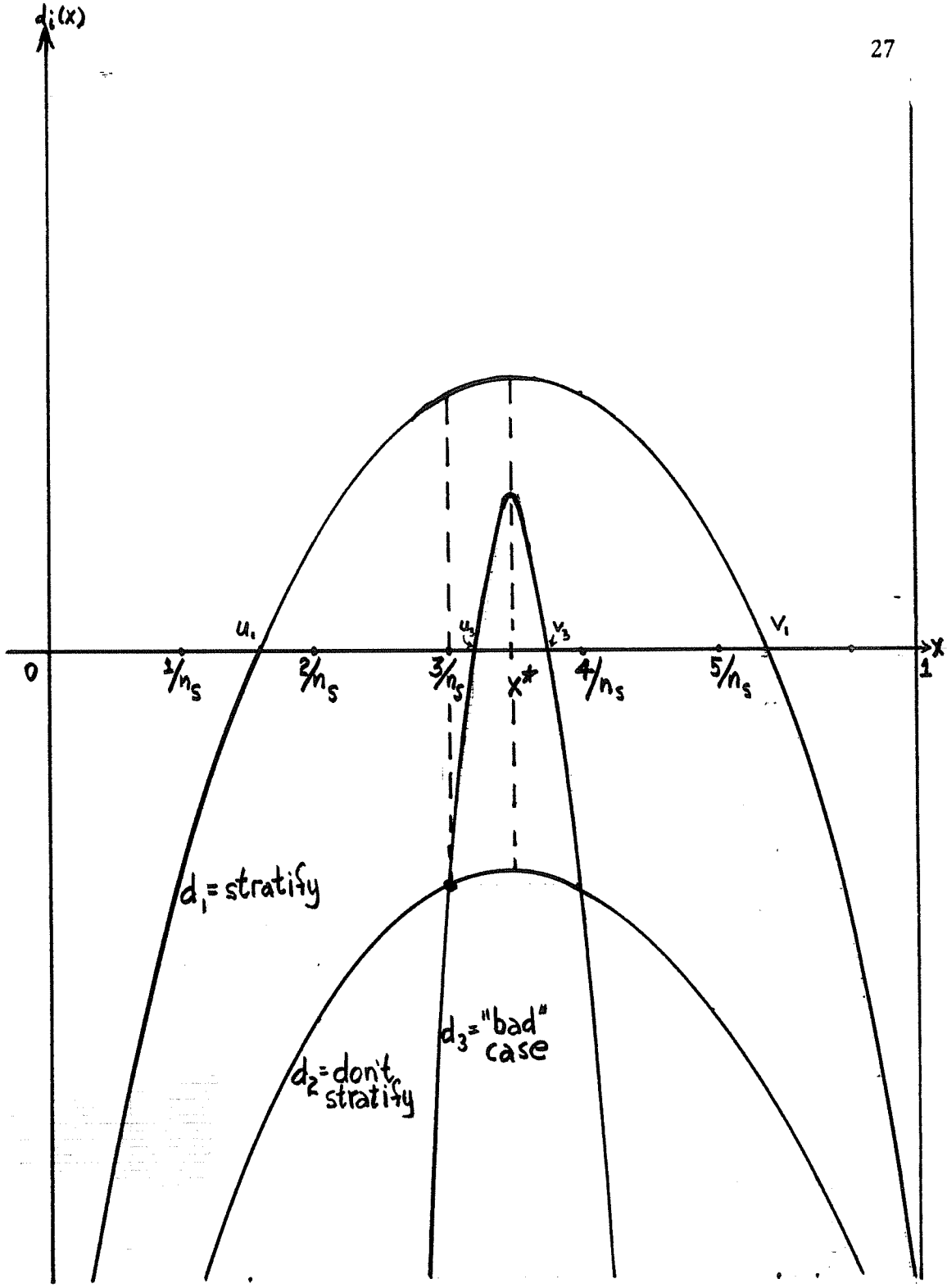


Figure 4.1: Graphs of $d(x) = \sigma_0^2 - L\left(\frac{\sigma_1^2}{x} + \frac{\sigma_2^2}{1-x}\right)$, $x \in [0,1]$ for three cases $(i = 1,2,3)$

If we let n_S remain fixed and let $x=n_1/n_S$ vary continuously, then we can define the function d on [0,1] by

$$d(x) = \sigma_o^2 - L\left(\frac{\sigma_1^2}{x} + \frac{\sigma_2^2}{1-x}\right) . \tag{4.18}$$

By Theorem 4.1 for p = 2, we get that d(x)>0 for some x,in [0,1] namely n_1^*/n_S, if and only if the inequality (4.17) holds. Hence, if (4.17) holds, then by the continuity of d, there will be an interval of values, (u,v), for x, in which stratification will be advantageous. In any case, the function d(x) will attain its maximum value on [0,1] when

$$x = \frac{\sigma_1}{\sigma_1 + \sigma_2} \text{ , where } x = \frac{n_1^*}{n_S} \text{ , } n_1^* \text{ as in theorem 4.1.} \tag{4.19}$$

Graphically, this is described in Figure 4.1.

In reality, bisection is only advantageous if there is an $x = n_1/n_S$, with n_1 an integer, for which $d(x) > 0$. The condition (4.17) implies that

$$d(x^*) = \sigma_o^2 - L\,(\sigma_1 + \sigma_2)^2 > 0, \tag{4.20}$$

where $x^* = \sigma_1/(\sigma_1 + \sigma_2) = n_1^*/n_S$.

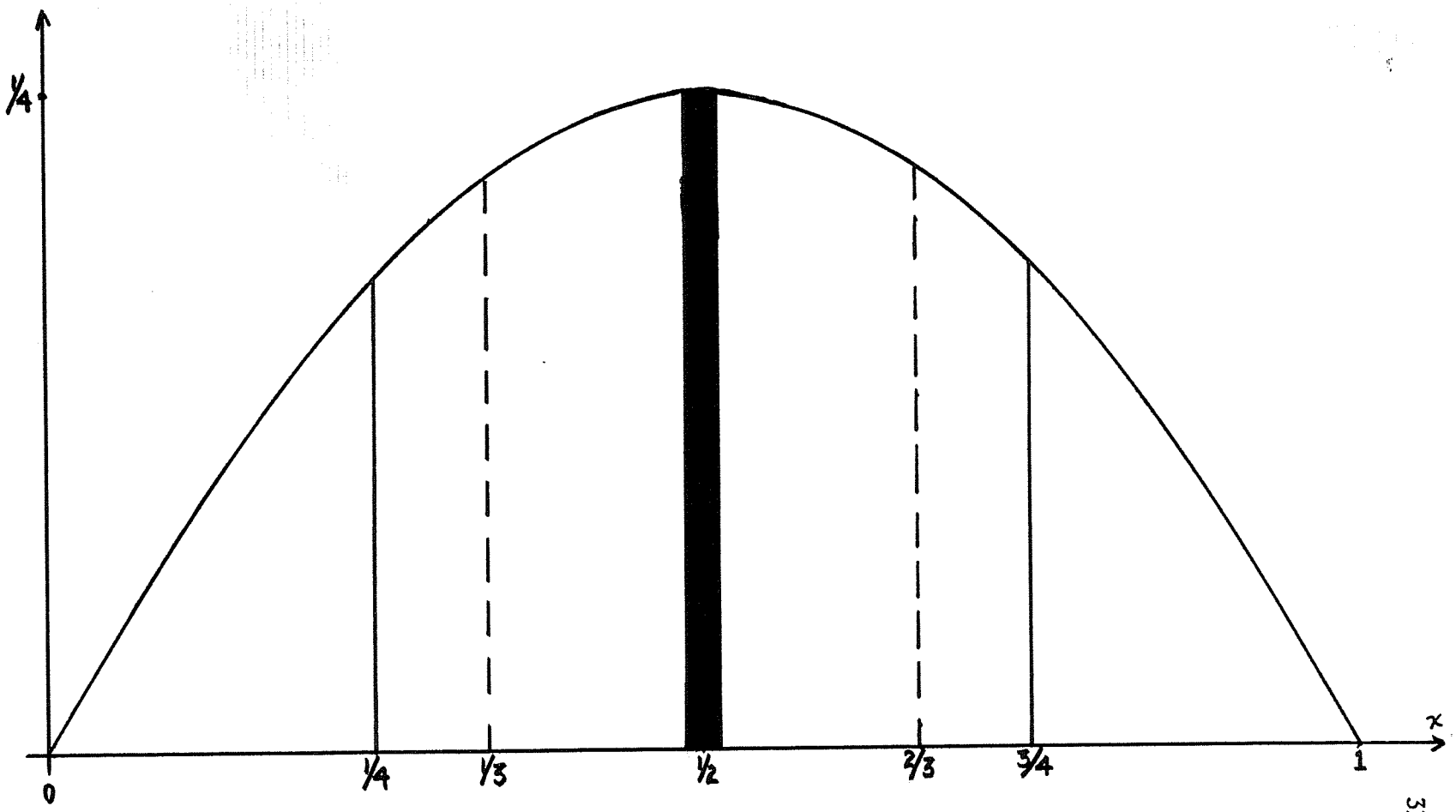


Figure 4.2. Bisection, trisection, and quadrisection of $f(x) = x(x-1)$ on $[0,1]$

The MCSS procedure, by this sequential process attempts to find a final estimator, $\hat{\theta}^*$, the sum of the estimators of the partition of R, $(R_1, R_2, \ldots, R_p)$ which satisfies the optimum condition (1.7).

There are a few limitations to the MCSS method. One of these is that it is uneconomical to examine more than a few possible stratifications of any given region; so that the class of estimators in (1.7) may need to be small. That is, for a given class of stratification (or partition) schemes, the decision rule may yield that it is not advantageous to stratify (by the suggested scheme). However, there may exist a partition of that stratum in which it is advantageous to stratify. Consider, for example, $\theta = \int_0^1 x(1-x)dx$. By the decision rule (4.16) bisection is rejected, because of the symmetry of the integrand, but trisection or quadrisection will be accepted (see Figure 4.2). Hence care should be used (as with any Monte Carlo method) in selecting the stratification scheme before using the MCSS method.

The decision rule as stated in (4.16) can not be applied in practice, because the values for σ_o^2 and σ_S^2 are almost always unknown. Therefore, we must estimate them. The estimator of σ_o^2 can, for example, be (for an initial sample of m_o points)

$$s^2_{o,m_o} = \frac{1}{m_o - 1} \sum_{r=1}^{m_o} (\tau_{or} - \hat{\theta}_o)^2 \quad , \tag{4.26}$$

where $\tau_{or} = \tau_o(\underset{\sim}{\xi}^o_r)$ and the $\underset{\sim}{\xi}^o_r$ $(r=1,2,\ldots,m_o)$ are independently identically distributed, each in the probability space $(R_o, \underset{\sim}{R}_o, \mu_o)$; the estimator of σ_S^2 can be (for initial samples of $m_1, \ldots, m_p$ points)

$$(4.27) \qquad \Big(\sum_{u=1}^{p} s_{u,m_u}\Big)^2 = \Big(\sum_{u=1}^{p}\Big[\frac{1}{m_u-1}\sum_{u=1}^{m_u}(\tau_{ur}-\hat{\theta}_u)^2\Big]^{1/2}\Big)^2 ,$$

where $\tau_{ur} = \tau_u(\underset{\sim}{\xi}^u_r)$ and, for each $u=1,2,\ldots,p$, the $\underset{\sim}{\xi}^u_r$ with $r=1,2,\ldots,m_u$, are independently identically distributed, each in $(R_u, \underset{\sim}{R}_u, \mu_u)$. This yields the practical

MCSS Decision Rule. Stratification of the stratum R_o is recommended if

$$(4.28) \qquad s^2_{o,m_o} > L\Big(\sum_{u=1}^{p} s_{u,m_u}\Big)^2 ,$$

where $L = \ell_o/\ell_S$.

Otherwise, we sample from R_o directly.

Remark: The inequality (4.28) is the statistical analogue of (4.16). Here, σ^2_o is replaced by its unbiased estimator s^2_{o,m_o} and σ^2_S is replaced by the (biased) estimator $(\Sigma_{u=1}^{p} s_{u,m_u})^2$. See remark (2) on page 20.

To guarantee termination of the stratification process, we overide the MCSS decision rule with the

MCSS Stratum Size Rule. For some $0 < \eta < 1$; if R_o is stratified into $U_{u=1}^{p} R_u$, and $\min\{\text{vol}(R_u) : u=1, 2,\ldots, p\} < \eta\ \text{vol}(R)$, then do not stratify R_o.

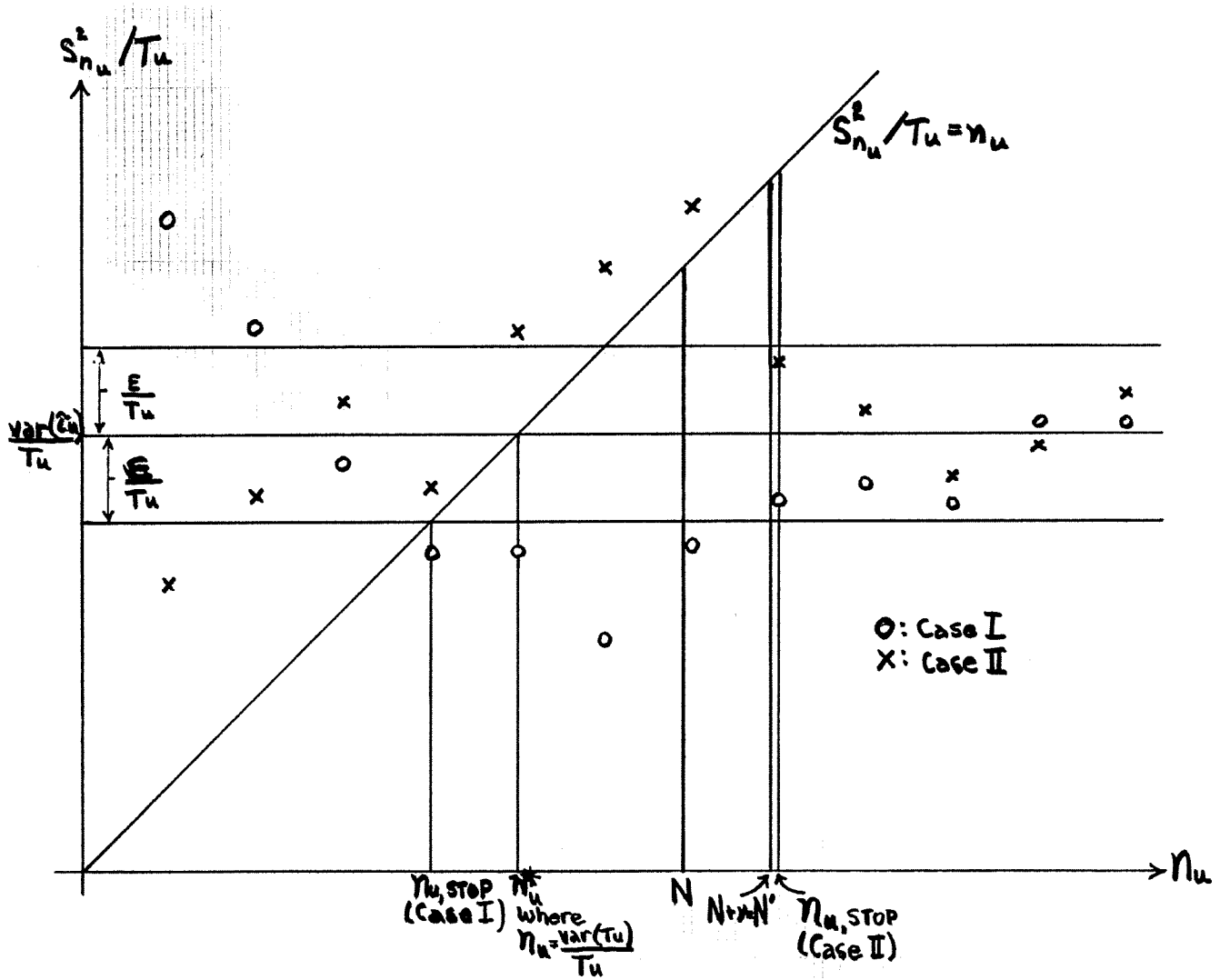


Figure 4.3. Stopping Rule. (See explanations on p. 20, 35, and 37.)

Theorem 4.2.

The total number of strata required, P, in the MCSS procedure is finite.

Proof:

$$\text{vol}(R) = \sum_{u=1}^{P} \text{vol}(R_u) \geq \eta P \, \text{vol}(R).$$

Therefore, $P \leq 1/\eta$. ⊣

The Expected Sample Size

As is the case with any statistical sequential procedure, the number of samples required for the MCSS method, $n = \Sigma_{u=1}^{p} n_u$, is a random variable. Its size depends upon the given error, ε, the number of standard deviations, t_α, the variance of the estimator, and the samples drawn in the particular experiment. We attempt to approximate the expected sample size, $E(n)$. (It is also called the average sample number (ASN) function, see [WAA] p. 25.)

Let $n = \sum_{u=1}^{p} n_u$, where n_u = the least multiple of some ν (given), such that the stopping rule (3.18) is satisfied, that is, $n_u > s^2_{u,n_u}/T_u$. We have that $E(n) = \sum_{u=1}^{p} E(n_u)$. Now, by Lemma 5.2, $s^2_{u,n_u} \to \text{var}(\tau_u)$ with probability one as $n \to \infty$, so that given any $\varepsilon, \gamma > 0$ and u, u=1,...,p, there exists an $N = N(\varepsilon, \gamma)$ such that either $n_u \leq N + \nu$; or $n_u > N + \nu$, and $n_u > (\text{var}(\tau_u) - \varepsilon)/T_u$ and

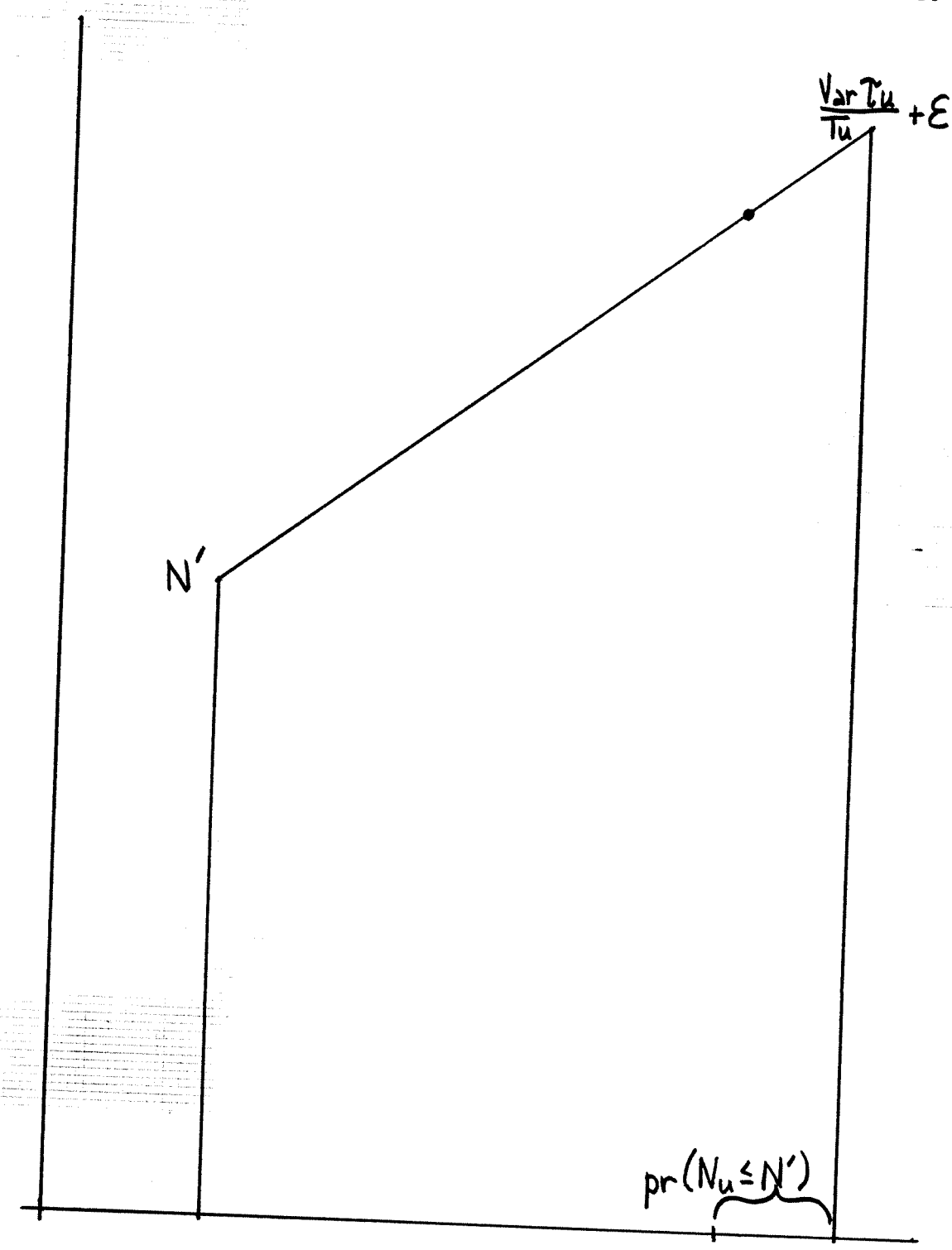


Figure 4.4. Convex Combination

$n_u - \nu < (\text{var}(\tau_u) + \varepsilon)/T_u$ with probability $(1-\gamma)$ (see Figure 4.3). Letting $N + \nu = N'$, we have that

$$E(n_u) = \sum_{m=1}^{\infty} m \; pr(n_u=m)$$

$$= \sum_{m \leq N'} m \cdot pr\,(n_u=m) + \sum_{m>N'} m \cdot pr\,(n_u=m).$$

In the first sum $m \leq N'$ explicitly, and in the second, letting $V = (\text{var}(\tau_u) + \varepsilon)/T_u + \nu$, we have that $pr\,(n_u=m|m \leq V) = 1-\gamma$ and $pr\,(n_u=m|m > V) = \gamma$. We get that

$$E(n_u) \leq N' \; pr\,(n_u \leq N') + V \; pr(N' < n_u)$$

$$+ \sum_{m>V} m \; pr\,(n_u=m).$$

Hence,

$$(4.29) \quad E(n_u) \leq (N' + V)\,(1-\gamma) + \sum_{m>V} m \; pr\,(n_u=m).$$

Although

$$\sum_{m>V} pr\,(n_u=m) = pr\,(n_u > V) = \gamma,$$

we don't have any other information on this distribution. All we can say is that if such information as

$$pr\,(n_u=m|m>V) \leq \frac{c}{m^{p+1}},$$

for some $p > 1$ and c a constant, then

$$\sum_{m>V} m \; p\,(n_u=m) \leq \sum_{m>V} \frac{c}{m^p} \leq \frac{c}{p+1} \left(\frac{1}{V}\right)^{p+1}$$

which is finite. Without such information, there, in fact, should be

no upper bound for $E(n_u)$. For example, if pr $(n_u=m|m>V) = 1/m^2$, then

$$\sum_{m>V} m \text{ pr } (n_u=m) = \sum_{m>V} \frac{1}{m} = \infty.$$

The Labor Ratio

The labor ratio was defined in (4.16) to be

$$L = \frac{\ell_S}{\ell_o} \quad , \tag{4.30}$$

where

ℓ_o is the amount of labor per point to calculate $\hat{\theta}_o$ and

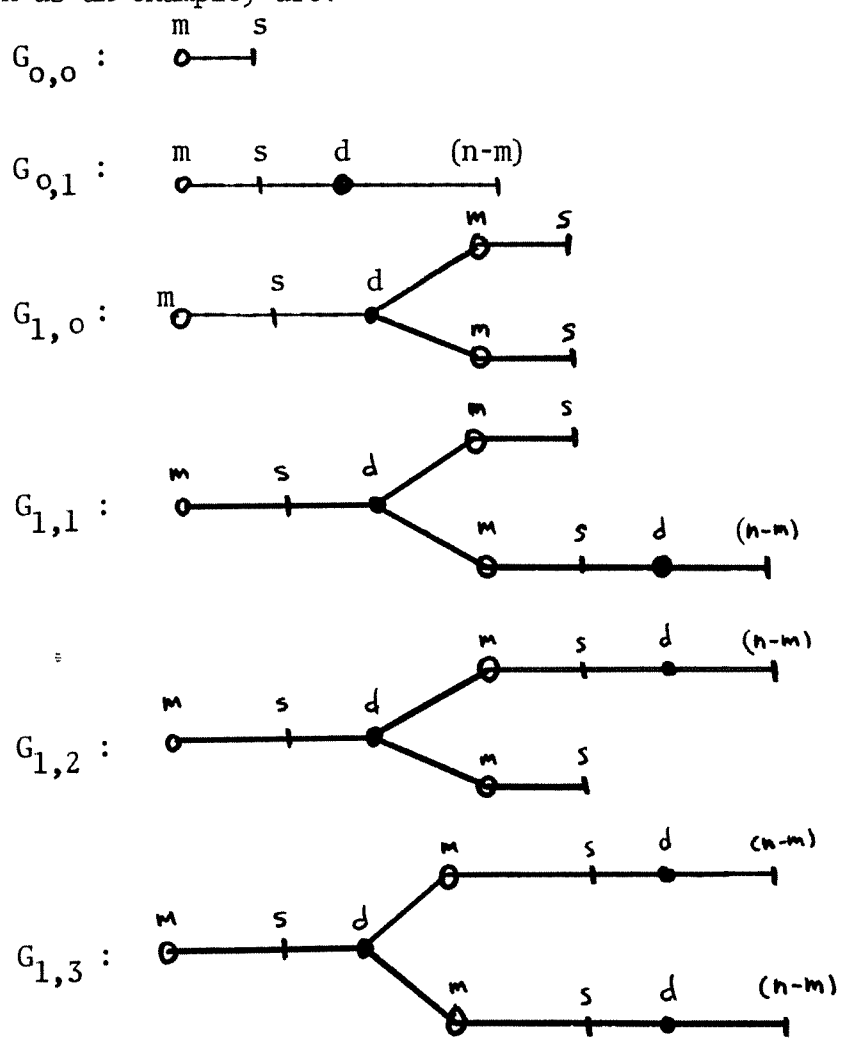
ℓ_S is the amount of labor per point to calculate $\hat{\theta}_S$.

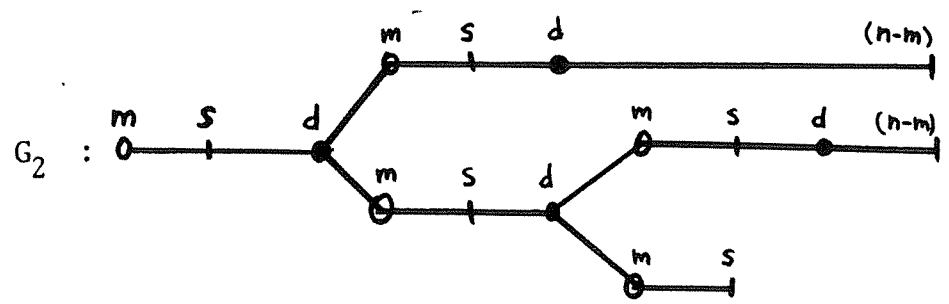
The quantities ℓ_o and ℓ_S are evaluated during each iteration of the MCSS procedure and calculated in terms of the number of essential operations required to calculate $\hat{\theta}_o$ and $\hat{\theta}_S$, respectively. Using the current numerical analysis convention (refer to [ISE-KEH] p. 34), the number of essential operations is the number of multiplications and divisions, where the exponentiation operation is treated as repeated multiplication. The quantities ℓ_o and ℓ_S depend on the number of dimensions of the integrand and region of integration, the number of essential operations required to evaluate the integrand,* to generate a pseudorandom number and scale it, to perform a square root, to approximate the mean and variance of the estimator $\hat{\theta}_o$ or $\hat{\theta}_S$, to perform stopping and decision rules, and the number of stratifications used by the given partition scheme. Since we are not taking into account such matters as

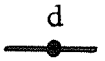
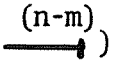
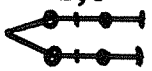
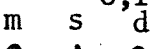
*see the footnote on page 41.

addition, subtraction, transfers, comparisons, memory references etc., ℓ_o and ℓ_s are only formalized estimates of labor.

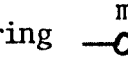
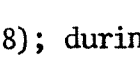
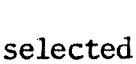
We can describe the course of a computation by a graph. We denote the sampling of m points to estimate the means and variances of our estimators by —m—, the application of the decision rule by —d—, the application of the stopping rule by —s—, and the further sampling of (n - m) points to the satisfaction of the stopping rule by —(n-m)—. The letters m, s, d, (n-m) are symbols only and do not represent specific numbers. Noting that we do not consider a given partition again, once it is rejected, we see that the simpler possible graphs (taking the bisection stratification as an example) are:





Consider any given decision rule application, say the  of $G_{o,1}$. The labor already expended is  and we have to compare the remaining labor w_o of $G_{o,1}$ (corresponding to ) with the corresponding labor w_S of the possible stratified computation. Clearly many possibilities exist. We choose (because it seems to be the best practical way) to compare $G_{o,1}$ with the result of a single stratification, followed by direct sampling, that is with graphs $G_{1,o}$, $G_{1,1}$, $G_{1,2}$, and $G_{1,3}$. The most likely of these is $G_{1,3}$, in practice. (The remaining labor w_S corresponds here to  .) Also, if we make our decision on the basis of comparison of $G_{o,1}$ with $G_{1,3}$, then no alternative event occurring after the  steps of $G_{o,1}$ have been executed can do anything but render stratification even more economical (for example, going to $G_{1,o}$ or $G_{1,1}$ or $G_{1,2}$, or to further stratifications such as G_2 etc.). Thus, this form of decision rule guarantees that (i) stratification will occur <u>if and only if</u> it effects an immediate economy of labor and (ii) any subsequent decision can only improve the economy. It does <u>not</u> guarantee that some complicated graph which, in fact, is more economical than $G_{o,1}$ will be reached by the decision procedure (if intermediate graphs are more costly than $G_{o,1}$: see

the example on p. 32 and Figure 4.2). Therefore, if any bias occurs, it is against stratification which should theoretically be done. The same discussion applies to any other application of the decision rule during the sequential process, for example from $G_{1,3}$ to G_2.

Let ℓ be the amount of labor expended in drawing a single sample point, evaluating the integrand there, updating the sum of values and sum of squares used in estimating the mean and variance of the estimator, and applying one of the two stopping rules. (During  the second rule is applied, see Section 5 and (5.8); during  , the first rule is applied; in each case, the labor is the same). Let r be the labor to apply the stopping and decision rules, and e be the labor to set up the strata for the decision rule.* In a given partition scheme, we consider the division of a given stratum into q substrata (for bisection q=2); and the decision rule will consider c such divisions (e.g. in a multidimensional scheme, we may bisect in c perpendicular directions—see Section 6), and therefore sample to estimate means and variances of cq=p substrata. The symbol  represents all p computations: if we do not stratify, all the results contribute to our estimate; if we do stratify, one of the blocks of q results is selected; this is represented by  .

*In general, the labor, although taken here to be constant, required to calculate the integrand $f(\underline{x})$ will depend on $\underline{x}$, and the labor to set up the sub-strata of $R_{\underline{u}}$ will depend on $\underline{u}$. The quantities ℓ and e should, therefore, be averaged estimates obtained in the course of sampling and computation.

Now, if we assume that $n_o \geq m_o$, $w_o = (n_o - m_o)\ell$, and if we assume that each $n_u \geq m_u = m$, then

$$w_S = e + qr + pqm\ell + \sum_{u=1}^{q} [n_u - m]\,\ell \ .$$

Letting $n_S = \sum_{u=1}^{q} n_u$, we get that

$$w_S = qr + e + n_S\,\ell + (p-1)\,qm\ell \ .$$

Since $\ell_o = w_o/(n_o - m)$ and $\ell_S = w_S/n_S$, we get that

$$\ell_o = \ell$$

and

$$\ell_S = \ell + \frac{1}{n_S}\,[(p-1)\,qm\ell + (qr+e)\,] .$$

Therefore, since the labor ratio $L = \ell_S/\ell_o$, we obtain that

$$L = 1 + \frac{1}{n_S}\,[(p-1)qm + (qr + e)/\ell\,] \ . \tag{4.31}$$

Remark: In practice we can only estimate L, for every u, because the value of n_S is usually unknown. In computing the labor ratio we estimate n_S by using Theorem 4.1 (we assume that the n_u will be chosen in the proportion of the n_u^* in (4.3), to yield the minimum variance (4.4); even though later the n_u are determined by the empirical stopping rule (3.18)), yielding $n_S = \sigma_S^2/T$, which is estimated by

$$n_S = \Big(\sum_{u=1}^{p} s_{u,m}\Big)^2/T \tag{4.32}$$

(Note that each σ_u^2 is estimated with m points, as $s_{u,m}^2$.) The assumption, that $n_o \geq m_o$ and $n_u \geq m$, is equivalent to saying that we look at $G_{o,1}$ and $G_{1,3}$, rather than, say, at $G_{o,o}$ or $G_{1,1}$.

We should remark also that if n_S is very large then L will be close to one, by (4.31). This is intuitively clear, as well; because, if it requires a large sample to achieve the desired tolerance, then the extra amount of work to stratify is negligible compared to the amount of work needed to draw a large sample size.

Clearly, from (4.31), L>1, so that stratified sampling requires more work than direct sampling. On the other hand, since $n_S > qm$, we obtain an upper bound for the labor ratio, namely,

$$L \leq p + (qr + e)/\ell qm. \tag{4.33}$$

Once we decide to sample directly from the region R_o we are done with that stratum and can go to the next one, if any. This is not so if we decide to stratify R_o into q substrata, $R_1,\ldots,R_q$, since each of these subregions, R_u, may or may not be partitioned again into q more substrata. Fortunately, we know, by Theorem 4.2, that with probability one this process does not carry on indefinitely.

5. THE STOPPING RULE FOR THE ESTIMATOR OF VAR(τ)

As we mentioned before, the value of var(τ) is usually unknown, because var(τ) depends upon the unknown quantity θ, that we are attempting to estimate. Therefore, we estimate var(τ) by the unbiased estimator

$$(5.1) \qquad s_n^2 = \frac{1}{n-1} \sum_{r=1}^{n} (\tau(\underset{\sim}{\xi}_r) - \hat{\theta}_n)^2 \ , \text{ for } n \geq 2 \ .$$

Naturally, this raises the question, how large of a sample, n, must we take in order to be reasonably confident that the estimate is good enough to apply the MCSS stopping rule (3.18) and the decision rule (4.28)?

One way in which to answer this question is to try to find the number of sample points, n, needed to give a probabilistic confidence interval for $|\text{var}(\tau) - s_n^2|$. Since the distribution of the random variables $\tau^2(\underset{\sim}{\xi})$ is usually difficult to determine, we appeal to a Chebyshev inequality.

Theorem 5.1.

If $\lambda > 0$, then for a given integer $n \geq 2$

$$(5.2) \qquad \text{pr} \{ |\text{var}(\tau) - s_n^2| \leq \lambda[\text{var}(s_n^2)]^{1/2} \} \geq 1 - \frac{1}{\lambda^2}$$

Proof:

By Chebyshev's inequality (see, e.g. [WIS] p. 75), if x is

a random variable with $E(x) < \infty$ and $var(x) > 0$, then for all $\lambda > 0$,

$$pr \{ | x - E(x)| \leq \lambda[var(x)]^{1/2} \} \geq 1 - \frac{1}{\lambda^2} .$$

Since $E(s_n^2) = var(\tau)$, we may put $x = s_n^2$ to yield (5.2). ~~H~~

Given a $\delta > 0$, if

$$\delta \geq \lambda[var(s_n^2)]^{1/2} \tag{5.3}$$

then

$$pr \{ |var(\tau) - s_n^2 | \leq \delta \} \geq \tag{5.4}$$

$$pr \{|var(\tau) - s_n^2| \leq \lambda[var(s_n^2)]^{1/2} \} \geq 1 - \frac{1}{\lambda^2} .$$

As is to be expected this leads us to another estimation problem. We know that (see [WIS] p. 199, and [KEM-STA] p. 277, volume 1)

$$var(s_n^2) = \frac{1}{n} (\mu_4 - \frac{n-3}{n-1} [var(\tau)]^2) , \tag{5.5}$$

where

$$\mu_4 = E[(\tau-\theta)^4] .$$

The $\text{var}(s_n^2)$ is, of course, unknown but can be estimated by the unbiased estimator (see [KEM-STA] p. 304, volume 1)

$$(5.6) \qquad V_n = \frac{1}{(n-2)(n-3)} \sum_{r=1}^{n} (\tau(\underline{\xi}_r) - \hat{\theta}_n)^4 +$$

$$\left[\frac{2}{(n+1)(n-1)^2} - \frac{3(n-1)}{(n+1)n(n-2)(n-3)}\right] \left[\sum_{r=1}^{n} (\tau(\underline{\xi}_r) - \hat{\theta}_n)^2\right]^2 ,$$

for $n \geq 4$.

As $n \to \infty$,

$$(5.7) \quad \left\{ \begin{array}{l} V_n \sim \hat{V}_n = \frac{1}{n}(m_{4,n} - s_n^4) \ , \\ \text{where} \quad m_{4,n} = \frac{1}{n} \sum_{r=1}^{n} (\tau(\underline{\xi}_r) - \hat{\theta}_n)^4 \ . \end{array} \right.$$

Substituting (5.7) into (5.3), we have the

MCSS stopping rule for the estimator s_n^2. ("Second Stopping Rule")

Continue sampling for $n = 4,5,6,\ldots$, until we find the first integer

$$(5.8) \qquad n \geq \left(\frac{\lambda}{\delta}\right)^2 (m_{4,n} - s_n^4) \ .$$

That the second stopping rule yields a finite procedure, with probability one, comes from the next theorem. First, we will need the following lemmas. They are standard results, but the proofs are included here for completeness.

Lemma 5.1. (see [BES] p. 58)

If $a,b,a_n(n=1,2,\ldots),b_n(n=1,2,\ldots)$ are random variables on a probability space $(R,\underset{\sim}{R},pr)$, and if $\ell im_{n\to\infty}\, a_n=a$ with probability one, and $\ell im_{n\to\infty}\, b_n=b$ with probability one, then, for any real constant c,

$$\lim_{n\to\infty} (a_n + cb_n) = a + cb \quad \text{with probability one,}$$

and

$$\lim_{n\to\infty} a_n b_n = ab \quad \text{with probability one.}$$

Proof: Let

$$A = \{x\varepsilon R: \lim_{n\to\infty} a_n(x) = a(x)\}$$

and

$$B = \{x\varepsilon R: \lim_{n\to\infty} b_n(x) = b(x)\} .$$

By the hypothesis

$$pr(A^c) = pr(B^c) = 0.$$

Let

$$C = \{x\varepsilon R: \lim_{n\to\infty} (a_n(x) + cb_n(x)) = a(x)+cb(x)\}$$

Since,

$$A \cap B \subseteq C ,$$

so that

$$C^c \subseteq A^c \cup B^c ;$$

$$pr(C^c) \leq pr(A^c) + pr(B^c) = 0$$

yield the first conclusion. The second follows by applying the same argument with

$$C = \{ x \in R : \lim_{n\to\infty} a_n(x)\, b_n(x) = a(x)\, b(x) \} . \qquad \text{H}$$

Lemma 5.2.

For s_n^2 defined as in (3.5),

$$\lim_{n\to\infty} s_n^2 = \mathrm{var}(\tau) \quad \text{with probability one.}$$

Proof:

By (1.4) and (3.5),

$$(5.9) \qquad \frac{n-1}{n} s_n^2 = \frac{1}{n} \sum_{r=1}^{n} \tau_r^2 - \frac{2}{n^2} \Big(\sum_{r=1}^{n} \tau_r \Big)^2 + \frac{1}{n^2} \Big(\sum_{r=1}^{n} \tau_r \Big)^2 .$$

By Kolmogorov's strong law of large numbers ([LOM] p. 239) and the properties of τ (see (1.2) and (1.3)), we see that,

$$(5.10) \qquad \begin{cases} \lim_{n\to\infty} \frac{1}{n} \sum_{r=1}^{n} \tau_r = \theta \quad \text{with probability one} \\ \text{and} \\ \lim_{n\to\infty} \frac{1}{n} \sum_{r=1}^{n} \tau_r^2 = [\mathrm{var}(\tau) + \theta^2] \quad \text{with probability one.} \end{cases}$$

Applying Lemma 5.1 to (5.9) and (5.10) we obtain the lemma. H

Lemma 5.3.

For $m_{4,n}$ defined as in (5.7),

$$\lim_{n\to\infty} m_{4,n} = \mu_4 \quad \text{with probability one.}$$

Proof:

By (5.7), and letting $m'_{t,n} = \sum_{r=1}^{n} \tau_r^t$, we have that

$$(5.11) \qquad m_{4,n} = \frac{1}{n} m'_{4,n} - \frac{4}{n^2} m'_{3,n} m'_{1,n} + \frac{6}{n^3} m_{2,n} (m'_{1,n})^2 - \frac{4}{n^4} (m'_{1,n})^4 + \frac{1}{n^4} (m'_{1,n})^4 .$$

As in Lemma 5.2, we see from the strong law of large numbers that, with probability one,

$$(5.12) \quad \begin{cases} \lim_{n\to\infty} \frac{1}{n} m'_{4,n} = \mu_4 + 4\theta\mu_3 + 6\theta^2 \operatorname{var}(\tau) + \theta^4 \\ \text{and} \\ \lim_{n\to\infty} \frac{1}{n} m'_{3,n} = \mu_3 + 3\theta \operatorname{var}(\tau) + \theta^3 , \end{cases}$$

where $\mu_3 = E[(\tau-\theta)^3]$ and $\mu_4 = E[(\tau-\theta)^4]$. Thus, by Lemma 5.1, (5.10), (5.11), and (5.12), we obtain the present lemma. H

It should be noted that results similar to Lemmas 5.2 and 5.3 are proven in the literature (see, e.g. [CRH] p. 351), for convergence in probability, that is s_n^2 and $m_{4,n}$ are consistent estimators.

Although the Lemmas are given here for convergence with probably one, they are standard results and their proofs are only included here for completeness.

Theorem 5.2

If $\mu_4 = E[(\tau-\theta)^4] < \infty$, then

$$pr[n < \infty] = 1.$$

Proof:

By (5.8),

$$pr[n=\infty] = pr[N < (\tfrac{\lambda}{\delta})^2 (m_{4,N} - s_N^4), \text{ for all } N>4]$$

$$\leq pr[\lim_{N\to\infty} (m_{4,N} - s_N^4) = \infty] .$$

By Lemma 5.1, 5.2, and 5.3,

$$\lim_{N\to\infty} (m_{4,N} - s_N^4) = \lim_{N\to\infty} (m_{4,N}) - [\lim_{N\to\infty} (s_N^2)]^2$$

$$= \mu_4 - [var(\tau)]^2 \quad \text{with probability one.}$$

Since $0 \leq \mu_4 < \infty$ and $0 \leq var(\tau) < \infty$, we must have that $\mu_4 - [var(\tau)]^2 < \infty$. Therefore,

$$pr[\lim_{N\to\infty} (m_{4,N} - s_N^4) = \infty] = 0 ;$$

whence $pr[n=\infty] = 0$. H

Remarks:

1) If the primary estimator, τ, of θ is the crude Monte Carlo estimator and if $f \in L^4(R)$ (that is, $\int_R |f(x)|^4 dx < \infty$), then $\mu_4 < \infty$.

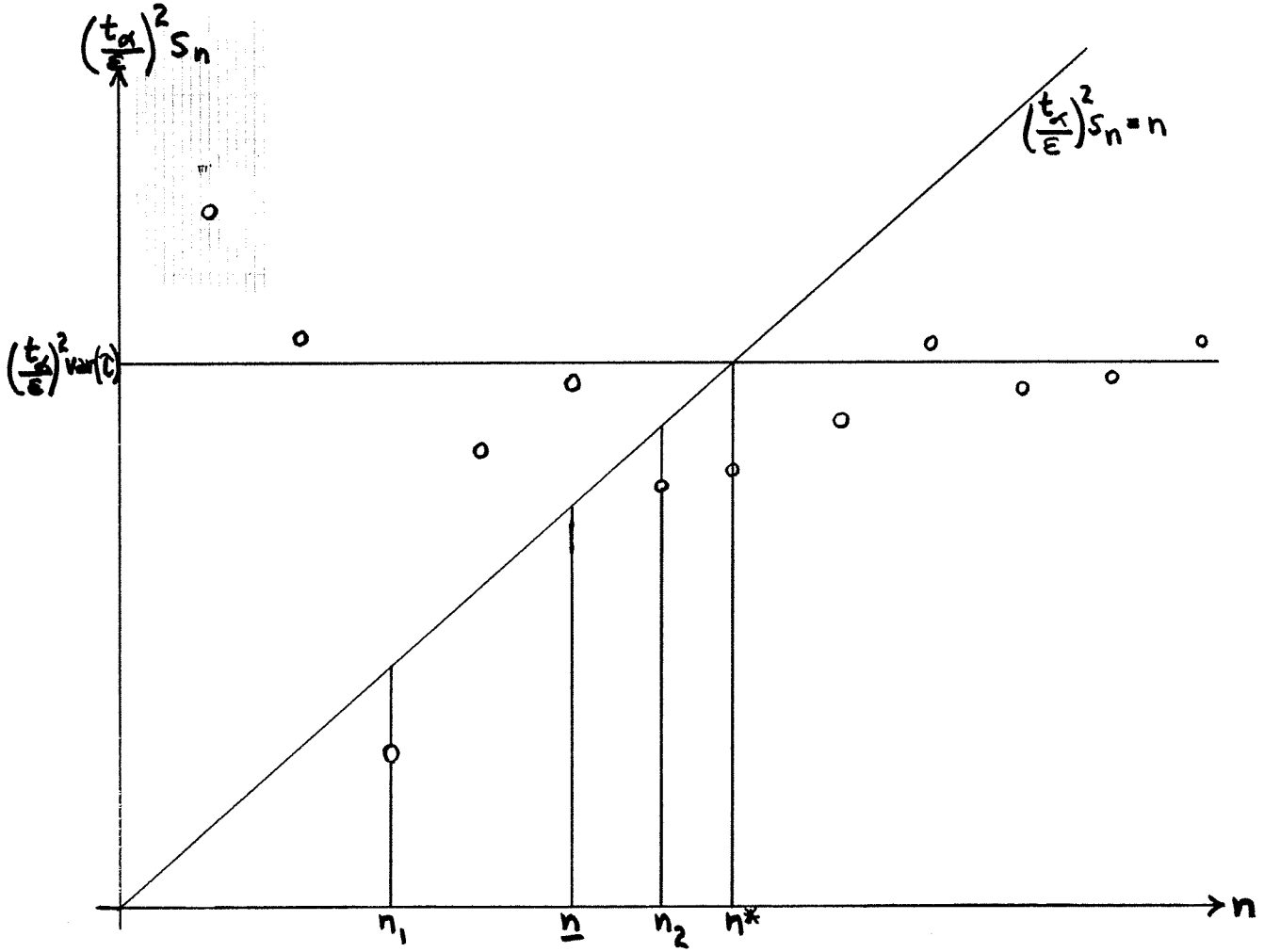


Figure 5.1. MCSS Stopping rules. (Compare Figure 4.3, and explanations on pages 20 and 52.)

2) Following the same type of argument as we did on pages 35 through 38, we find that the expected sample size necessary to satisfy (5.8) is approximately $(\lambda/\delta)^2 (\mu_4 - [\mathrm{var}(\tau)]^2)$.

The second MCSS stopping rule (see (5.8)) determines an estimate for the lower bound on the number of samples needed before we apply the first MCSS stopping rule (3.18) and decision rule (4.28). That is, the stopping rule for s_n^2 attempts to prevent the MCSS process from stopping too soon.

Consider the example shown in Figure 5.1. Without the estimated lower bound, $\underline{n}$, from (5.8), we would take n_1 samples and stop, since (3.18) is satisfied. However, with the lower bound, $\underline{n}$, we must take at least $\underline{n}$ sample points before we apply the stopping rule. So that, in this case, we would take n_2 samples before having (3.18) satisfied. This is much closer to the actual number n^* of samples needed in this example, than is n_1.

There is a drawback to this procedure. The estimated lower bound $\underline{n}$ may severely underestimate the true lower bound n^*. Take again the situation described in Figure 5.1. If $\underline{n}$ is less than n_1, then the method would stop after only n_1 observations. This would cause a large underestimation of $\mathrm{var}(\tau)$, and hence, we would think that we had a better estimate of θ than we actually have. What the second stopping rule does is to lessen considerably the probability of severely underestimating $\mathrm{var}(\tau)$. (It cannot

guarantee this, however.) If $\underline{n}$ is greater than n^*, we lose some time, but the accuracy of var(τ) does not deteriorate.

Furthermore, the estimate, $m_{4,n}$, of the fourth moment, μ_4, used in (5.8), is very unstable. So that, the second stopping rule only provides a rough guide to the actual lower bound for the number of samples needed before we apply the rules (3.18) and (4.28)

6. THE IMPLEMENTATION OF THE MCSS PROCEDURE

In this section we will deal with the description and analysis of some specific cases of the MCSS procedure. The cases are crude, control variate, and antithetic variate estimators (see [HAMJ-HAD] pp. 50-66) with a bisection-type stratification scheme.

Let us recall (see (1.1)), that the problem is to estimate $\theta = \int_R f(\underline{x})\, \underline{dx}$. We will assume that R is a k-cell (see [RUW], p. 27); that is, if $a_i < b_i$, $i=1,\ldots,k$ and $\underline{x} = (x_1,\ldots,x_k)$ then

$$R = \{ \underline{x} : a_i \leq x_i < b_i, \text{ for } i=1,\ldots,k \} .$$

If R is not a k-cell, then, since R is a compact set, we can find a k-cell R' containing it. Thus, we can extend $f(\underline{x})$ to R' as zero outside R, and rename R' as our new R.

The type of bisection scheme used bisects a given region, say R_o, on one of its coordinate axes, say that of x_j, at the point $c_j = (a_j + b_j)/2$, so that the bisection of R_o produces two strata

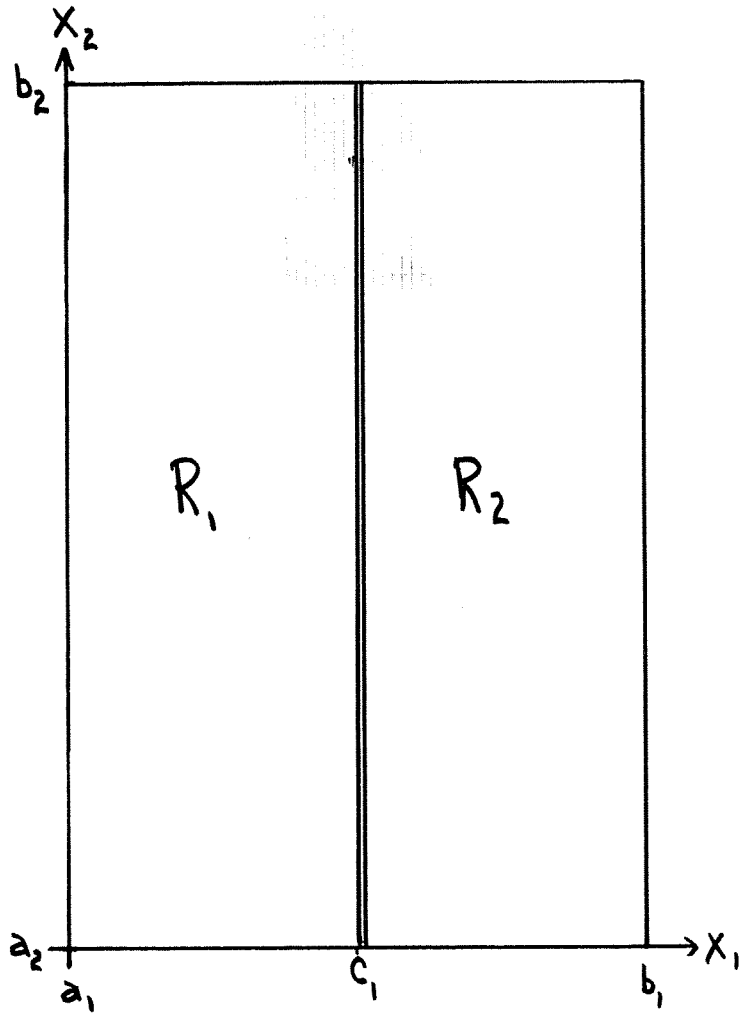


Figure 6.1: Bisecting on X_1 at C_1.

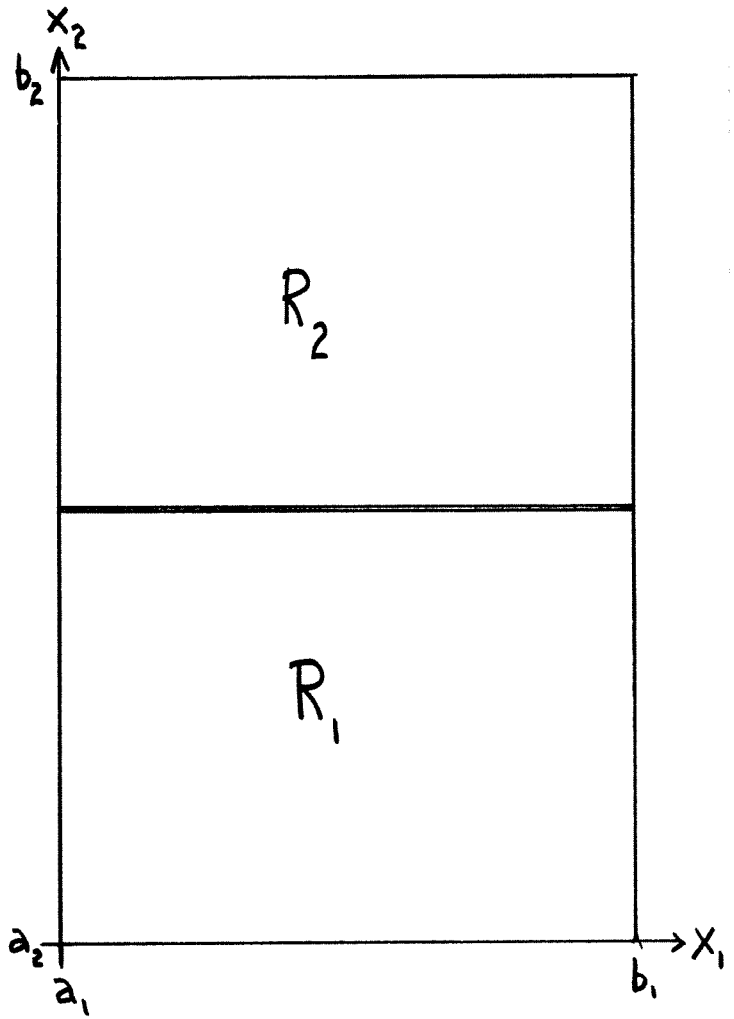


Figure 6.2: Bisecting on X_2 at C_2.

$$R_1 = \{ \underline{x} : a_j \leq x_j < c_j, \text{ and } a_i \leq x_i < b_i \text{ , for all } i \neq j \}$$

and

$$R_2 = \{ \underline{x} : c_j \leq x_j < b_j, \text{ and } a_i \leq x_i < b_i \text{ , for all } i \neq j \}$$

where $R_1 \cup R_2 = R_o$ and R_1 and R_2 are disjoint. (See Figures 6.1 and 6.2.) Letting vol(R) denote the hypervolume of the region R, that is $\text{vol}(R) = \int_R \underline{dx}$. When R is a k-cell, then $\text{vol}(R) = \prod_{i=1}^{k}(b_i - a_i)$. We should note that $\text{vol}(R_1) = \text{vol}(R_2) = 1/2\ \text{vol}(R)$.

In general, the crude Monte Carlo estimator with stratified sampling for p strata is defined to be

$$\hat{\theta}_C = \sum_{u=1}^{p} \hat{\theta}_{C,u,n_u} \tag{6.1}$$

where

$$\hat{\theta}_{C,u,n_u} = \frac{1}{n_u} \sum_{r=1}^{n_u} \tau_{C,u}(\underline{\xi}_r) \text{ ,} \tag{6.2}$$

and

$$\tau_{C,u} = \text{vol}(R_u)\ f(\underline{\xi}) \text{ ,} \tag{6.3}$$

and $\underline{\xi} \sim U(R_u)$, which means that $\underline{\xi}$ is a random point chosen from a multivariate uniform distribution over the stratum R_u and having a probability density function: $p(\underline{\xi}) = [\text{vol}(R_u)]^{-1}$, if $\underline{\xi} \in R_u$, and $p(\underline{\xi}) = 0$, otherwise. Since R is a k-cell, $\underline{\xi} \sim U(R)$, for $\underline{\xi} = (\xi_1, \ldots, \xi_k)$, means that $\xi_i \sim U(a_i, b_i)$, for i=1,...,k; that is, for i=1,...,k, $p(\xi_i) = (b_i - a_i)^{-1}$ if $\xi_i \in (a_i, b_i)$ and $p(\xi_i) = 0$,

otherwise. The same is true for each substratum R_u.

Theorem 6.1.

Let $\theta = \int_R f(\underline{x})\ \underline{dx}$, where R is a k-cell. If $\hat{\theta}_C$ is defined as in (6.1), then $\hat{\theta}_C$ is an unbiased estimator of θ, that is

$$E(\hat{\theta}_C) = \theta \ , \tag{6.4}$$

and

$$\mathrm{var}(\hat{\theta}_C) = \sum_{u=1}^{p} \mathrm{var}(\hat{\theta}_{C,u,n_u}) = \sum_{u=1}^{p} \frac{1}{n_u} \mathrm{var}(\tau_{C,u}) \ , \tag{6.5}$$

where

$$\mathrm{var}(\tau_{C,u}) = \mathrm{vol}(R_u) \int_{R_u} f^2(\underline{x})\ \underline{dx} - \theta_u^2 \ . \tag{6.6}$$

Proof: Since

$$E(\tau_{C,u}) = \int_{R_u} \tau_{C,u}\, p(\underline{x})\ \underline{dx} = \int_{R_u} \mathrm{vol}(R_u)\, f(\underline{x})\ \underline{dx}/\mathrm{vol}(R_u) =$$

$$\int_{R_u} f(\underline{x})\ \underline{dx} = \theta_u$$

we can apply (1.2), (1.4), (1.5), and (1.12), yielding the result (6.4). From the definitions

$$\mathrm{var}(\tau_{C,u}) = E[(\tau_{C,u} - \theta_u)^2] = E(\tau_{C,u}^2) - \theta_u^2$$

$$= \mathrm{vol}(R_u) \int_{R_u} f^2(\underline{x})\ \underline{dx} - \theta_u^2 \ ,$$

as in (6.6). Now apply (1.5) and (1.12) to get (6.5). H-

The control-variate sampling technique is useful when we can find an "easy" function $\phi(\underline{x})$ which approximates the integrand $f(\underline{x})$ over the domain of integration R. A function $\phi(\underline{x})$ will be called easy if we can theoretically integrate $\int_R \phi(\underline{x})\ \underline{dx}$. The control-variate estimator with stratified sampling for p strata is defined to be

$$\hat{\theta}_{CV} = \sum_{u=1}^{p} \hat{\theta}_{CV,u,n_u} + \Phi \tag{6.7}$$

where

$$\hat{\theta}_{CV,u,n_u} = \frac{1}{n_u} \sum_{r=1}^{n_u} \tau_{CV,u}\ (\underline{\xi}_r)\ , \tag{6.8}$$

$$\tau_{CV,u} = \mathrm{vol}(R_u)\ [f(\underline{\xi}) - \phi(\underline{\xi})], \tag{6.9}$$

$$\Phi = \int_R \phi(\underline{x})\ \underline{dx}\ , \tag{6.10}$$

$$\underline{\xi} \sim U(R_u),\ \text{and}\ R_u = \{\underline{x}:\ a_{uj} \leq x_j < b_{uj},\ j=1,\ldots,k\ \}$$

Examining (6.9), we can see that the control variate technique is the same as the crude sampling technique for the function $(f-\phi)(\underline{x})$ with a constant added-in to the result. Thus, the following theorem is almost an immediate consequence of theorem 6.1.

Theorem 6.2.

Let θ be defined as in Theorem 6.1 and $\hat{\theta}_{CV}$ be defined as in (6.7). Then $\hat{\theta}_{CV}$ as an unbiased estimator of θ, that is,

$$E(\hat{\theta}_{CV}) = \theta, \tag{6.11}$$

and

$$\mathrm{var}(\hat{\theta}_{CV}) = \sum_{u=1}^{p} \mathrm{var}(\hat{\theta}_{CV,u,n_u}) = \sum_{u=1}^{p} \frac{1}{n_u} \mathrm{var}(\tau_{CV,u}), \tag{6.12}$$

where

$$\mathrm{var}(\tau_{CV,u}) = \mathrm{vol}(R_u) \int_{R_u} [f(\underline{x})-\phi(\underline{x})]^2 \underline{dx} - (\theta_u - \Phi_u)^2 \tag{6.13}$$

and

$$\Phi_u = \int_{R_u} \phi(\underline{x}) \underline{dx} .$$

Proof:

By comparing (6.1)-(6.3) with (6.7)-(6.9), respectively, and using (6.10), we see that $\hat{\theta}_{CV}-\Phi$ is an estimator $\hat{\theta}_C$ for

$$\theta-\Phi = \int_R (f-\phi)(\underline{x}) \underline{dx} .$$

Thus, by Theorem 6.1, (6.4)-(6.6) imply that

$$E(\hat{\theta}_{CV} - \Phi) = \theta-\Phi ,$$

and

$$\mathrm{var}(\hat{\theta}_{CV} - \Phi) = \sum_{u=1}^{p} \mathrm{var}(\hat{\theta}_{CV,u,n_u}) = \sum_{u=1}^{p} \frac{1}{n_u} \mathrm{var}(\tau_{CV,u}) ,$$

where

$$\text{var}(\tau_{CV,u}) = \text{vol}(R_u) \int_{R_u} (f-\phi)^2(\underline{x})\underline{dx} - (\theta_u - \Phi_u)^2 ,$$

and the theorem follow. H

As we can see from (6.13), the variance of $\hat{\theta}_{CV}$ can be made much smaller than the variance of $\hat{\theta}_C$ if we choose $\phi(\underline{x})$ such that $|f(\underline{x}) - \phi(\underline{x})|$ is much smaller than $|f(\underline{x})|$ over the domain of integration R.

The antithetic-variate technique consists of finding a linear transformation of the integrand, $f(\underline{x})$, which will transform it to a nearly constant function, then applying crude sampling to the transformed function (see [HAMJ-MOK]).

Although, there are many antithetic estimators that can also be used, as we will discuss in Section 12, the particular antithetic-variate estimator for $\theta_u = \int_{R_u} f(\underline{x})\underline{dx}$, that is now being considered in the MCSS algorithm is

$$\tau_{A,u} = \frac{1}{2} \text{vol}(R_u) \, [f(\underline{\xi}) + f(\underline{\xi}^*)] , \tag{6.14}$$

where

$$\underline{\xi} \sim U(R_u), \; R_u = \{\underline{x}: a_{uj} < x_j < b_{uj}, \; j=1,\ldots,k \}$$

and

$$\underline{\xi}^* = (a_{u1} + b_{u1} - \xi_1, \ldots, a_{uk} + b_{uk} - \xi_k) ;$$

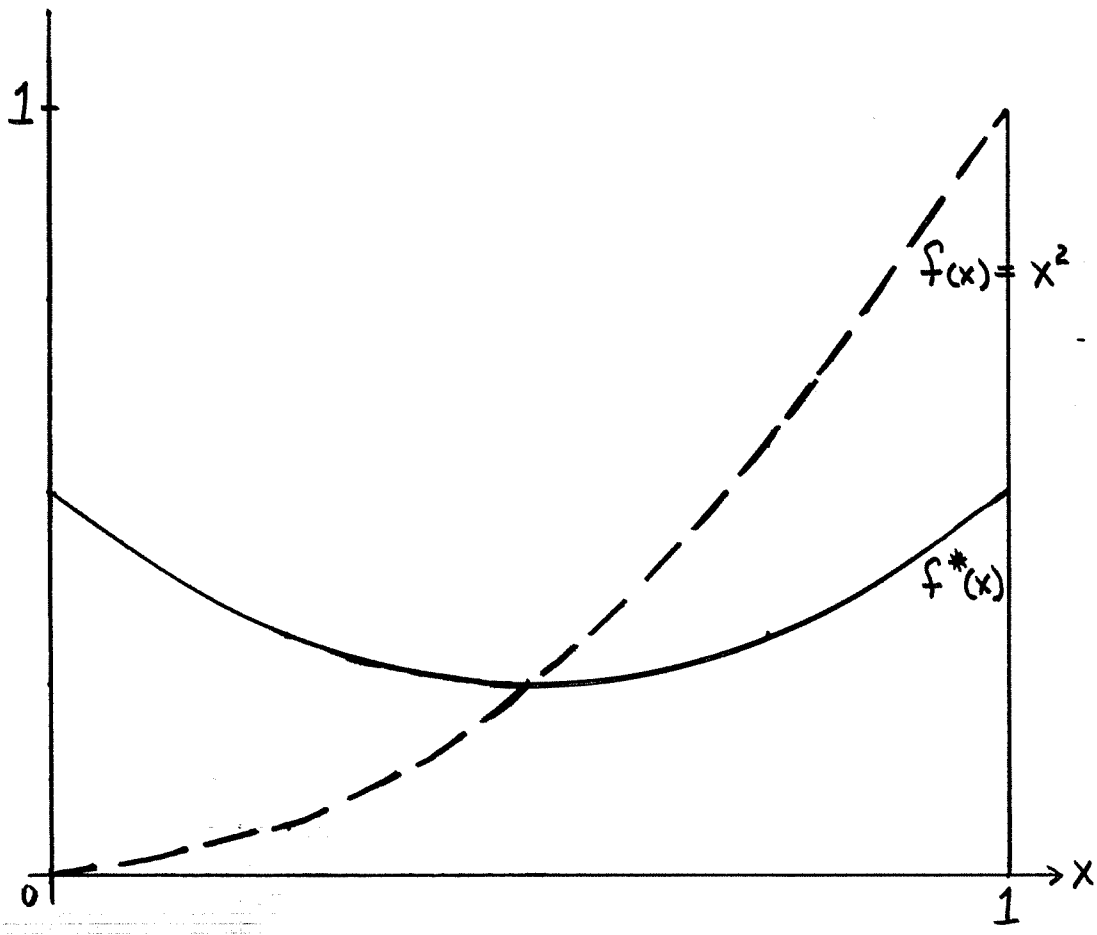


Figure 6.3. The Antithetic variate estimator.

the estimator for θ, with stratified sampling for p strata is

$$\hat{\theta}_A = \sum_{u=1}^{p} \hat{\theta}_{A,u,n_u} \tag{6.15}$$

where

$$\hat{\theta}_{A,u,n_u} = \frac{1}{n_u} \sum_{r=1}^{n_u} \tau_{A,u}(\underline{\xi}_r) \; . \tag{6.16}$$

We can interpret the antithetic-variate estimator as transforming the integrand into a new function, $\mathcal{W}_A f = f^*$, which when integrated over the same region of integration yield the same value for θ (this will be shown in the next theorem), and applying the crude Monte Carlo estimator (6.3) to this new function f*. Consider, for example, $\theta = \int_0^1 x^2 \, dx$. When we apply (6.14) to $f(x) = x^2$, we get the estimator $\frac{1}{2}[\xi^2 + (1-\xi)^2]$, $\xi \sim U(0,1)$. We, then, have as our new function $f^*(x) = \frac{1}{2}[x^2+(1-x)^2]$. Estimating $\int_0^1 f^*(x)dx$ by the crude Monte Carlo estimator (6.3) is the same as estimating $\int_0^1 x^2 \, dx$ by τ_A (see (6.14)). This is illustrated in Figure 6.3.

When we stratify with the antithetic-variate estimator, we usually get a different function, f*, for each stratum, that is we usually do <u>not</u> use the same f* over the entire region of integration. In our example, if we bisect the region of integration, [0,1), we get that, in [0,1/2), $f_1^*(x) = \frac{1}{2}[x^2+ (\frac{1}{2} -x)^2]$ and, in [1/2,1), $f_2^*(x) = \frac{1}{2}[x^2+ (3/2 - x)^2]$. This is graphed in

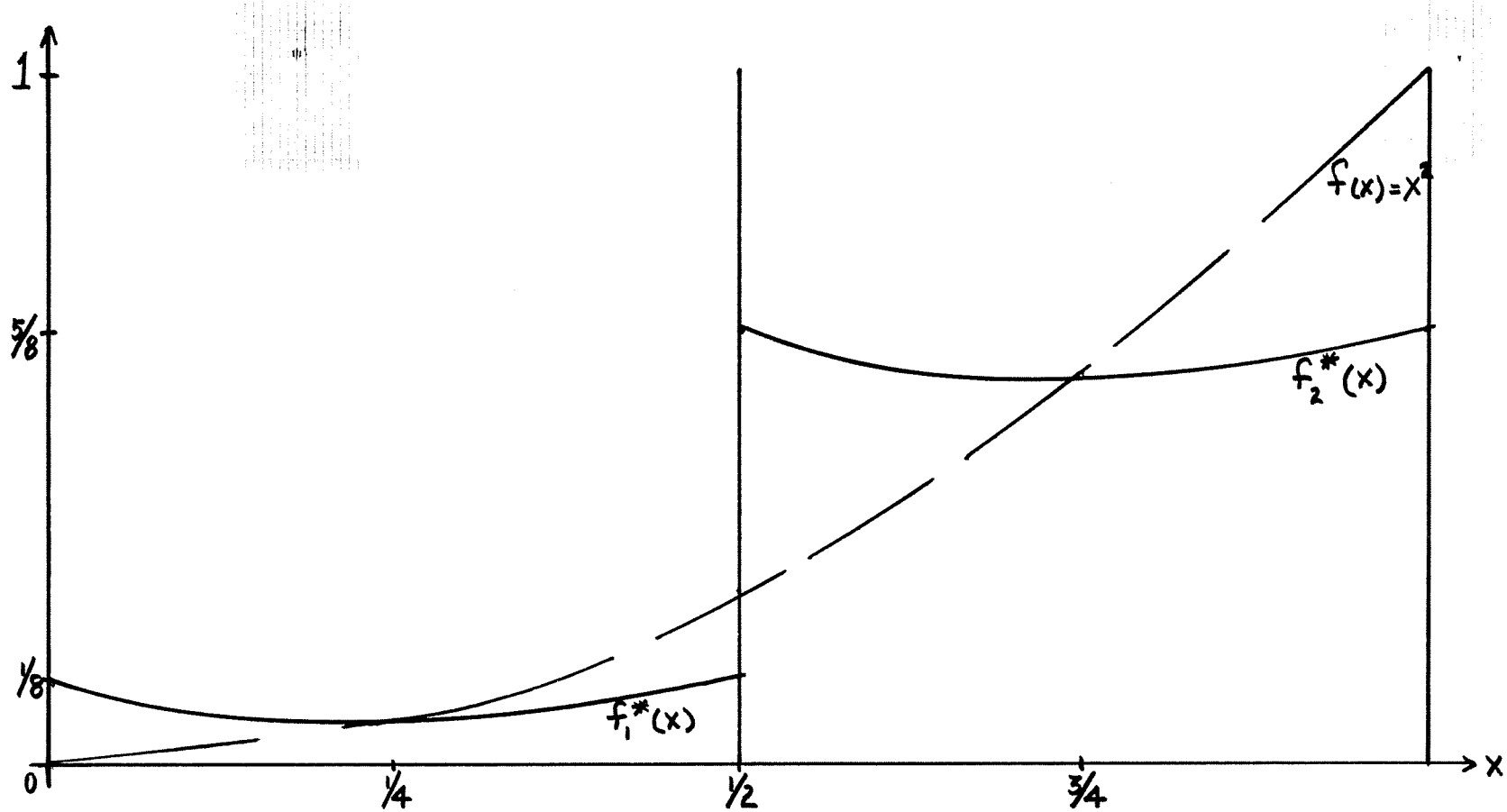


Figure 6.4. The Antithetic variate with bisection.

Figure 6.4.

Theorem 6.3 .

If θ is as before and $\hat{\theta}_A$ is defined as in (6.15) and (6.16), then

$$E(\hat{\theta}_A) = \theta \ , \tag{6.17}$$

and if the $\tau_{A,u}$ are uncorrelated, then

$$\mathrm{var}(\hat{\theta}_A) = \sum_{u=1}^{p} \frac{1}{n_u} \mathrm{var}(\tau_{A,u}) \ , \tag{6.18}$$

where

$$\mathrm{var}(\tau_{A,u}) = \frac{1}{2} \mathrm{vol}(R_u) \int_{R_u} [f^2(\underline{x}) + f(\underline{x}) f(\underline{x}^*)] \underline{dx} - \theta_u^2 \ , \tag{6.19}$$

and

$$\underline{x}^* = (a_{ul} + b_{ul} - x_1, \ldots, a_{uk} + b_{uk} - x_k) \ .$$

Proof:

From (6.14) we have that

$$E(\tau_{A,u}) = \int_{R_u} \frac{1}{2} [f(\underline{x}) + f(\underline{x}^*)] \underline{dx} \ .$$

But, since R_u is a k-cell, $R_u = \{\underline{x} : a_{uj} < x_j < b_{uj}, \ j=1,\ldots,k \}$

$$\int_{R_u} f(\underline{x}^*)\underline{dx} = \sum_{j=1}^{k} \left[\int_{b_{uj}}^{a_{uj}} d(a_{uj}+b_{uj}-x_j) \right] f(a_{u1}+b_{u1}-x_1,\ldots,a_{uk}+b_{uk}-x_k)$$

$$= \sum_{j=1}^{k} \left[\int_{a_{uj}}^{b_{uj}} dz_j \right] f(z_1,\ldots,z_k) = \int_{R_u} f(\underline{x})\underline{dx},$$

where the notation $\sum_{j=1}^{k} \int_{E_j} dy_j$ denotes $\int_{E_1} dy_1 \cdots \int_{E_k} dy_k$.

Therefore,

$$E(\tau_{A,u}) = \int_{R_u} f(\underline{x})\underline{dx} = \theta_u .$$

Now apply Lemma 3.2 to get (6.17).

$$\mathrm{var}(\tau_{A,u}) = \int_{R_u} \tau_{A,u}^2 \, [\mathrm{vol}(R_u)]^{-1} \, \underline{dx} - \theta_u^2$$

$$\int_{R_u} \tau_{A,u}^2 \, [\mathrm{vol}(R_u)]^{-1} \, \underline{dx} = \frac{1}{4} \, \mathrm{vol}(R_u) \int_{R_u} [f(\underline{x})+f(\underline{x}^*)]^2 \, \underline{dx}$$

$$= \frac{1}{2} \, \mathrm{vol}\,(R_u) \int_{R_u} [f^2(\underline{x}) + f(\underline{x})\, f(\underline{x}^*)] \, \underline{dx} . \qquad \text{H}$$

We now apply Lemma 3.3 to get (6.18).

The motivation for using the estimator τ_A comes from the next theorem and its corollaries.

Theorem 6.4.

Let us define the transformation $\mathcal{W}_A$ by

$$\mathcal{W}_A\,[f(\underline{x})] = \frac{1}{2}\,\mathrm{vol}(R)[f(\underline{x}) + f(\underline{x}^*)]\ ,$$

where

$$\underline{x}^* = (a_1 + b_1 - x_1, \ldots, a_k + b_k - x_k)\ ,$$

$$R = \{\ \underline{x} : a_i < x_i < b_i,\ i=1,\ldots,k\ \}\ .$$

If $f(\underline{x})$ is such that

$$f(\underline{x}) + f(\underline{x}^*) = K\ ,$$

for some constant K; then

(6.20) $$\mathcal{W}_A\,[f(\underline{x})] = \theta, \text{ for all } \underline{x}\in R\ ;$$

so that, since $\tau_A = \mathcal{W}_A f(\underline{\xi})$,

(6.21) $$\mathrm{var}(\tau_A) = 0\ .$$

Proof:

By Theorem 6.3, we have that $E(\tau_A) = \theta$. Furthermore,

$$E(\tau_A) = E\left(\frac{1}{2}\,\mathrm{vol}(R)\ [f(\underline{x}) + f^*(\underline{x})]\right)$$

$$= \int_R \frac{1}{2}\,[f(\underline{x}) + f^*(\underline{x})]\underline{dx}$$

$$= \frac{1}{2}\,\mathrm{vol}(R)\ K\ , \text{ by the hypothesis .}$$

Hence,

$$K = [\tfrac{1}{2}\,\mathrm{vol}(R)]^{-1}\,\theta\ .$$

Therefore, we get (6.20):

$$\mathcal{W}_A[f(\underline{x})] = [\tfrac{1}{2}\,\mathrm{vol}(R)]\ [\tfrac{1}{2}\,\mathrm{vol}(R)]^{-1}\,\theta = \theta$$

Now, (6.21) follows trivially since

$$\mathrm{var}(\tau_A) = E(\tau_A - \theta)^2 = 0\ . \qquad \text{H}$$

Corollary 6.1.

Let τ_A be defined as in Theorem 6.4, if $f(\underline{x})$ is antisymmetric about the centroid of R, that is

$$f(c_1+ z_1,\ldots,c_k+ z_k) = -\ f(c_1- z_1,\ldots,c_k- z_k)\ ,$$

where the centroid of R is $(c_1,\ldots,c_k)$, with $c_i = \frac{1}{2}\,(a_i+b_i)$, for $i=1,\ldots,k$, then (6.20) and (6.21) hold.

Proof :

Letting $x_i = c_i+ z_i$, for $i=1,\ldots,k$, we have that

$$c_i - z_i = 2c_i - x_i = a_i+ b_i - x_i,\ \text{for } i=1,\ldots,k\ .$$

Thus, by the antisymmetry of f

$$f(x_1,\ldots,x_k) + f(a_1+ b_1- x_1,\ldots,a_k+ b_k- x_k) = 0\ . \qquad \text{H}$$

Corollary 6.2.

With τ_A as in Theorem 6.4, if $f(\underline{x})$ is a linear function, that is

$$f(\underline{x}) = \gamma + \sum_{i=1}^{k} \beta_i x_i ,$$

then (6.20) and (6.21) hold.

Proof:

Here,

$$f(\underline{x})+f(\underline{x}^*) = 2\gamma + \sum_{i=1}^{k} \beta_i x_i - \sum_{i=1}^{k} \beta_i(a_i+b_i-x_i)$$

$$= 2\gamma - \sum_{i=1}^{k} \beta_i(a_i+ b_i);$$

but this last expression is a constant. ⊞

Remark. The last corollary states that the estimator, τ_A, of θ is exact for linear functions. This is clearly not the case for quadratic functions. Thus, in numerical quadrature terminology we would say that τ_A has degree of precision one.

Lemma 6.1.

If $f(\underline{x}) \neq f(\underline{x}^*)$ on a subset of R of positive volume, where

$$\underline{x}^* = (a_1+ b_1- x_1,\ldots,a_k+ b_k- x_k) ,$$

and if τ_A is defined as in (6.14) and τ_C as in (6.3), then

$$\text{var}(\tau_A) < \text{var}(\tau_C);$$

and $\text{var}(\tau_A) = \text{var}(\tau_C)$ if and only if $f(\underline{x}) = f(\underline{x}^*)$ almost everywhere in R.

Proof:

By (6.19),

$$\text{var}(\tau_A) = \frac{1}{2}\,\text{vol}(R)\,[\int_R f^2(\underline{x}) + f(\underline{x})\,f(\underline{x}^*)\,\underline{dx}] - \theta^2 ,$$

and by (6.6)

$$\text{var}(\tau_C) = \text{vol}(R)\int_R f^2(\underline{x})\,\underline{dx} - \theta^2 .$$

Now, by Schwart'z inequality,

$$\int_R f(\underline{x})f(\underline{x}^*)\underline{dx} \le [\int_R f^2(\underline{x})\underline{dx}]^{1/2}[\int_R f^2(\underline{x}^*)\underline{dx}]^{1/2} = \int_R f^2(\underline{x})\underline{dx}$$

and

$$\int_R f(\underline{x})f(\underline{x}^*)\underline{dx} = \int_R f^2(\underline{x})\underline{dx}$$

if and only if

$$f(\underline{x}) = f(\underline{x}^*) \quad \text{almost everywhere in R.}$$

Therefore, we obtain the desired results. H

Now, let us examine when it would be more advantageous to use the antithetic rather than the crude Monte Carlo estimator.

Let $\hat{\theta}_{A,n} = n^{-1} \sum_{r=1}^{n} \tau_A(\underline{\xi}_r)$ and $\hat{\theta}_{C,n} = n^{-1} \sum_{r=1}^{n} \tau_C(\underline{\xi}_r)$ denote the antithetic-variate and crude Monte Carlo estimators, respectively, for n observations. Clearly, it is advantageous to use the antithetic-variate estimator rather than the crude Monte Carlo estimator, when the total work to compute $\hat{\theta}_{A,n_A}$, w_A, is less than the total work to compute θ_{C,n_C}, w_C, to get the same desired accuracy.

Let T be the desired tolerance; so that, it requires $n_A = \text{var}(\tau_A)/T$ samples for $\hat{\theta}_A$ and $n_C = \text{var}(\tau_C)/T$ samples for $\hat{\theta}_C$, to achieve the same desired accuracy. Now, let ℓ_A be the amount of labor to evaluate τ_A, and ℓ_C be the amount of labor to evaluate τ_C. Since for every one computation of τ_A we require <u>two</u> function evaluations (see (6.14)), whereas τ_C requires only <u>one</u> function evaluation (see (6.3)), we have that

$$\ell_A = 2\ell_C \ .$$

Therefore, $w_A < w_C$ if and only if

$$w_A = n_A \ell_A < n_C \ell_C = w_C \ ;$$

or equivalently,

$$\text{var}(\tau_A)\ \ell_A < \text{var}(\tau_C)\ \ell_C \ .$$

Using $\ell_A = 2\ell_C$, we get

Theorem 6.5

It is advantageous to use the antithetic variate estimator, $\hat{\theta}_A$ rather than the crude Monte Carlo estimator, $\hat{\theta}_C$, if and only if

(6.22) $$2\ \mathrm{var}(\tau_A) < \mathrm{var}(\tau_C)\ ;$$

or equivalently, if and only if

(6.23) $$\mathrm{vol}(R) \int_R f(\underline{x}) f(\underline{x}^*) \underline{dx} < \theta^2 \ .$$

Remarks: 1) The inequality (6.23) can be written in the equivalent forms.

(6.24) $$\mathrm{cov}(\tau_C, \tau_D) < 0,$$

where

$\tau_D = \mathrm{vol}(R) \cdot f(\underline{\xi}^*)$, and τ_C is defined as in (6.3);

or again, if ρ denotes the correlation coefficient,

(6.25) $$\rho = \frac{\mathrm{cov}(\tau_C, \tau_D)}{\mathrm{var}(\tau_C)} < 0 \ ,$$

since $\mathrm{var}(\tau_D) = \mathrm{var}(\tau_C)$.

2) A good practical criterion for using the antithetic variate estimator would therefore be that ρ was significantly negative.

3) This result is new. The apparent similarity of (6.24) to the result in [HAMJ - HAD] on page 57 is coincidental; they are looking at the variances rather than comparing labor.

7. BASIC RELATIONSHIPS

Before we proceed with the description of the MCSS algorithm for the estimators mentioned in Section 6, a few relationships must be established. These relationships are used in the procedure and, as we shall see, reduce the number of samples required by the usual sequential procedures.

Definition: $a_n \cong b_n$ if and only if

$$\text{pr}\{ \lim_{n\to\infty} (a_n - b_n) = 0 \} = 1 ;$$

that is, $\lim_{n\to\infty} (a_n - b_n) = 0$ with probability one

Theorem 7.1

Let R_o be any given stratum of R, R_1 and R_2 be such that $R_o = R_1 \cup R_2$ with R_1, R_2 disjoint.

Then

$$\hat{\theta}_{t,o,n_o} \cong \hat{\theta}_{t,1,n_1} + \hat{\theta}_{t,2,n_2} \tag{7.1}$$

where

$t = C$, CV, or A, and $n_o = n_1 + n_2$.

Proof:

This theorem will be proven for the case when t=C. The other cases follow in a similar manner.

For brevity, let $\hat{\theta}_{u,n} = \hat{\theta}_{C,u,n_u}$ for u=0,1,2.

Now, for u=0,1,2,

$E(\hat{\theta}_{u,n}) = \theta_u$, by Theorem 6.1 ,

and $\hat{\theta}_{C,u,n_u}$ is an average of independent identically distributed random variables satisfying (1.2)-(1.5). So, by the strong law of large numbers (see [LOM] p. 239)

$$\ell im_{n\to\infty} \hat{\theta}_{u,n} = \theta_u, \text{ with probability one,}$$

for u=0,1,2.

Now upon applying lemma 5.1, we get

$$\ell im_{n\to\infty} (\hat{\theta}_{1,n} + \hat{\theta}_{2,n}) = \theta_1 + \theta_2 \text{ , with probability one.}$$

But, since $R_o = R_1 \cup R_2$,

$$\theta_o = \theta_1 + \theta_2 ;$$

so that

$$\ell im_{n\to\infty}(\hat{\theta}_{1,n} + \hat{\theta}_{2,n}) = \theta_o \text{ , with probability one.}$$

Since we also have

$$\ell im_{n\to\infty} \hat{\theta}_{o,n} = \theta_o \text{ , with probability one;}$$

upon applying Lemma 5.1 again we get

$\lim_{n\to\infty} (\hat{\theta}_{1,n} + \hat{\theta}_{2,n} - \hat{\theta}_{0,n}) = 0$, with probability one. H

Next, we need an estimator for $\text{var}(\tau_{t,u})$, for t = C,CV, and A. Let $\text{var}(\tau_{t,u})$ be estimated by

$$(7.2) \qquad s^2_{t,u,n_u} = \frac{1}{n_u - 1} \sum_{r=1}^{n_u} (\tau_{t,u,r} - \hat{\theta}_{t,u,n_u})^2, \text{ for } n_u \geq 2 ,$$

where $\tau_{t,u,r} = \tau_{t,u}(\underset{\sim}{\xi}_r)$ and t = C,CV, or A . Then

$$(7.3) \qquad E(s^2_{t,u,n_u}) = \text{var}(\tau_{t,u}) \text{ , for t=C, CV, and A.}$$

This is proven in exactly the same manner as Lemma 3.1 by using (6.4), (6.11), and (6.17).

Theorem 7.2.

If a given stratum R_o is bisected on the x_j axis at $c_j = \frac{1}{2}(a_j + b_j)$ and if t=C, CV, and A, and $n_o = n_1 + n_2$; then

$$(7.4) \qquad s^2_{t,o,n_o} \cong (2 - \frac{1}{n_1}) s^2_{t,1,n_1} + (2 - \frac{1}{n_2}) s^2_{t,1,n_2} + (\hat{\theta}_{t,1,n_1} - \hat{\theta}_{t,2,n_2})^2 + \hat{Q}_t ,$$

where

$\hat{Q}_t = 0$ when t = C or CV ,

$\hat{Q}_A = n_o^{-1} \sum_{r=1}^{n_o} \hat{Q}_r$,

$$\hat{Q}_r = [\tfrac{1}{2}\,\mathrm{vol}(R_o)]^2\,[f(\underline{\xi}_{1r})-f(\underline{\xi}_{2r})]\,[f(\underline{\xi}^*_{2r})-f(\underline{\xi}^*_{1r})]$$

and (omitting the index r for clarity)

$$\underline{\xi}_1 = (\xi_1,\ldots,\xi_k)\ ,\quad \underline{\xi}_1 \sim U(R_1),\ \text{i.e.}$$

$$\xi_i \sim U(a_i,b_i),\ \text{for } i\neq j \text{ and } i=1,\ldots,k,\quad \xi_j \sim U(a_j,\ c_j)\ ,$$

$$\underline{\xi}^*_1 = (a_1+\ b_1-\ \xi_1,\ldots,a_j+\ c_j-\ \xi_j,\ldots,\ a_k+\ b_k-\ \xi_k)\ ,$$

$$\underline{\xi}_2 = (\xi_1,\ldots,\ \xi_j\ +\ c_j-\ a_j,\ldots,\ \xi_k)\ ,$$

$$\underline{\xi}^*_2 = (a_1+\ b_1-\xi_1,\ldots,\ a_j+\ b_j-\ \xi_j,\ldots,\ a_k+\ b_k-\ \xi_k\ )\ .$$

Remark: We observe that the points $\underline{\xi}_1$ and $\underline{\xi}_2$ are not uncorrelated (they are rigidly connected), so that (6.18) does not hold, in this case. To prove this theorem we will first need

Lemma 7.1

Under the same hypothesis as in Theorem 7.2, we have

$$(7.5)\qquad \mathrm{var}(\tau_{C,o}) = 2[\mathrm{var}(\tau_{C,1}) + \mathrm{var}(\tau_{C,2})\ ] + (\theta_1-\ \theta_2)^2\ ;$$

letting $\Phi_u = \int_{R_u} \phi(\underline{x})\underline{dx}$, we get

$$(7.6)\quad \mathrm{var}\ (\tau_{CV,o}) = 2[\mathrm{var}(\tau_{CV,1})+\ \mathrm{var}(\tau_{CV,2})]+[(\theta_1-\Phi_1)-(\theta_2-\Phi_2)]^2;$$

and

$$(7.7)\quad \mathrm{var}(\tau_{A,o}) = 2[\mathrm{var}(\tau_{A,1}) + \mathrm{var}(\tau_{A,2})] + (\theta_1 - \theta_2)^2 + Q_A,$$

where $$Q_A = \frac{1}{2}\,\mathrm{vol}(R_o)\,\{\int_{R_1} f(\underline{x})\,[f(\underline{x}_o^*) - f(\underline{x}_1^*)]\,\underline{dx}$$

$$+ \int_{R_2} f(\underline{x})\,[f(\underline{x}_o^*) - f(\underline{x}_2^*)\underline{dx}\,\},$$

$\underline{x}_o^* = (a_1+b_1-x_1,\ldots,a_k+b_k-x_k)$, $\underline{x}_1^* = (a_1+b_1-x_1,\ldots,a_j+c_j-x_j,\ldots,$

$a_k+b_k-x_k)$, and $\underline{x}_2^* = (a_1+b_1-x_1,\ldots,c_j+b_j-x_j,\ldots,a_k+b_k-x_k)$.

Proof of Lemma 7.1:

By (6.6), we have for crude sampling that

$$\mathrm{var}(\tau_{C,o}) + \theta_o^2 = \mathrm{vol}(R_o) \int_{R_o} f^2(\underline{x})\underline{dx},$$

whereas, since $\mathrm{vol}(R_1) = \mathrm{vol}(R_2) = \mathrm{vol}(R_o)/2$,

$$2[\mathrm{var}(\tau_{C,1})+\theta_1^2 + \mathrm{var}(\tau_{C,2})+\theta_2^2] = \mathrm{vol}(R_o)\,[\int_{R_1} f^2(\underline{x})\underline{dx} + \int_{R_2} f^2(\underline{x})\underline{dx}]$$

$$= \mathrm{vol}(R_o) \int_{R_o} f^2(\underline{x})\underline{dx}, \text{ since } R_o = R_1 \cup R_2.$$

Therefore

$$\mathrm{var}(\tau_{C,o}) = 2[\mathrm{var}(\tau_{C,1}) + \mathrm{var}(\tau_{C,2})] + 2(\theta_1^2 + \theta_2^2) - \theta_o^2 .$$

Since, $R_o = R_1 \cup R_2$ yields $\theta_o = \theta_1 + \theta_2$, we have

$$2(\theta_1^2 + \theta_2^2) - \theta_o^2 = 2(\theta_1^2 + \theta_2^2) - (\theta_1 + \theta_2)^2 = \theta_1^2 - 2\theta_1\theta_2 + \theta_2^2 = (\theta_1 - \theta_2)^2 .$$

This proves (7.5).

The control variate case (7.6) is proven in the same manner with $f^2(\underline{x})$ replaced by $[f(\underline{x}) - \phi(\underline{x})]^2$ and θ_u replaced by $\theta_u - \Phi_u$ for $u=0,1,2$.

For the antithetic variate case, we have, by (6.19),

$$\mathrm{var}(\tau_{A,o}) + \theta_o^2 = \frac{1}{2}\,\mathrm{vol}(R_o) \int_{R_o} [f^2(\underline{x}) + f(\underline{x})\, f(\underline{x}_o^*)]\,\underline{dx}$$

Now,

$$2[\mathrm{var}(\tau_{A,1}) + \theta_1^2 + \mathrm{var}(\tau_{A,2}) + \theta_2^2] = \frac{1}{2}\,\mathrm{vol}(R_o)\{\int_{R_1} [f^2(\underline{x}) + f(\underline{x}) f(\underline{x}_1^*)]\,\underline{dx}$$

$$+ \int_{R_2} [f^2(\underline{x}) + f(\underline{x}) f(\underline{x}_2^*)]\,\underline{dx}\ \}$$

$$= \frac{1}{2}\,\mathrm{vol}(R_o)\left[\int_{R_o} f^2(\underline{x})\,\underline{dx} + \int_{R_1} f(\underline{x}) f(\underline{x}_1^*)\,\underline{dx} + \int_{R_2} f(\underline{x}) f(\underline{x}_2^*)\,\underline{dx}\ \right]$$

Therefore,

$$\mathrm{var}(\tau_{A,o}) = 2[\mathrm{var}(\tau_{A,1}) + \mathrm{var}(\tau_{A,2})] + (\theta_1 - \theta_2)^2 + \frac{1}{2}\mathrm{vol}(R_o)\left[\int_{R_o} f(\underline{x}) f(\underline{x}_o^*)\,\underline{dx}\right.$$

$$\left. - \int_{R_1} f(\underline{x}) f(\underline{x}_1^*)\,\underline{dx} - \int_{R_2} f(\underline{x}) f(\underline{x}_2^*)\,\underline{dx}\ \right] .$$

$$\mathrm{var}(\tau_{A,o}) = 2[\mathrm{var}(\tau_{A,1}) + \mathrm{var}(\tau_{A,2})] + (\theta_1 - \theta_2)^2 + Q_A \ ,$$

where

$$Q_A = \tfrac{1}{2}\,\mathrm{vol}(R_o)\left[\int_{R_o} f(\underline{x}) f(\underline{x}_o^*)dx - \int_{R_1} f(\underline{x}) f(\underline{x}_1^*)dx - \int_{R_2} f(\underline{x}) f(\underline{x}_2^*)dx\right];$$

or, upon splitting $\int_{R_o}$, we get that

$$Q_A = \tfrac{1}{2}\,\mathrm{vol}(R_o)\int_{R_1} f(\underline{x})\,[f(\underline{x}_o^*) - f(\underline{x}_1^*)]\underline{dx} + \int_{R_2} f(\underline{x})\,[f(\underline{x}_o^*) - f(\underline{x}_2^*)\underline{dx}]$$

H -

Proof of Theorem 7.2 :

For t=c, $E(s_{C,o}^2) = \mathrm{var}(\tau_{C,o})$, by (7.3); whence

$$E\left[\left(2 - \tfrac{1}{n_1}\right)s_{C,1}^2 + \left(2 - \tfrac{1}{n_2}\right)s_{C,2}^2 + (\hat{\theta}_{C,1} - \hat{\theta}_{C,2})^2\right] = 2[\mathrm{var}(\tau_{C,1}) + \mathrm{var}(\tau_{C,2})] +$$

$$(\theta_1 - \theta_2)^2 \ ,$$

since $\hat{\theta}_{C,1}$ and $\hat{\theta}_{C,2}$ are independent and

$$E[(\hat{\theta}_{C,1} - \hat{\theta}_{C,2})^2] = E(\hat{\theta}_{C,1}^2) - 2E(\hat{\theta}_{C,1})E(\hat{\theta}_{C,2}) + E(\hat{\theta}_{C,2}^2)$$

$$E(\theta_{C,u}^2) = \frac{1}{n_u}\,\mathrm{var}(\tau_{C,u}) + \theta_u^2 \ , \quad \text{for } u=1,2.$$

By applying Lemma 7.1, Equation (7.5), the result follows from (1.5), the strong law, and its extensions in Lemmas 5.1, 5.2.

For t= CV, the result follows in a manner analogous to the preceding case. For the case t=A, we have that, since $\underline{\xi}_2$ depends on $\underline{\xi}_1$, (still omitting the index r for the random point)

$$E(\hat{Q}) = E([\tfrac{1}{2} \text{vol}(R_o)]^2 [f(\underline{\xi}_1)-f(\underline{\xi}_2)][f(\underline{\xi}_2^*)-f(\underline{\xi}_1^*)]) ;$$

$$(7.8) \qquad E(\hat{Q}) = \tfrac{1}{2} \text{vol}(R_o)\{\int_{R_1} f(\underline{x})[f(a_1+b_1-x_1,\ldots,a_k+b_k-x_k)$$

$$- f(a_1+b_1-x_1,\ldots,a_j+c_j-x_j,\ldots,a_k+b_k-x_k)]\underline{dx}$$

$$+ \int_{R_1} f(x_1,\ldots,x_j+c_j-a_j,\ldots,x_k) [f(a_1+b_1-x_1,\ldots,$$

$$a_j+c_j-x_j,\ldots,a_k+b_k - x_k) -f(a_1+b_1-x_1,\ldots,a_k+b_k-x_k)]\underline{dx} \} .$$

We use the substitution $y_j=x_j+c_j-a_j$ in the second integral, to get that

$$\int_{R_1}\underline{dx} = \int_{a_1}^{b_1} dx_1 \ldots \int_{a_j}^{c_j} dx_j \ldots \int_{a_k}^{b_k} dx_k = \int_{a_1}^{b_1} dx_1 \ldots \int_{c_j}^{b_j} dy_j \ldots \int_{a_k}^{b_k} dx_k$$

$$= \int_{R_2} dx_1 \ldots dy_j \ldots dx_k ;$$

and hence, the second integral equals

$$\int_{R_2} f(x_1,\ldots,y_j,\ldots,x_k)\ [f(a_1+b_1-x_1,\ldots,a_j+b_j-y_j,\ldots,a_k+b_k-x_k)$$

$$- f(a_1+b_1-x_1,\ldots,c_j+b_j-y_j,\ldots,a_k+b_k-x_k)]dx_1\ldots dy_j\ldots dx_k \ .$$

Replacing y_j by x_j and substituting into (7.8), we get that (restoring index r)

$$E(\hat{Q}_r) = \frac{1}{2}\,\mathrm{vol}(R_o)\ \{\ \int_{R_1} f(\underline{x})[f(\underline{x}_o^*)-f(\underline{x}_1^*)]\underline{dx}\ +$$

$$\int_{R_2} f(\underline{x})[f(\underline{x}_o^*) - f(\underline{x}_2^*)]\underline{dx}\ \}\ .$$

$$= Q_A\ ,\ \text{by Lemma 7.1, whence } E(\hat{Q}_A)=Q_A \text{ also.}$$

The remainder of the proof follows exactly as in the case when t=C. ⊣

The importance of Theorems 7.1 and 7.2 is that, if we sample from regions R_1 and R_2, then we need not sample from region R_o to determine its sample mean and variance for the estimate of $\theta_o = \int_{R_o} f(\underline{x})\underline{dx}$, because the samples from R_1 and R_2 will yield them. This, of course, yields a reduction in the total number of function evaluations needed.

The following theorem is very useful for the sequential computation of s_n^2. It is known that, if we used the formula $s_n^2 = (n-1)^{-1} \sum_{r=1}^{n} \tau^2(\xi_r) - \theta^2$, we would obtain large roundoff

errors, whereas if we used formula (7.2) we would not, but would require the storing of the $\tau(\underline{\xi}_r)$'s. The following theorem establishes the validity of a formula which enables us to compute s_n^2 with a roundoff error comparable to that arising from the use of formula (7.2), yet requiring very little storage. For a further discussion of this point, see [NEP].

Theorem 7.3.

Let $x_1,\ldots,x_N$ be any set of real numbers and $\bar{x}(N) = N^{-1} \sum_{r=1}^{N} x_r$; then

$$(7.9) \qquad \sum_{r=1}^{N} (x_r - \bar{x}(N))^2 = \sum_{r=1}^{N-1} u_r \ ,$$

where

$$u_r = \frac{1}{r(r+1)} \left[r\, x_{r+1} - \sum_{s=1}^{r} x_s \right]^2 .$$

Remark:

The formula (7.9) is the Helmert transformation. The proof is given in [WEB], but is included here for completeness.

Proof (by induction on N):

$$\sum_{r=1}^{2} (x_r - \bar{x}(2))^2 = \sum_{r=1}^{2} \left[x_r - \tfrac{1}{2}(x_1 + x_2)\right]^2$$

$$= \tfrac{1}{2}(x_1 - x_2)^2 = u_1 \ .$$

Hence (7.9) holds for N=2. Assume (7.9) holds for N=2,3,...,n-1, that is

$$(7.10) \qquad \sum_{r=1}^{n-1} (x_r - \bar{x}(n-1))^2 = \sum_{r=1}^{n-2} u_r \ .$$

Now

$$\bar{x}(n) = \frac{1}{n} \sum_{r=1}^{n} x_r$$

$$= \frac{n-1}{n} \left(\frac{1}{n-1} \sum_{r=1}^{n-1} x_r\right) + \frac{1}{n} x_n$$

$$= \frac{n-1}{n} \bar{x}(n-1) + \frac{1}{n} x_n \ .$$

Since $\sum_{r=1}^{n-1} [x_r - \bar{x}(n-1)] = 0$,

$$\sum_{r=1}^{n} (x_r - \bar{x}(n))^2 = \sum_{r=1}^{n} \left(x_r - \frac{n-1}{n} \bar{x}(n-1) - \frac{1}{n} x_n\right)^2$$

$$= \sum_{r=1}^{n-1} \left[\left(x_r - \bar{x}(n-1) - \frac{1}{n}(x_n - \bar{x}(n-1))\right]^2 + \left[\frac{n-1}{n}(x_n - \bar{x}(n-1))\right]^2\right.$$

$$= \sum_{r=1}^{n-1} [x_r - \bar{x}(n-1)]^2 + \frac{n-1}{n} [x_n - \bar{x}(n-1)]^2$$

$$= \sum_{r=1}^{n-1} [x_r - \bar{x}(n-1)]^2 + \frac{1}{(n-1)n} \left[(n-1)x_n - \sum_{s=1}^{n-1} x_s\right]^2$$

$$= \sum_{r=1}^{n-2} u_r + u_{n-1} \,, \qquad \text{by (7.10) and the definition of } u_r \,,$$

$$= \sum_{r=1}^{n-1} u_r \,. \qquad \text{H}$$

Corollary.

The estimator of $\text{var}(s_N^2)$

$$(7.11) \qquad \frac{1}{N}[m_{4,N} - (\frac{N-1}{N})^2 s_N^4] = \frac{1}{N^2} \sum_{r=1}^{N-1} w_r$$

where $$w_r = \frac{1}{r(r+1)} [r(\tau_{r+1} - \hat{\theta})^2 - \sum_{s=1}^{r} (\tau_s - \hat{\theta})^2]^2$$

Proof:

Let $z_r = \tau_r - \hat{\theta}$.

$$\frac{1}{N}[m_{4,N} - (\frac{N-1}{N})^2 s_N^4] = \frac{1}{N} [\frac{1}{N} \sum_{r=1}^{N} z_r^4 - (\frac{1}{N} \sum_{s=1}^{N} z_s^2)^2]$$

$$= \frac{1}{N^2} [\sum_{r=1}^{N} \{ z_r^2 - (\frac{1}{N} \sum_{s=1}^{N} z_s^2) \}^2]$$

$$= \frac{1}{N^2} \sum_{r=1}^{N-1} w_r \,, \text{ by Theorem 7.3.} \qquad \text{H}$$

Lemma 7.2.

If $R = U_{u=1}^{p} R_u$ and the R_u are all disjoint, and

$$T_u = \frac{T}{\mathrm{vol}(R)} \mathrm{vol}(R_u) \qquad (u=1,\ldots,p); \tag{7.12}$$

then

$$\sum_{u=1}^{p} T_u = T.$$

Proof:

$$\sum_{u=1}^{p} T_u = \frac{T}{\mathrm{vol}(R)} \sum_{u=1}^{p} \mathrm{vol}(R_u) = \frac{T}{\mathrm{vol}(R)} \mathrm{vol}(R) . \qquad \text{H}$$

8. THE MCSS ALGORITHM

With the basic notation and theorems at hand, we are now prepared to describe the MCSS algorithm.

The MCSS Algorithm for Crude, Control Variate, and Antithetic Variate Estimators with Bisection-Type Stratification

Main Program

1) [Read input parameters] Read k, a_i,b_i for i=1,...,k, ε, t_α, FC, c, MAXm, m_o, Δm, t, MAXLEV, NOSTOP, NCA, NPTMIN, TIMAX;

(k =the dimensionality of the integral,

(a_i,b_i)=the ith side of the k-cell R, the region of integration, for i=1,...,k,

ε =the desired error bound,

t_α =the desired number of standard deviations for the confidence interval,

FC =the number of multiplications and divisions to evaluate $f(\underline{x})$,

c =the number of coordinate axes in which bisection of a stratum will be performed, $1 \leq c \leq k$,

MAXm =the maximum number of samples that will be drawn before applying the stopping rules and the decision rule,

m_o =the initial number of samples,

Δm =the increment, so that $m \leftarrow m+\Delta m$,

t =the type of estimator, C, CV, or A,

MAXLEV =the maximum length of the strata storage LIFO lists,

NOSTOP =nonnegative integer such that if $vol(R_i)/vol(R) > (1/2)^{NOSTOP}$ we do not stop, but continue to stratify R_i,

NCA =0, when random choice of coordinates desired, =1 when coordinates are to be chosen in a cyclic manner, (if c=k, the value of NCA is ignored),

NPTMIN =the minimum number of points to be used in sampling directly,

TIMAX =the maximum amount of time, in seconds, to be used in sampling directly)

2) [Echo check on data] Print input parameters;

3) Call MCSS with the above input parameters and return the estimate $\hat{\theta}$, of θ and the estimate of one-half of the confidence interval, $t_\alpha \cdot s(\hat{\theta})$;

4) [If control variate estimator desired, then add its integral to the estimator] Read Φ; If $\Phi \neq 0$, $\hat{\theta} \leftarrow \theta + \Phi$;

5) Print out $\hat{\theta}$, $t_\alpha \cdot s(\hat{\theta})$, ε.

Subroutine MCSS (R, k, ε, t_α, FC, c, MAXm, m_o, Δm, t, MAXLEV, NOSTOP, NCA, NPTMIN, TIMAX, $\hat{\theta}$, $s(\hat{\theta})$)

Input: $R = \{\underline{x} : a_i < x_i < b_i, i=1,\ldots,k\}$, k,..., TIMAX are input parameters defined in the main program.

Output: $\hat{\theta}$ the estimate of θ and $s(\hat{\theta})$ the estimate of the standard error of $\hat{\theta}$.

(This subroutine performs the sequential bisection type stratification.)

1) [Calculate labor ratio constants] $\ell_o \leftarrow 4k+FC+4$; ($\ell_o$= labor constant for direct sampling) $\ell_{s1} \leftarrow 40.6c + .6$; $\ell_{s2} \leftarrow 134c + 20$; ($\ell_{s1}$ and ℓ_{s2} are labor constants for stratified sampling. The derivation of these values will be shown in the next section.)

2) [Initialize] NPTTOT←0; (NPTTOT=the running sum of the total number of samples) $\hat{\theta} \leftarrow 0$; ($\hat{\theta}$ = estimate of θ) $s^2(\hat{\theta}) \leftarrow 0$; ($s^2(\hat{\theta})$ = estimate of var($\hat{\theta}$)) LEVEL ←0; (LEVEL = the pointer which indicates the last element on the last-in-first-out (LIFO) lists which store the information saved on the previously examined strata.) TOL←ε^2/t_α^2 ; TOLI ←TOL;

3) Call VOLTOL (R,k,VOLRJ,TOLI,1); (R={x: $a_i<x_i<b_i$, i=1,...,k}, a k-cell, the region of integration, vol(R) = $\int_R \underline{dx}$, and TOLI = ε^2/t_α^2)

4) If c=k, go to (5);

   4.1) If NCA=0, pick c coordinate directions at random and without repetitions, store in NDIR(i), i=1,...,c;

   4.2) If NCA=1, pick c coordinate directions in cyclic fashion, that is for i=1,...,c do (NDIR(i)←(NCA-1) mod(k); NCA←NCA+1;)

5) If LEVEL=0, MAXm ←2·MAXm ; (This doubles the upper bound on the number of samples needed for stopping and decision rules. The effect is to provide a larger sample size in the strata in

which the variance of the estimator is large. As will be shown later, the strata in which the variance is large, are stored first and worked on last. Thus, when LEVEL=0 we will be working on that stratum with the largest variance. Initially, this stratum is R.)

6) [Initialize] $\hat{v}(s^2) \leftarrow 0$; ($\hat{v}(s^2)$=the estimate for var($s_o^2$)) $N \leftarrow 0$; (N= the running total of the number of samples taken in a given region) $m \leftarrow m_o$; (m = the number of samples to be used in applying the stopping and decision rules)

7) [Sample size loop] $n_o \leftarrow 2 \cdot m$; (n_o = the sample size for each of the 2c strata of the given partition) $\Sigma s_o^2 \leftarrow 0$;

8) [Coordinate direction loop] For j=1,...,c, do the following:

8.1) If c=k, JDIR$\leftarrow$j;

8.2) If c<k, JDIR$\leftarrow$NDIR(j);

8.3) Call MEANVR (R_o,k,m,Δm,JDIR,N,$\hat{\theta}_1$(JDIR),$\hat{\theta}_2$(JDIR),s_1^2(JDIR), s_2^2(JDIR),v(s^2),$\hat{Q}$(JDIR); (R_o={ $\underline{x}$: $a_i<x_i<b_i$, i=1,...,k } and MEANVR returns the values θ_1, θ_2, s_1^2, s_2^2, v(s^2) and $\hat{Q}$)

8.4) s^2(JDIR)$\leftarrow(2-\frac{1}{m})(s_1^2(\text{JDIR})+s_2^2(\text{JDIR}))+((\hat{\theta}_1(\text{JDIR})-\hat{\theta}_2(\text{JDIR}))/n_o)^2 + \hat{Q}(\text{JDIR})/n_o$; (Here we are applying Theorem 7.2, to compute s_o^2 .)

8.5) $\Sigma s_o^2 \leftarrow s^2(\text{JDIR}) + \Sigma s_o^2$;

9) $s^2 \leftarrow \Sigma s_o^2/c$; $N \leftarrow N+2c \cdot m$;

10) [Apply the second stopping rule (5.8) to determine if additional samples are necessary to achieve a better estimate of the variance.] If LEVEL=0, $\lambda \leftarrow 3$; If LEVEL$\neq$0, $\lambda \leftarrow 2$; (See the note following (5).) If $v(s^2) < (TOLI/\lambda^2)$, go to (12);

11) $m \leftarrow \Delta m + m$; If $m < MAXm$, go to (7);

12) $\Sigma\hat{\theta}_o \leftarrow 0$; VOL$\leftarrow$VOLRJ/2; NPTTOT N + NPTTOT; DELMAX$\leftarrow$ -1.0; MAXDIR $\leftarrow$ 0;

13) [Compute estimates] For j=1,...,c, do the following:

13.1) If c=k, JDIR$\leftarrow$j;

13.2) If c<k, JDIR$\leftarrow$NDIR(j);

13.3) $\hat{\theta}_1(JDIR) \leftarrow \hat{\theta}_1(JDIR)$ VOL/m;
$\hat{\theta}_2(JDIR) \leftarrow \hat{\theta}_2(JDIR)$ VOL/m;
$s_1^2(JDIR) \leftarrow s_1^2(JDIR)$ $(VOL)^2/(m-1)$;
$s_2^2(JDIR) \leftarrow s_2^2(JDIR)$ $(VOL)^2/(m-1)$;
$s^2(JDIR) \leftarrow s^2(JDIR)$ $(VOLRJ)^2$;

13.4) $\Sigma\hat{\theta}_o \leftarrow \hat{\theta}_1(JDIR) + \hat{\theta}_1(JDIR) + \Sigma\hat{\theta}_o$; (See Theorem 7.1.)
$s_1 \leftarrow [SS1(JDIR)]^{1/2}$; $s_2 \leftarrow [SS2(JDIR)]^{1/2}$;

13.5) [Find the coordinate direction, JDIR, where the bisection type stratification yields the largest reduction in the labor needed for the estimator.] If DELMAX $\geq s^2(JDIR)/(s_1+s_2)^2$, go to (13.3);

13.6) DELMAX$\leftarrow s^2(JDIR)/(s_1+s_2)^2$; MAXDIR$\leftarrow$JDIR; $\hat{\theta}_1 MAX \leftarrow \hat{\theta}_1(JDIR)$; $\hat{\theta}_2 MAX \leftarrow \hat{\theta}_2(JDIR)$; $S_1^2 MAX \leftarrow s_1^2(JDIR)$; $S_1^2 MAX \leftarrow s_1^2(JDIR)$;

14) $s^2(\hat{\theta}_o) \leftarrow s_o^2/N$; ($s^2(\hat{\theta}_o)$ = the estimate of the variance of the estimator, $\hat{\theta}_o$.) $v(s^2) \leftarrow v(s^2) \cdot ((VOL)^2/N)^2$;

15) [Calculate the upper bound for the confidence interval for the variance of the estimator, see (5.4)] $s^2(\hat{\theta}_o) \leftarrow s^2(\hat{\theta}_o) + \lambda^2 \cdot v(s^2)/N$; $s_o^2 \leftarrow s^2(\hat{\theta}_o) \cdot N$;

16) If VOLRJ/VOLR $>(1/2)^{NOSTOP}$, go to (29);

17) [Stopping Rule, see (3.8)] If $s^2(\hat{\theta}_o) >$ TOLI, go to (23);

18) [No additional points needed, add new estimate to the previous one.] $\hat{\theta} \leftarrow \hat{\theta} + \hat{\theta}$; $s^2(\hat{\theta}) \leftarrow s^2(\hat{\theta}_o) + s^2(\hat{\theta})$;

19) [Are we done?] If LEVEL=0, go to (35);
(A "true" response indicates that there is no more information stored on the previously examined strata, i.e. we have examined all of them.)

20) [Not finished, retrieve the information on the next stratum in the LIFO lists.] For j=1,...,k, do ($a_j \leftarrow A_j$(LEVEL); $b_j \leftarrow B_j$(LEVEL);) $\hat{\theta}_1$MAX$\leftarrow$E(LEVEL); S_1^2MAX$\leftarrow$V(LEVEL); m$\leftarrow$K(LEVEL); (for the definitions see step (30))

21) [Move pointer] LEVEL$\leftarrow$LEVEL-1; (This has the effect of "erasing" the last pieces of information stored on the LIFO lists.)

22) Call VOLTOL (R_o, k, VOLRJ, TOLI, 2); ($R_o = \{\underline{x} : a_i \leq x_i < b_i$, i=1,...,k }, the values VOLRJ = vol(R_o), TOLI=vol(R_o)/vol(R)$\cdot \varepsilon^2/t_\alpha^2$ are returned) go to (32);

23) [Calculate the number of points needed to achieve the desired accuracy] NPT$\leftarrow s_o^2$/TOLI; $n_s \leftarrow (s_1+s_2)^2$/TOLI;

24) [Calculate the labor ratio] $L \leftarrow 1 + 2.m/n_s(2c-1) + (2m/n_s\ell_{s1} + \ell_{s2}/n_s)/(\ell_o+(k+10)/(NPT-N))$;

25) [Decision rule] If DELMAX >L, go to (29);

26) NPT←NPT-N; If NPT > TIMAX·10^5, go to (29); (This is a check to see if bisection might be advantageous later, even though the decision rule did not recommend it now. When NPT is so large, little extra labor is lost.)

27) [Don't stratify, calculate the estimates using direct sampling] Call CRUDMC (R_o, k, VOLRJ, TOLI, t, NPT, N, s_o^2, θ', $s^2(\hat{\theta}_o)$);

28) $\hat{\theta}_o \leftarrow (\theta'$ VOLRJ + $\hat{\theta}_o \cdot n_o)/(NPT + N)$; NPTTOT←NPT+NPTTOT; go to (18);

29) If LEVEL>MAXLEV, go to (27); If (VOLRJ/VOLR)< 10^{-8}, go to (27); (sample directly if store level overflow or vol(R_o) very small)

30) [Begin stratification procedure; save information on the stratum where the variance is the larger and set up the other stratum.] LEVEL←LEVEL+1; For i=1,...,k, do the following:

30.1) A_i(LEVEL)←a_i; B_i(LEVEL)←b_i;

30.2) If i ≠ MAXDIR, go to (30.1);

30.3) If $s_1^2(i) > s_2^2(i)$, go to (30.7);

30.4) A_i(LEVEL)← $\frac{1}{2}$ (a_i+b_i);

30.5) E(LEVEL)←$\hat{\theta}_2$MAX; V(LEVEL)← s_2^2MAX;

30.6) $b_i \leftarrow A_i$(LEVEL);

30.7) $B_i(\text{LEVEL}) \leftarrow \frac{1}{2}(a_i + b_i)$;

30.8) $E(\text{LEVEL}) \leftarrow \hat{\theta}_1\text{MAX}$; $V(\text{LEVEL}) \leftarrow S_1^2\text{MAX}$;

30.9) $a_i \leftarrow B_i(\text{LEVEL})$; $\hat{\theta}_1\text{MAX} \leftarrow \hat{\theta}_2\text{MAX}$; $s_1^2\text{MAX} \leftarrow s_2^2\text{MAX}$;

31) $K(\text{LEVEL}) \leftarrow m$; Call VOLTOL($R_o$, k, VOLRJ, TOLI, 3);

32) [Is the new stratum within desired accuracy?] $s^2(\hat{\theta}_o) \leftarrow s_1^2\text{MAX}/m$;
If $(\text{VOLRJ/VOLR}) > (\frac{1}{2})^{\text{NOSTOP}}$, go to (4); If $s^2(\hat{\theta}_o) > \text{TOLI}$, go to (4);

33) [New stratum within desired accuracy.] $\text{NPT} \leftarrow n_o \cdot c - m$;
(sample directly at least NPT more points in the new stratum)
Call CRUDMC (R_o, k, NPT, m, $S_1^2\text{MAX}$, θ', $s(\hat{\theta}_o)$)

34) $\hat{\theta}_o \leftarrow (\theta' \cdot \text{VOLRJ} + \hat{\theta}_1\text{MAX} \cdot m)/(\text{NPT}+m)$; $\text{NPTTOT} \leftarrow \text{NPTTOT}+m$;
go to (18)

35) $s(\hat{\theta}) \leftarrow [s^2(\hat{\theta})]^{1/2}$; return.

Subroutine MEANVR (R_o, k, m_o, Δm, m, JDIR, N, $\hat{\theta}_1(\text{JDIR})$, $\hat{\theta}_2(\text{JDIR})$, $s_1^2(\text{JDIR})$, $s_2^2(\text{JDIR})$, $\hat{v}(s^2)$, $\hat{Q}(\text{JDIR})$)

Input: $R_o = \{\underline{x}: a_i < x_i < b_i,\ i=1,\ldots,k\}$, k is the dimension of the space, $\hat{\theta}_1$, $\hat{\theta}_2$, s_1^2, s_2^2, $\hat{Q}$ are the running sums of the estimates when the bisection is made on the coordinate axis, JDIR, v(s) is the running sum of the estimate of var(s^2).

Output: $\hat{\theta}_1$, $\hat{\theta}_2$, s_1^2, s_2^2, $v(s^2)$, $\hat{Q}$.

1) i←JDIR; CJ ← $\frac{1}{2}$ (a_i+b_i); HALF←CJ-a_i; If m>m_o,go to (3);

2) [Initialize totals] $\hat{\theta}_1$← 0; $\hat{\theta}_2$← 0; s_1^2 ←0; s_2^2 ←0;
$\hat{Q}$(JDIR)← 0; KK←m_o; KL←0; go to (4);

3) [Not first time] KK←Δm; KL←m-Δm; If t=A, KL ← $\frac{1}{2}$ KL;

4) If t=A, KK ← $\frac{1}{2}$ KK; (For the antithetic variate we will go half as many times thru the loop, because there are twice as many function evaluations for the estimator.)

5) For j=1,...,KK do the following:

5.1) Call RANPT (R_o,JDIR, 1, HALF, CJ, k, t, $\underline{\xi}$);
Y1←F($\underline{\xi}$,k);

5.2) If t=C, go to (5.4);

5.3) Call ANTHET (R_o,JDIR,1,HALF,CJ,k,t,$\underline{\xi}$);
YA1←F($\underline{\xi}$,k);

5.4) Call RANPT (R_o, JDIR, 2, HALF, CJ, k, t, $\underline{\xi}$);
Y2 ← F($\underline{\xi}$, k);

5.5) If t=C, go to (5.8);

5.6) Call ANTHET (R_o, JDIR, 2, HALF, CJ, k, t, $\underline{\xi}$);
YA2 ← F($\underline{\xi}$, k);

5.7) Q(JDIR) ← (Y1-Y2)·(YA2-YA1) + Q(JDIR);
Y1 ← Y1 + YA1; Y2 ←Y2 + YA2; (see Theorem 7.2)

5.8) N ←N + 2; If t=A, N←N+2;

5.9) If j=1, go to (5.11); If KM< 0, go to (5.11);

5.10) KP ← KM + 1; $v(s^2)$ ←$v(s^2)$ + (KM · (Y1-$\hat{\theta}_1$/KP)^2- s_1^2)^2/(KM·KP)+ (KM·(Y2-$\hat{\theta}_2$/KP)^2- s_2^2)^2/(KM·KP); (This uses the corollary to Theorem 7.3.)

5.11) KM←KL+j-1; If KM≤0, go to (5.13); KP←KM+1;

5.12) $s_1^2 \leftarrow s_1^2 + (KM \cdot Y1 - \hat{\theta}_1)^2/(KM \cdot KP)$; $s_2^2 \leftarrow s_2^2 +$ $(KM \cdot Y2 - \hat{\theta}_2)^2/(KM \cdot KP)$; (This uses Theorem 7.3, the Helmert Transformation.)

5.13) $\hat{\theta}_1 \leftarrow \hat{\theta}_1 + Y1$; $\hat{\theta}_2 \leftarrow \hat{\theta}_2 + Y2$;

6) Return.

Subroutine VOLTOL (R_o, k, VOLRJ, TOLI, IGOTO)

Input: $R_o = \{ \underline{x} : a_i \leq x_i < b_i, i=1,\ldots,k \}$, IGOTO = 1,2,or 3, if IGOTO=1, then TOLI = $(\varepsilon/t_\alpha)^2$.

Output: VOLRJ = $\int_{R_o} \underline{dx}$ and TOLI = the desired tolerance of R_o.

1) If IGOTO = 3, go to (3)

2) VOLRJ ←1; For i=1,...,k, do VOLRJ ←VOLRJ $\cdot (b_i - a_i)$; go to (4);

3) VOLRJ ← $\frac{1}{2}$ VOLRJ; (Since we just bisected stratum, the volume of it is halved.) go to (5);

4) If IGOTO ≠ 1, go to (5); TOL ←TOLI; VOLR← VOLRJ; return.

5) If (VOLRJ/VOLR) > .001, TOLI ← TOL · (VOLRJ/VOLR);
If (VOLRJ/VOLR) < .001, TOLI ←.001 · TOL; (Without this last condition, the tolerance for such values of vol(R_o) proved in practice, to be much too strict.) return.

Subroutine CRUDMC (R_o, k, VOLRJ, TOLI, g, NPT, N, s_o^2 , θ', $s^2(\hat{\theta}_o)$)

Input: $R_o = \{x : a_i<x_i<b_i, i=1,...k\}$, k, VOLRJ, TOLI, t= C or A, NPT = size of the sample before applying the stopping rule, N, s_o^2, $s^2(\hat{\theta}_o)$, TIMAX = maximum time allotted, in seconds.

Output: θ', $s^2(\hat{\theta}_o)$. (the direct sampling estimates)

(This algorithm determines the estimates by using Anscombe's sequential scheme [ANF])

1) TIMEON←TIME; (get the starting time and store it)

2) [Initialize] θ'←0; SSQ←0; NTIMES = 0;

3) If NPT<1, return; If t=A, NN←NPT/2; If t=C, NN←NPT;

4) For i=1,..., NN, do the following:

4.1) Call RANPT (R_o, 0, 0, 0, 0, k, t, $\underline{\xi}$);

4.2) Y ← F($\underline{\xi}$, k);

4.3) If t=C, go to (4.6);

4.4) Call ANTHET (R_o, 0, 0, 0, 0, k, t, $\underline{\xi}$);

4.5) Y ←F($\underline{\xi}$, k) + Y;

4.6) NM ←i-1 + NTIMES · NN, NP←NM+1;

4.7) If NM<0, go to (4.9);

4.8) SSQ←SSQ + $(NM \cdot Y - \theta')^2/NP \cdot NM)$;

4.9) θ'← θ' + Y ;

5) NTIMES←NTIMES + 1; If NPT·NTIMES< NPTMIN, go to (4);

6) $s^2(\hat{\theta}_o) \leftarrow (s_o^2 \cdot N + SSQ \cdot (VOLRJ)^2)/(NPT \cdot NTIMES + N)^2$;

7) [Stopping Rule] If $s^2(\theta_o) \leq$TOLI, go to (11);

8) TIMTOT ← TIME - TIMEON;(elapsed time in seconds)

9) If TIMTOT < TIMAX, go to (4);

10) Print out error message: "time limit exceeded" ;

11) NPT ← NTIMES NPT; return.

Subroutine RANPT (R_o, JDIR, LOR, HALF, CJ, k, t, $\underline{\xi}$)

Input: R_o, JDIR, LOR = 1 or 2, CJ = $\frac{1}{2}(a_i+b_i)$ and HALF = $\frac{1}{2}(b_i-a_i)$, where i= JDIR, t=C or A.

Output: $\underline{\xi} = (\xi_1,\ldots,\xi_k)$ is the random point uniformly distributed on R_o.

1) j ← JDIR; AC ← a_j;

2) If LOR = 2 and t = A, go to (6);

3) If LOR = 2, AC ← CJ;

4) For i=1,...,k do the following:

4.1) If i=j, go to (4.3);

4.2) ξ_i ← RANUN · (b_i-a_i) + a_i; go to (4.4);

4.3) ξ_i ← RANUN · HALF + AC;

4.4) XS(i) ← ξ_i;

5) Return;

6) For i=1,...,k, do ξ_i ← XS(i);

7) ξ_j ← XS(j) + CJ - a_j; return.

Entry ANTHET

8) For i=1,...,k do the following:

8.1) If i=j and LOR=1, go to (8.3);

8.2) $\xi_i \leftarrow a_i + b_i$ - XS(i); go to (8.1);

8.3) If LOR=1, $\xi_i \leftarrow a_i +$ CJ - XS(i);

8.4) If LOR=2, $\xi_i \leftarrow$ CJ + b_i - XS(i);

9) Return.

Function RANUN

Output: A pseudo-random number approximately uniformly distributed on [0,1].

1) RANUN $\leftarrow$(RANUN $\cdot 5^{15} + 1$) mod $2^{35}/(2^{35}-1)$; return. (RANUN = 5^{13}, initially. The constants 5^{15} and 5^{13} are used because they are the "best" in the sense of producing a sequence with a high frequency wave length;see [COR-MAR])

Function F($\underline{\xi}$, k)

Input: $\underline{\xi} = (\xi_1,\ldots,\xi_k)$.

Output: F($\underline{\xi}$).

The user supplies the integrand f, if t=C or A then F$\leftarrow$ f($\underline{\xi}$), if t=CV, then F $\leftarrow$(f-ϕ)($\underline{\xi}$), where the control variate, ϕ, is supplied by the user.

9. STORAGE REQUIREMENTS AND THE LABOR RATIO FOR THE MCSS ALGORITHM

The storage requirements for the MCSS algorithm depend on the number of dimensions, k, of the region of integration and the maximum length, MAXLEV, of the lists storing the information on the substrata to be examined. In practice, MAXLEV = 25 has proven to be sufficiently large, however the user can increase this parameter if the problem requires more storage. Specifically, the MCSS algorithm requires

$$2 \cdot \text{MAXLEV}\ (k+1) + 7k + 250 \tag{9.1}$$

words. When MAXLEV = 25 and k = 10, the amount of storage needed is only 870 words. If k = 100, with MAXLEV as before, then 6,000 words would be needed. This amount of storage is not too large, since most of the modern computers have storage capacities of 32,000 words or more.

The formula for the labor ratio, L, is obtained by applying (4.31). Here, since we are using bisection, q=2 and since we are considering the bisection in c coordinate directions, p=2c. We let g be the number of essential operations (ops.) to generate a pseudo-random number, FC be the number of ops. to evaluate $f(\underline{x})$, and z be the number of ops. to take a square root of a given floating point number. It can be seen from the algorithm that

it takes:

$k \cdot g$ ops. to generate a random variable $\underline{\xi} = (\xi_1, \ldots, \xi_k)$,

FC ops. to evaluate the integrand there, *

4 ops. to update the sum of squares,

$k + 10$ ops. to calculate the hypervolume of the region of integration and compute the mean and variance of the estimator.

Therefore,

$$\ell = k \cdot g + FC + 4 + (k+10)/(n_o - 2cm), \tag{9.2}$$

where $(n_o - 2cm)$ is the number of samples drawn <u>after</u> applying the stopping rules and 2cm is the number <u>before</u> applying them.

Now, in doing bisection-type stratification at c coordinate axes, we can see that it takes:

10 cm ops. to compute the sum of squares that is in the estimator of $\text{var}(s^2)$,

$2m/\Delta m$ ops. to apply the second stopping rule,

$(3c+1)m/\Delta m + 5c + 10$ ops. to calculate s_o^2 and $s^2(\hat{\theta}_u)$,

$2(cz+c)$ ops. to apply the decision rule,

$4c(10+z)$ ops. to set up the strata for the decision rule. *

Hence, if $\Delta m = 10$, and as on the Univac 1108 $g=4$ and $z=10$,

$$qr+e = 2r+e = 40.6 \text{ cm} + .6m + 134c + 20 . \tag{9.3}$$

* See the footnote on page 41.

By (4.31), (9.2), and (9.3) we obtain that the labor ratio

$$(9.4) \qquad L = 1 + \frac{1}{n_s}\,[2(2c-1)m + (40.6\ cm + .6m + 134c + 20)\ /$$

$$\{4k + FC + 4 + (k+10)/(n_o - 2cm)\}]\ ,$$

where n_s is the number of samples for stratification.

10. NUMERICAL RESULTS

The MCSS algorithm was applied to the problem to evaluating various different types of multiple integrals. This section is devoted to interpreting and displaying the results obtained from applying the algorithm. In addition, comparisons will be made with other known procedures. The following experiments were run on the Univac 1108 computer at the University of Wisconsin Computing Center.

Example 1: $\int_0^1 \int_0^1 4\, x_1\, x_2\, dx_1\, dx_2 = 1$

In the first experiment, the crude estimator was used along with the following input parameters: $m_o = 50$, $\Delta m = 10$, MAXm=250, c=2, NOSTOP=0, NCA=0, NPTMIN=0 (i.e., the NOSTOP, NCA, and NPTMIN options were not used) $\varepsilon = .01$, $t_\alpha = 1.0$, FC = 3, TIMAX = 1 second.

Let us notice that the function $4\, x_1\, x_2$ is symmetric about the line $x_1=x_2$ and increases monotonically along that line from $x_1=x_2=0$ to $x_1=x_2=1$. The level curves of the integrand are shown in Figure 10.1. The MCSS procedure stratified the region of integration as indicated in Figure 10.2. Notice that the partitions are symmetric about the line $x_1=x_2$; this corresponds to the behavior of the integrand.

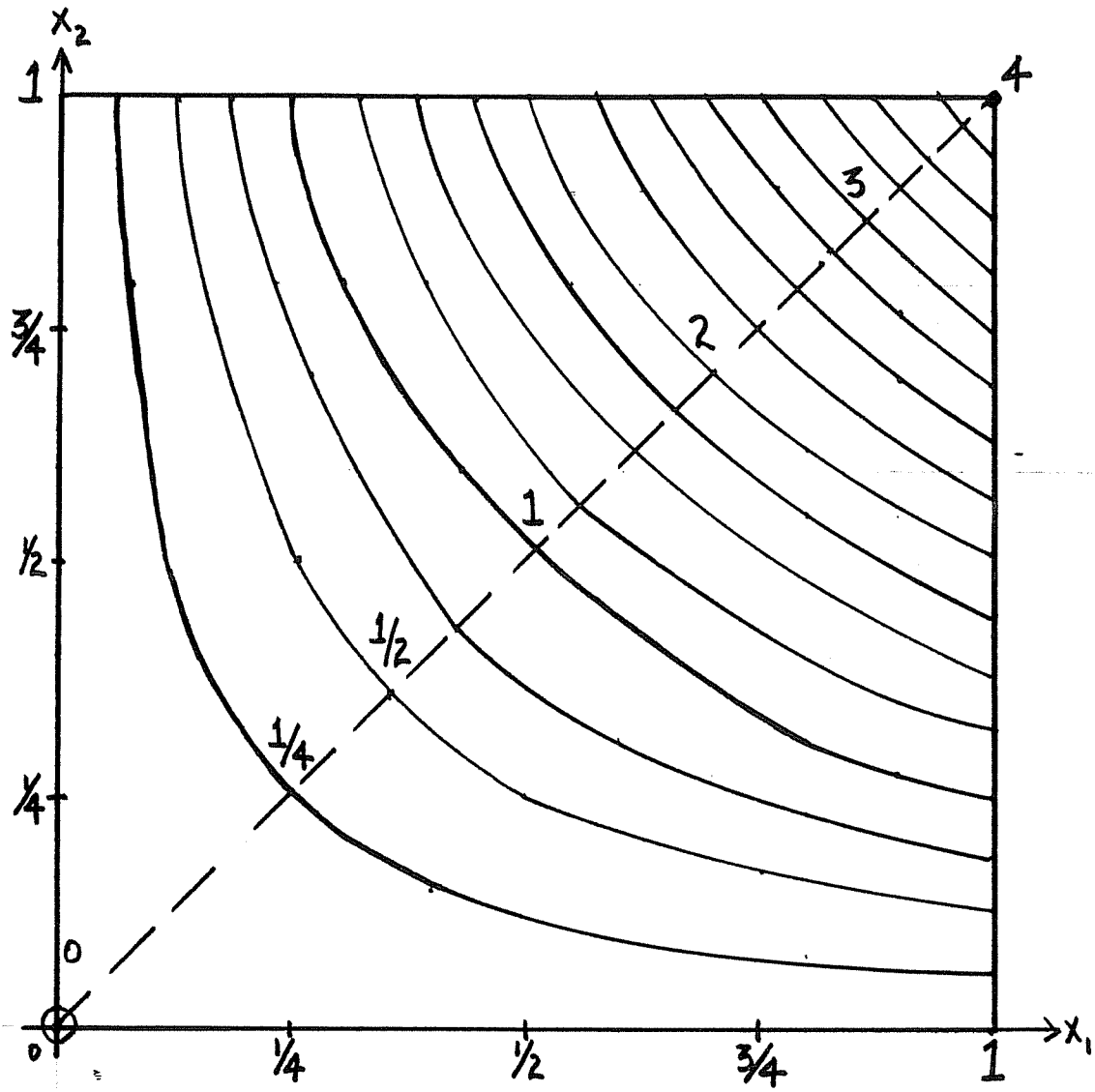


Figure 10.1: The integrand $4x_1x_2$

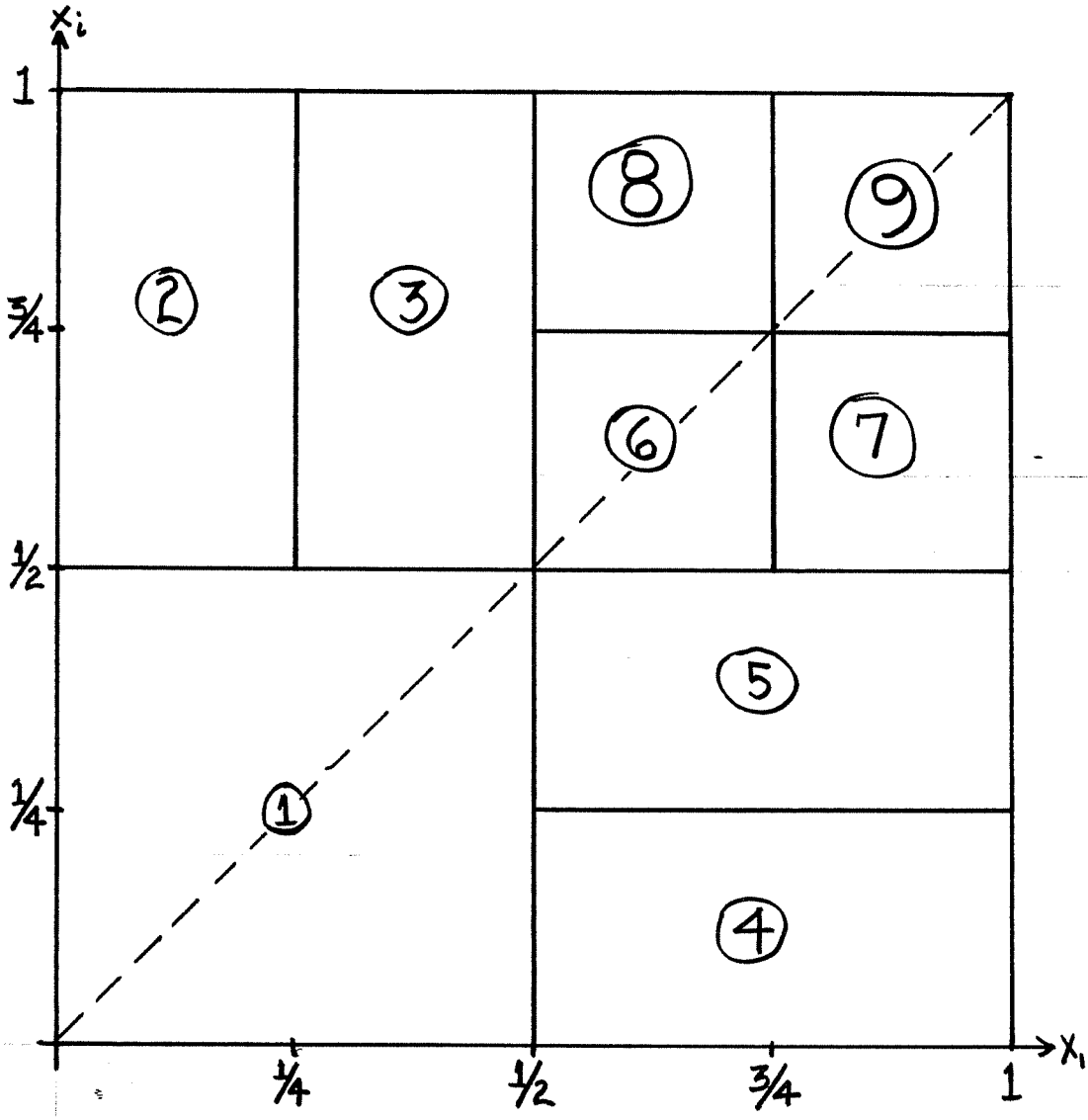


Figure 10.2: The stratification

We will now examine, in detail, just exactly how the MCSS procedure arrived at this partition. First, one word about the notation. We will denote a stratum $R_o = \{ \underline{x} : a_i \leq x_i \leq b_i, i=1,2 \}$ by $(a_1,b_1) \times (a_2,b_2)$.

Starting with $R_o = (0,1)x(0,1)$ and bisecting along the coordinate x_1, we have that

$R_1(1) = (0,\frac{1}{2})x(0,1)$ $\qquad$ $R_2(2) = (\frac{1}{2},1)x(0,1)$

$\hat{\theta}_1(1) = .232$ $(\theta_1(1) = .25)$ $\qquad$ $\hat{\theta}_2(1) = .766$ $(\theta_2(1)=.75)$

$s_1^2(1) = .0334$ $(\text{var}(\tau_1)=.0486)$ $\qquad$ $s_2^2(1) = .167$ $(\text{var}(\tau_2)=.215)$

$s_o^2(1) = .682$ $(\text{var}(\hat{\theta}_o)=.778)$

Bisecting along x_2, we have similarly:

$R_2(2) = (0,1)x(0, \frac{1}{2})$ $\qquad$ $R_2(2) = (0.1)x(\frac{1}{2},1)$

$\hat{\theta}_1(2) = .276$ $(.25)$ $\qquad$ $\hat{\theta}_2(2) = .730$ $(.75)$

$s_1^2(2) = .0491$ $(.0486)$ $\qquad$ $s_2^2(2) = .163$ $(.215)$

$s_o^2(2) = .625$ $(.778)$

The second stopping rule was satisfied with N=200, so that $m=m_o=50$ for each stratum. Now apply the stopping rule, we see that

$$s^2(\hat{\theta}_o) = .55 \times 10^{-2} > T = 10^{-4};$$

so we don't stop.

The coordinate x_1 yields the greatest value of the ratio $s_o^2(i)/(s_1(i) + s_2(i))^2$, i=1,2. (Theoretically, the ratio is identical for i=1,2 and equals 1.66). Since $s_o^2(1)/(s_1(1) + s_2(1))^2 =$ 1.95 and the labor ratio L=1.04, stratification along the coordinate x_1 is recommended.

Next, we store the information from the stratum $R_2(1)$, since $s_1^2(1) < s_2^2(1)$. Now, we set $R_o = R_1(1)$ and bisect along x_1, we get

$R_1(1) = (0,\frac{1}{4}) \times (0,1)$ $\qquad$ $R_2 = (\frac{1}{4}, \frac{1}{2}) \times (0,1)$

$\hat{\theta}_1(1) = .0558 \quad (.0625)$ $\qquad$ $\hat{\theta}_2(1) = .158 \quad (.1875)$

$s_1^2(1) = .301 \times 10^{-2} \quad (.304 \times 10^{-2})$ $\qquad$ $s_2^2(1) = .821 \times 10^{-2} \quad (.135 \times 10^{-1})$

$s_o^2(1) = .0327 \quad (.0481)$

Bisecting along x_2, we have

$R_1(2) = (0,\frac{1}{2}) \times (0,\frac{1}{2})$ $\qquad$ $R_2(2) = (0,\frac{1}{2}) \times (\frac{1}{2},1)$

$\hat{\theta}_1(2) = .0808 \quad (.0625)$ $\qquad$ $\hat{\theta}_2(2) = .197 \quad (.1875)$

$s_1^2(2) = .335 \times 10^{-2} \quad (.304 \times 10^{-2})$ $\qquad$ $s_2^2(2) = .985 \times 10^{-2} \quad (.135 \times 10^{-1})$

$s_o^2(2) = .0400 \quad (.0481)$

Again, N=200 satisfies the second stopping rule; for the other stopping rule we have that $s^2(\hat{\theta}_o) = .388 \times 10^{-3} > .5 \times 10^{-4} = \frac{1}{2} T$. Hence we do not stop. The ratio $s_o^2(i)/(s_1(i) + s_2(i))^2$ is greatest for i=2, although theoretically they are the same. Applying the

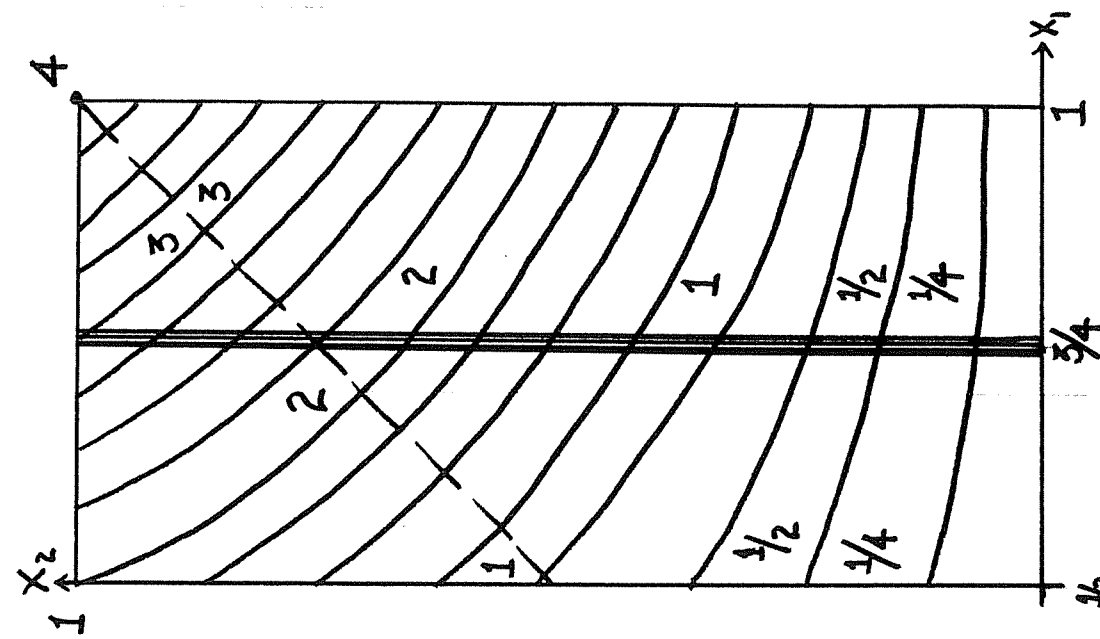


Figure 10.4: Bisecting along x_1

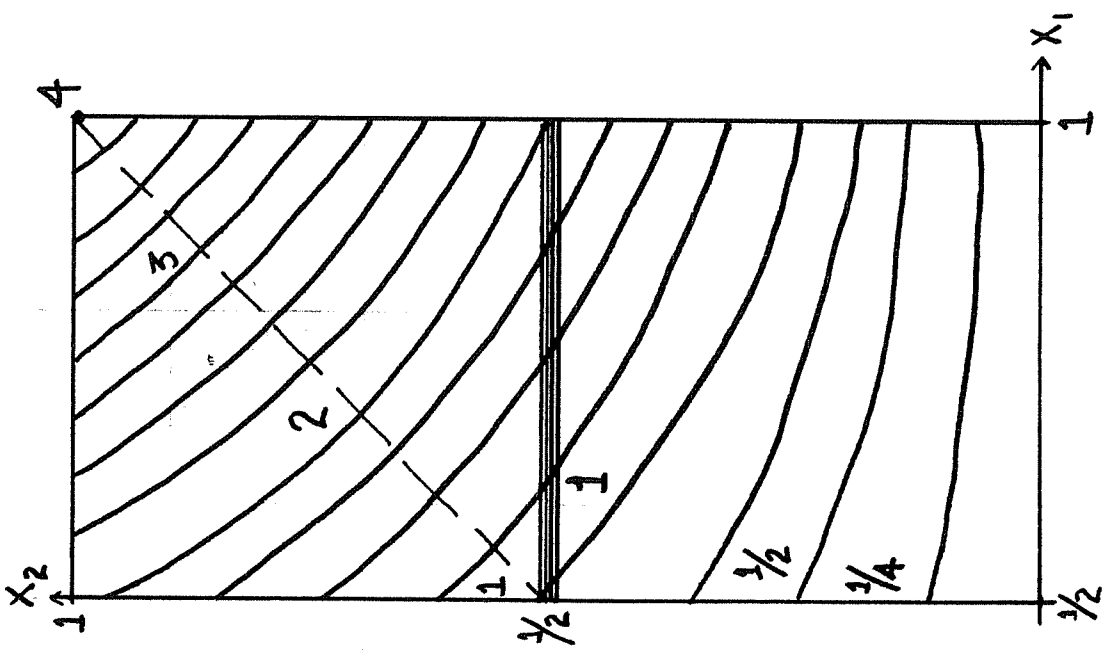


Figure 10.3: Bisecting along x_2

decision rule yields that stratification is recommended.

The stratum with the large sample variance $(0,\frac{1}{2})x(\frac{1}{2},1)$ is stored and we now sample from $(0,\frac{1}{2})x(0,\frac{1}{2})$. For this stratum the stopping rule does not suggest stopping, but the decision rule does not recommend stratifying. So we sample directing using the crude estimator to get the estimate $\hat{\theta}_1$=.0662 (θ_1=.0625).

We proceed to retrieve the last stratum stored $(0,\frac{1}{2})x(\frac{1}{2},1)$. The stopping and decision rules suggest bisecting forming the strata labeled 2 and 3 in Figure 10.2. Since the stopping rule is satisfied for each of the strata, we add their estimate $\hat{\theta}_2$=.0473 (.0469) and $\hat{\theta}_3$=.143 (.141) to the running sum, $\Sigma_{u=1}^{3}\ \theta_u$=.256 (.250).

So far, the region $(0,\frac{1}{2})x(0,1)$ has been estimated. This leaves the stratum $(\frac{1}{2},1)x(0,1)$. The decision process indicates bisection along the coordinate x_2. (This agrees with the theoretical result.) This time, there is a clear advantage to stratify along x_2. Let us see why.

Intuitively, we can see that bisecting along x_2 splits the region $(\frac{1}{2},1)x(0,1)$ into one stratum with lower values of the integrand than the other stratum (see Figure 10.3),while bisecting does not. (See Figure 10.4.) Notice, too, that the bisection along x_2 partitions $(\frac{1}{2},1)x(0,1)$ into two strata such that the value of the integrand increases more rapidly in one than in the other; while if we bisect along x_1, this difference is not as great.

Theoretically, if we bisect along x_2 we get:

$\theta_1(2) = .1875$ $\theta_2(2) = .5625$

$var(\tau_1(2)) = .01345$ $var(\tau_2(2)) = .0239$

Whereas, bisecting along x_1 we have:

$\theta_1(1) = .3125$ $\theta_2(1) = .4375$

$var(\tau_1(1)) = .034$ $var(\tau_2(1)) = .066$

First, we notice that $|\theta_1(2) - \theta_2(2)| < |\theta_1(1) - \theta_2(1)|$ and, secondly, $var(\tau_1(2)) + var(\tau_2(2)) < var(\tau_1(1) + var(\tau_2(1))$.

Going next to the region $(\frac{1}{2},1)x(0,\frac{1}{2})$, the program bisects it along x_2. (Theoretically, there is no preference.) Then each one is sampled directly. (See Figure 10.2, strata 4 and 5.) The region that remains is $(\frac{1}{2},1)x(\frac{1}{2},1)$. This is first bisected along x_2. Then each half is bisected along x_1.

Finally, in the stratum $(\frac{3}{4},1)x(\frac{3}{4},1)$, the decision rule indicates that this region be sampled directly. The estimate obtained is $\hat{\theta}_9 = .1914$ ($\theta_9 = .1925$).

Adding θ_9 to the running sum, we get the estimate of θ, $\hat{\theta}_C = 1.007$ ($\theta=1$). The computed standard error is equal to .007 (actual s.e. = .0044) which is less than the desired error, $\varepsilon = .01$. The MCSS procedure took 5,182 samples; while it would take 40,000 samples, if we used the crude Monte Carlo estimator without stratification to achieve the same standard error.

In the next experiment we use the antithetic variate estimator defined in (6.14) to estimate $\theta = \int_0^1 \int_0^1 4x_1x_2dx_1dx_2$. Except for the type of estimator, we use the same input parameters as before. The partition of the region of integration is shown in Figure 10.5, and the results are presented in the following table:

u	$\hat{\theta}_{A,u}$	θ_u	$\lvert\hat{\theta}_{A,u}-\theta\rvert$	$s^2(\hat{\theta}_{A,u})$	n_u
1	.3111	.3125	.0014	$.347\text{x}10^{-5}$	450
2	.4372	.4375	.0003	$.334\text{x}10^{-5}$	450
3	.0615	.0625	.0010	$.399\text{x}10^{-5}$	450
4	.1881	.1875	.0006	$.382\text{x}10^{-5}$	450
Totals	.9979	1.0000	.0033	$.146\text{x}10^{-4}$	1800

Computed standard error = .0038 (actual s.e. = .003) number points needed if only direct sampling was used = 25,000.

The partition in this case is different from the crude case, because the antithetic variate transforms the integrand: see Section 6. Note, too, that $2\ \text{var}(\tau_A) = 2/9 < \text{var}(\tau_C) = 7/9$ so that, by Theorem 6.5, the antithetic variate estimator is more efficient than the crude estimator. The results of the experiment certainly indicate this, as well.

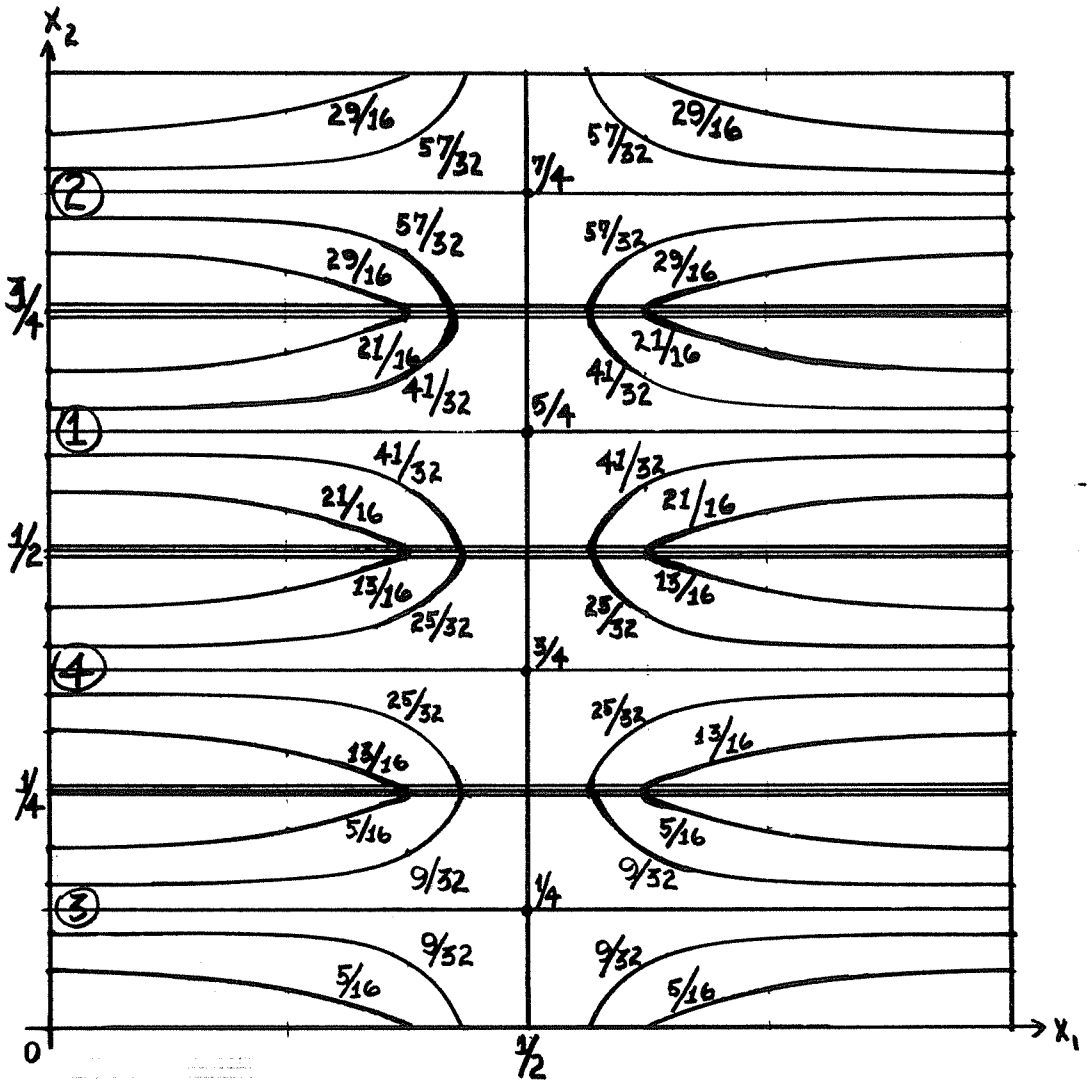


Figure 10.5. The Antithetic variate partition and the level curves of the transformed integrand.

Example 2: $\theta = \int_{U^{10}} \prod_{i=1}^{10} i\, x_i^{i-1}\, dx_i = 1.0$, where $U^{10} = \underset{i=1}{\overset{10}{X}} [0,1]$.

The integrand, in this example, ranges from 0 at (0,0,...,0) to 3.6×10^6 at (1,1,...,1) and is monotonically increasing along each coordinate x_i. Furthermore, since $\partial f/\partial x_i = i(i-1)x_i^{i-2} \prod_{j=1, j\neq i}^{10} x_j^{j-1}$, the rate of change for each variable x_i increases on U^{10} as i increases. This does play an important role in the choosing of coordinates to bisect.

In the first experiment we used the following input parameters: k=10, m_o=50, Δm=10, MAXm=150, c=10, t=A, NOSTOP=3, NCA=NPTMIN=0, ε=.1, t_α=1, FC=45, TIMAX=5. It should be noted that since $2\ \mathrm{var}(\tau_A) = 2.00 \times 10^4 < \mathrm{var}(\tau_C) = 2.01 \times 10^4$ there is only a slight advantage in using the antithetic estimator.

Table 10.1 shows the last ten strata chosen by the MCSS algorithm and their estimates. Notice that the coordinates x_1, x_2, x_3, x_4 and x_5 are bisected much less than the coordinates x_6, x_7, x_8, x_9, and x_{10}, and that x_8, x_9, and x_{10} are bisected more frequently than the others.

The stratification yielded the following results:

$\hat{\theta}_A = .944$ $\quad |\hat{\theta}_A - \theta| = .056$ $\quad \sum_{u=1}^{39} |\hat{\theta}_{A,u} - \theta_u| = .075$

number of strata = 39 number of samples = 205,677

Stratum	30	31	32	33	34	35	36	37	38	39
(a_1,b_1)	(0,1)									(0,1)
(a_2,b_2)	(0,1)		(0,1/2)	(1/2,1)	(0,1/2)		(1/2,1)			(1/2,1)
(a_3,b_3)	(1/2,1)									(1/2,1)
(a_4,b_4)	(1/2,1)									(1/2,1)
(a_5,b_5)	(1/2,3/4)		(3/4,1)							(3/4,1)
(a_6,b_6)	(3/4,1)		(1/2,3/4)		(3/4,1)					(3/4,1)
(a_7,b_7)	(3/4,1)									(3/4,1)
(a_8,b_8)	(3/4,1)							(3/4,7/8)	(7/8,1)	(7/8,1)
(a_9,b_9)	(3/4,1)				(3/4,7/8)	(7/8,1)	(3/4,1)		(3/4,7/8)	(7/8,1)
(a_{10},b_{10})	(3/4,7/8)	(7/8,1)	(3/4,1)				(3/4,7/8)		(7/8,1)	(7/8,1)
$\hat{\theta}_{A,u}$	.0197	.0708	.0192	.0529	.0206	.0658	.0581	.0501	.0368	.1136
θ_u	.0207	.0738	.0173	.0518	.0213	.0662	.0575	.0555	.0365	.1131
$\lvert\hat{\theta}_{A,u}-\theta_u\rvert$	.0010	.0030	.0019	.0011	.0007	.0004	.0006	.0054	.0003	.0005

Table 10.1 The last ten strata of the partition using the sample variance. (After stratum 30 only the interval where a change has been made is indicated, except in the last stratum.)

Stratum	34	35	36	37	38	39	40	41	42	43
(a_1,b_1)	$(0,1)$									$(0,1)$
(a_2,b_2)	$(0,1)$								$(0,\frac{1}{2})$	$(\frac{1}{2},1)$
(a_3b_3)	$(\frac{1}{2},1)$									$(\frac{1}{2},1)$
(a_4,b_4)	$(\frac{1}{2},1)$									$(\frac{1}{2},1)$
(a_5,b_5)	$(\frac{1}{2},\frac{3}{4})$	$(\frac{3}{4},1)$		$(\frac{1}{2},\frac{3}{4})$		$(\frac{3}{4},1)$				$(\frac{3}{4},1)$
(a_6,b_6)	$(\frac{1}{2},\frac{3}{4})$			$(\frac{3}{4},1)$						$(\frac{3}{4},1)$
(a_7,b_7)	$(\frac{3}{4},1)$									$(\frac{3}{4},1)$
(a_8,b_8)	$(\frac{3}{4},1)$							$(\frac{3}{4},\frac{7}{8})$	$(\frac{7}{8},1)$	$(\frac{7}{8},1)$
(a_9,b_9)	$(\frac{3}{4},1)$						$(\frac{3}{4},\frac{7}{8})$	$(\frac{7}{8},1)$		$(\frac{7}{8},1)$
(a_{10},b_{10})	$(\frac{3}{4},1)$	$(\frac{3}{4},\frac{7}{8})$	$(\frac{7}{8},1)$	$(\frac{3}{4},\frac{7}{8})$	$(\frac{7}{8},1)$	$(\frac{3}{4},\frac{7}{8})$	$(\frac{7}{8},1)$			$(\frac{7}{8},1)$
$\hat{\theta}_{A,u}$	.0186	.0157	.0537	.0200	.0810	.0770	.0665	.0507	.0365	.1156
θ_u	.0187	.0151	.0540	.0207	.0738	.0767	.0667	.0559	.0377	.1131
$\lvert\hat{\theta}_{A,u}-\theta_u\rvert$	.0001	.0006	.0003	.0007	.0072	.0003	.0002	.0052	.0012	.0025

Table 10.2 The last ten strata of the partition using the theoretically computed variance. (After stratum 34 only the interval where a change has been made is indicated, except in the last stratum.)

computed standard error = .017 (actual std. err. = .029)

number of samples needed to achieve the same actual standard error using direct sampling is approximately 22,000,000

This result demonstrates how powerful stratification can be compared to direct sampling. In this experiment, the MCSS procedure required 1/100th of the number of function evaluations needed to do a direct sampling antithetic variate procedure.

The above partition is only an approximation to the optimal one in the sense of (1.7). To find the optimum partition the MCSS program was run using the theoretically computed values of the variance of the estimator. Table 10.2 shows the final ten of these strata. Notice, first, that the last stratum here is the same as in the last experiment where we used the sample variance. Also, note that the coordinates x_8, x_9, and x_{10} are bisected more than the others.

An estimate of θ was taken using this partition and the theoretically computed variances. The results are:

$\hat{\theta} = .987$ $\quad |\hat{\theta} - \theta| = .013$ $\quad \sum_{u=1}^{43} |\hat{\theta}_u - \theta_u| = .066$

number of strata = 43 number of samples = 203,042

actual standard error = .023

As expected, this result is better than the previous one. But,

in comparing the actual standard errors and the number of samples in the two experiments we see that the MCSS procedure using the sample variances did indeed produce a partition very near the optimum one.

In order to compare the results of the MCSS procedure with other ones, two additional experiments were attempted. The first one consisted of using the crude Monte Carlo estimator and sampling uniformly from U^{10}. The results are:

$$\hat{\theta} = .733 \qquad |\hat{\theta}-\theta| = .267$$

number of samples = 415,00 computed standard error = .22

(actual std. err. = .11)

Notice that even though the number of samples used by this method is twice that of the MCSS method, the results are much worse.

The next experiment attempted to evaluate the integral by using the multiple numerical quadrature algorithm, NIMDQD, available at the University of Wisconsin Computing Center (see [TAL]). This is an adaptive and iterative scheme using Simpson's Rule recursively. The procedure partitions the region of integration according to the behavior of the integrand and iterates until the desired error bound is reached. However, one iteration for a multiple integral whose region of integration is a 10-cell requires $5^{10} = 9,765,625$ function evaluations. This would take at least 100 minutes on the Univac 1108, so that this experiment was never completed.

Example 3: $\theta = \int_{U^{20}} (\exp(x_1 x_2 \ldots x_{20}) - 1) dx_1 dx_2 \ldots dx_{20} = .953817 \times 10^{-6}$

where $U^{20} = X_{i=1}^{20}[0,1)$.

This example was taken from a paper by Handscomb [HAD]. The integrand is a smooth function, as was the integrand in the previous example, but differs from it in that the present integrand only ranges from 0 to e-1 ($\doteq$ 1.718).

The first experiment uses the following input parameters: k=20, m_o=50, Δm=10, MAXm=500, c=1, NCA=1, (this means that first x_1 is bisected and tested, then $x_2, \ldots,$ and after x_{20}, x_1 etc.) NOSTOP=5, NPTMIN=500, $\varepsilon = .1 \times 10^{-6}$, t_α=1, and TIMAX=5.
The antithetic variate estimator is used because 2 var(τ_A) = $.285 \times 10^{-9}$ >var(τ_c) = $.286 \times 10^{-9}$.

The results are:

$\hat{\theta}_A = .855 \times 10^{-6}$ $\quad$ $|\hat{\theta}_A - \theta| = .098 \times 10^{-6}$

$\sum_{u=1}^{55} |\hat{\theta}_{A,u} - \theta_u| = .198 \times 10^{-6}$ $\quad$ number of strata=55

number of samples = 80,206 $\quad$ computed standard error = $.501 \times 10^{-7}$

(actual standard error = $.496 \times 10^{-7}$) the number of samples need to achieve the same standard error by direct sampling = 115,000.

In the next experiment we increased the desired accuracy to $\varepsilon = .05\text{x}10^{-6}$ and increased the number of directions searched to $c = 10$, when they are picked randomly without repetitions (i.e. NCA=0). The results are:

$\hat{\theta}_A = .911\text{x}10^{-6}$ $\qquad$ $|\hat{\theta}_A - \theta| = .043\text{x}10^{-6}$

$\sum_{u=1}^{68} |\hat{\theta}_{A,u} - \theta_u| = .136\text{x}10^{-6}$ $\qquad$ number of strata = 68

number of samples = 234,352 $\qquad$ computed standard error = $.241\text{x}10^{-7}$

(actual std.err. = $.210\text{x}10^{-7}$)

the number of samples for direct sampling would be = 648,000

Here, we decreased the actual standard error by a factor of 2.36, whereas we only took 2.93 times the number of samples as in the first experiment. For direct sampling, we would have needed 5.65 times the number of samples.

If the control variate $\phi(\underline{x}) = x_1 x_2 \ldots x_{20}$ is applied to θ, then we have to estimate $\int_{U^{20}} (f-\phi)(\underline{x})\underline{dx}$, which leads us to our next example.

Example 4. $\theta - \phi = \int_{U^{20}} [\exp(x_1 x_2 \ldots x_{20}) - 1 - x_1 x_2 \ldots x_{20}]\underline{dx} =$

$.14355\text{x}10^{-9}$,

where $\Phi = \int_{U^{20}} \phi(\underline{x})\underline{dx} = (1/2)^{20} = .953674\text{x}10^{-6}$,

and θ is defined in example 3.

The function $\phi(\underline{x}) = x_1x_2...x_{20}$ is an obvious and a good choice for the control variate, because it is the first nonzero term in the Taylor Series expansion of $[\exp(x_1x_2...x_{20})-1]$ about the origin and because $\Phi/\theta = .999845$.

The input parameters are the sample as in the first experiment of the last example except that $\varepsilon = 1.0x10^{-10}$ and, of course, t=CV. The results are:

$\hat{\theta}_{CV} = .953772x10^{-6}$ $\qquad$ $|\hat{\theta}_{CV} - \theta| = .511x10^{-10}$

$\hat{\theta}_{CV} - \Phi = .924x10^{-10}$ $\qquad$ number of strata = 48

number of samples = 143,398

(actual standard error = $.578x10^{-10}$)

computed standard error = $.6422x10^{-10}$

The number of samples for direct sampling would be =1,400,000.

($var(\tau_{CV}) = .5x10^{-14}$)

Example 5. $\qquad \theta = \int_{U^5} f(\underline{x})d\underline{x} = 1/54 = .01851851...,$

where $f(\underline{x}) = 1$, if $x \varepsilon H = [0,1)X[0,\frac{1}{2})X[0,\frac{1}{3})X[0,\frac{2}{3})X[\frac{1}{3},\frac{1}{2})$

and $f(\underline{x}) = 0$, otherwise.

In the previous examples the integrands were continuous and infinitely differentiable functions. Here, the integrand is

discontinuous on the region of integration.

The input parameters:

$k=5$, $m_o=50$, $\Delta m=10$, $MAXm=100$, $c=5$, $t=c$, $NOSTOP=3$,

$NCA=NPTMIN=0$, $\varepsilon=1{,}0\times10^{-4}$, $t_\alpha=1$, $FC=1$, and $TIMAX=1$

yielded the following results:

$\hat{\theta}_C = .0185158$ $\qquad$ $|\hat{\theta}_C-\theta| = .27\times10^{-5}$

$\sum_{u=1}^{101} |\hat{\theta}_{C,u}-\theta_u| = .27\times10^{-4}$ $\qquad$ number of strata=101

computed std.err. $=.109\times10^{-4}$

number of samples=120,145

(actual std.err.$= .875\times10^{-5}$)

number of samples direct sampling would need =232,000,000

($var(\tau_C)=.0181$)

That direct sampling would require almost 2,000 times the number of samples than the MCSS method is due to the effectiveness of the procedure to partition the region of integration. The region U^5 was stratified into strata where the function was zero and strata where the function was almost entirely non-zero there. For example these last two strata are:

$$R_{100}= (0.,.5)x(0.,.5)x(.3359,.3438)x(0.,.5)x(.375,.5),$$

$\hat{\theta}_{C,100} = \theta_{100} = 0,$

$R_{101} = (0.,.5)x(0.,.5)x(.3281,.3359)x(0.,.5)x(.375,.5)$

$\hat{\theta}_{C,101} = .8417 \times 10^{-4}, \quad \theta_{101} = .8138 \times 10^{-4}$.

In a direct sampling Monte Carlo procedure 98% of the samples, on the average, would yield a value of zero for the integrand. For the MCSS, the average is 38%.

Example 6 $\theta = \int_0^1 dx_1 \int_0^{(1-x_1^2)^{1/2}} dx_2 \int^{(1-x_1^2-x_2^2)^{1/2}} dx_3$

$$\int_0^{(1-x_1^2-x_2^2-x_3^2)^{1/2}} dx_4 = .308425 .$$

In this example we have a region of integration which is not a k-cell. We circumscribe $U^4 = X_{i=1}^4 [0,1)$ about the region of integration and define $f(\underline{x}) = 1$ if $\sum_{i=1}^4 x_i^2 \leq 1$ and $f(\underline{x}) = 0$, otherwise. Thus, we have the equivalent form

$$\int_{U^4} f(\underline{x}) \underline{dx} = \theta .$$

The input parameters are: k=4, m_o=50, Δm=5, MAXm=100, c=4, t=C, NOSTOP=5, ε=1.0x10^{-3}, t_α=1, FC=1, and TIMAX=1. The results are:

$\hat{\theta}_C = .307446$ $\quad\quad$ $|\hat{\theta}_C - \theta| = .979 \times 10^{-3}$

number of strata = 86 $\quad\quad$ number of samples = 133,266

computed standard error = $.631 \times 10^{-3}$

number of samples direct sampling would need to achieve the same standard error = 535,000 $\quad$ ($\text{var}(\tau_C) = .0181$)

This example was taken from the Modified Monte Carlo Quadrature (MMC) by Haber [HAS]. Haber's MMC procedure consists of, a priori, subdividing each interval of the k-cell, $[a_i, b_i)$, for i=1,...,k. The region of integration is partitioned according to its geometry rather than the behavior of the integrand. For this example, one of his experiments consisted of subdividing each interval [0,1) into 1/16-ths, so that U^4 is partitioned into 16^4(=65,536) strata. Then using the crude Monte Carlo estimator, two samples were drawn from each stratum. The results are:

$|\hat{\theta}(\text{MMC}) - \theta| = .144 \times 10^{-3}$ $\quad$ number of samples = 131,072

computed standard error = $.45 \times 10^{-3}$.

Since the integrand, $f(\underline{x})=1$, when $\sum_{i=1}^{4} x_i^2 \leq 1$ and $f(\underline{x})=0$, otherwise, is symmetric with respect to each of the coordinate axes, stratifying each axis identically, as did Haber, is an excellent choice for this integrand. Hence, the MMC method is ideal for this example; nevertheless the MCSS does not compare too

unfavorably.

All of the examples that Haber used were four dimensional multiple integrals. Why? For instance, one of the examples was the four dimensional equivalent to our example 3. If the MMC procedure was applied to example 3, it would require 2^{20}, or approximately one million, strata just to bisect each interval [0,1) once. Moreover, due to the nature of the integrand there exists other partitions which would be more efficient, that is, require less work and obtain more accurate answers.

Example 7: $\theta(k) = \int_{U^k} f(\underline{x})d\underline{x}$,

where $f(\underline{x})=1$, if $\sum_{i=1}^{k} x_i^2 \leq 1$, $f(\underline{x})=0$, otherwise, k=5 and 10,

and $\theta(5) = .164493$ and $\theta(10) = .002490$.

These are just the five and ten dimensional analogues of the last examples. The input parameters remain the same, except, of course, the value k. For k=5, the results are:

$\hat{\theta}_C = .164280$ $\quad\quad$ $|\hat{\theta}_C - \theta| = .213 \times 10^{-3}$

number of strata = 77 $\quad\quad$ number of samples = 124,029

computed standard error = $.546 \times 10^{-3}$

number of samples needed for direct sampling = 460,000

$(\text{var}(\tau_C) = .1374)$

For k=10, the results are:

$\hat{\theta}_C = .002528$ $\quad |\hat{\theta}_C - \theta| = .38\text{x}10^{-4}$

number of strata = 33 number of samples = 87,892

computed standard error = $.604\text{x}10^{-4}$

samples needed for direct sampling = 695,000

$(\text{var}(\tau_C) = .0025)$

Example 8. $\theta(k) = \int_0^1 dx_1 \int^{(1-x_1^2)^{1/2}} dx_2 \ldots$

$$\int_0^{(1-x_1^2 \ldots x_{k-1}^2)^{1/2}} dx_k \exp(-\sum_{i=1}^{k} x_i^2) ,$$

for k=4,5,...,10 .

This example comes from the report on the NIMDQD subroutine by Tavernini (see [TAL]). Only the case k=4 is mentioned in the report. However, the cases k=5,6,...,10 where also tested and compared with the MCSS procedure in order to determine, empirically, at which dimensions NIMDQD is more advantageous than MCSS and vice versa.

It should be noted that the results here will not give us any general idea as to what the number of dimensions it will be advantageous to use the MCSS, but only a vague notion. Also,

k	θ(k)	MCSS $\lvert\hat{\theta}_A-\theta(k)\rvert \times 10^{-3}$	Number of samples	Computed std.err. $\times 10^{-3}$	NIMDQD $\lvert J(k)-\theta(k)\rvert \times 10^{-3}$	$Ex10^{-3}$
4	.16299721	.38512 9,005*	23,990	.78	.54946 835*	1
5	.082467784	.28672 6,234*	39,632	.70	.31670 2,900*	1
6	.03890386	.68812 4,759*	46,406	.65	.21247 9,690*	1
7	.01724266	.14618 2,209*	51,203	.52	.10950 32,850*	1
8	.00722508	.18967 1,129*	60,420	.44	.04142 115,165*	1
9	.00287724	.17171 484*	73,924	.24	.01829 383,340*	1
10	.00109374	.03290 5,596*	160,171	.05	.0007 1,531,345*	1

Table 10.3 *Number of evaluations of the integrand.

the integral in this example is not difficult to evaluate, mainly because $\mathrm{var}(\tau_C(k))$ is small relative to $\theta(k)$, for $k=4,\ldots,10$.

Before the MCSS procedure is applied we transform the integral, as in the last example, into the equivalent form:

$$\int_{U^k} f(\underline{x})\underline{dx} = \theta(k) , \tag{10.1}$$

where $f(\underline{x}) = \exp(-\sum_{i=1}^{k} x_i^2)$ if $\sum_{i=1}^{k} x_i^2 \leq 1$ and $f(\underline{x}) = 0$, otherwise. The input parameters are:

$k=4,5,\ldots,10$, $m_o=50$, $\Delta m=10$, MAXm=100, c=k, t=A,

NOSTOP=5, $\varepsilon=1.0\times10^{-3}$, $t_\alpha=1$, FC=5,6,...,11, and TIMAX=1.

For the NIMDQD algorithm the inputs are the desired bound on the truncation error, $E=10^{-3}$ for $k=4,\ldots,10$, and the function for evaluating the upper and lower limits, $g_j(x_1,\ldots,x_j)=(1-x_1^2-\ldots x_{j-1}^2)^{\frac{1}{2}}$ and $h_j(x_1,\ldots,x_j)=0$, where $j=1,\ldots,k$, for each $k=4,\ldots,10$. Note that the NIMDQD procedure evaluates the originally stated integral, while the MCSS procedure evaluates the integral in (10.1).

Let J(k) be the NIMDQD procedure's estimate of $\theta(k)$. The results are shown in Table 10.3.

In the MCSS results we differentiated between the number of samples and number of function evaluation. The latter only refers to computing the function, $f(\underline{x}) = \exp(-x_1^2-x_2^2-\ldots-x_k^2)$, which requires k+10 essential operations (ops.),whereas evaluating $f(\underline{x})=0$, for

$\sum_{i=1}^{k} x_i^2 \leq 1$ requires k ops. since it is necessary to evaluate $\sum x_i^2$. On the other hand, the NIMDQD must evaluate $g_j(x_1,\ldots,x_j) = (1-x_1^2 \ldots x_{j-1}^2)^{1/2}$ which requires j+9 ops. This averages out to be $5^{-(k-1)}(k-1)^2$ (k/2+9) per function evaluation, which is not too significant when k is large.

Examining the results we can see that NIMDQD is superior to MCSS when k=4,5,or 6. When k=7 the NIMDQD estimate is slightly better than MCSS, but the NIMDQD requires 562,000 ops. to evaluate its integrand and the g_j's, while the MCSS requires 380,000 ops. to evaluate its integrand. For k=8,9, and 10, it is a trade-off between accuracy and labor. The NIMDQD procedure only iterated once, for k=9 and 10.

Note that for k>10 the number of function evaluations for the NIMDQD method becomes prohibitive, whereas for the MCSS method this is not the case.

Example 9: $\theta(k) = \int_{-5}^{5} dx_1 \ldots \int_{-5}^{5} dx_5 \prod_{i=1}^{k} [(2\pi)^{-\frac{1}{2}} \exp(-\frac{1}{2} x_i^2)] = 1.0,$

for k=5 and 10.

The integrand in this example is the normal probability function. Letting $D(k) = X_{i=1}^{k}(-3,3)$ and $H(k) = X_{i=1}^{k}\{(-5,-3] \cup [3,5)\}$, we have that integrating over D(k) yields 95%, for k=5, and 90%, for k=10, of the value of $\theta(k)$. Therefore, the optimum

strategy would seem to be to stratify and take more samples in D(k) than in H(k). The MCSS procedure using the following input parameters, in fact, did this.

k=5,10, m_o=50, Δm=10, MAXm=150, c=k, t=A, NOSTOP=5, NCA=NPTMIN=0, ε=.1, t_α=1, FC=k+11, and TIMAX=1.

The results for k=5 are:

$\hat{\theta}_A$ = .960 $\quad |\hat{\theta}_A-\theta|$ = .040

computed standard error=.022 number of strata = 42

number of samples=105,821

number of samples needed for direct sampling to get same computed s.e. = 370,000 (var(τ) = 177.65).

For k=10, the results are:

$\hat{\theta}_A$ = .904 $\quad |\hat{\theta}_A-\theta|$ =.096

computed standard error=.106 number of strata = 68

number of samples=453,872

number of samples needed to get the same s.e. by direct sampling = 2,850,000 (var(τ) = 31,920).

Example 10. $\theta = \int_R \int_R \exp(-2\sigma)/(\sigma^2 V^2)\, dv \cdot dv'$,

where $\sigma^2 = \sum_{i=1}^{3} (x_i - x_{i+3})^2$, R= right circular cylinder of

unit radius, eight unit lengths, and of volume

$V = 8\pi$. $\theta = 0.1862$.

This example is from the paper on antithetic variates by Hammersley and Morton [HAMJ-MOK]. The integrand is unbounded on RxR and is infinite on the set $H = \{ (x_1,\ldots,x_6) : x_i = x_{i+3}$, for i=1, 2,3 $\}$. Although the value of θ is finite, $var(\tau_c) = \infty$ on RxR. Thus, we cannot guarantee that the stopping rule will ever be satisfied nor does Theorem 3.1 hold.

Nevertheless, the MCSS procedure was tried just to see what would happen. The input parameters are:

k=6, m_o=50, Δm=10, MAXm=200, c=6, t=A, NOSTOP=5,

NCA=NPTMIN=0, ε=.01, t_α=1, FC=25, and TIMAX=5 .

The results are:

$\hat{\theta}_A = .1571$ $\qquad$ $|\hat{\theta}_A - \theta| = .0291$

number of strata=77 $\qquad$ number of samples=307,791

computed standard error=.0062

The MCSS algorithm partitioned the region of integration, RxR, so that the total hypervolume of the strata which includes the set H is very small compared to the vol(RxR). In addition, the probability of choosing a point in H is very small.

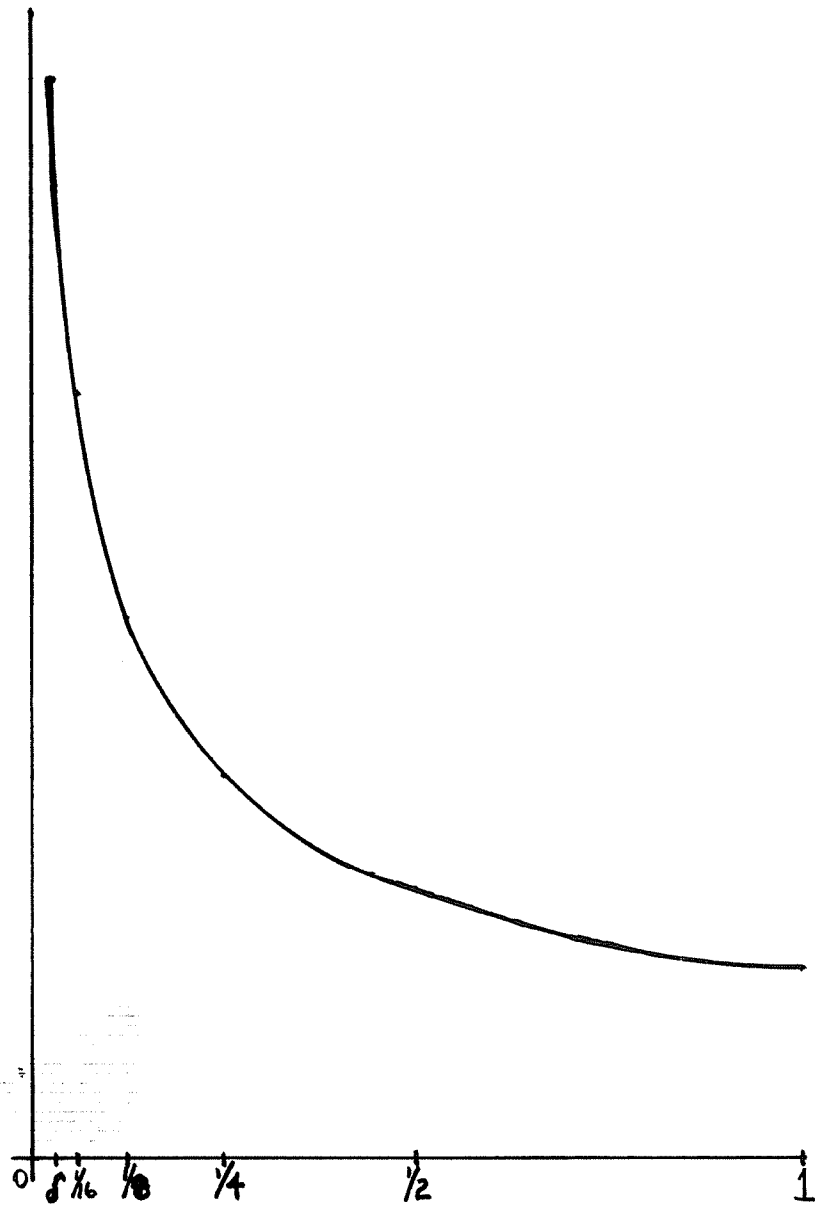


Figure 10.6. The partition of $\int_0^1 x^{-1/2}\,dx$

(Theoretically, it is zero; but, because we work with a finite word length computer, there are only a finite number, say u, of machine-attainable points in the cylindrical region R, and so u^2 points in RxR. The number of points in H is also u. If we assume that the sampling distribution is uniform over the u^2 attainable points of RxR, the probability of H becomes 1/u. In our experiment with the Univac 1108 computer, u is about $\pi \times 2^{183} \sim 10^{55}$.) Therefore, the contributions, from the strata which include H, to the estimate of θ, are very small.

In order to see more clearly what has happened in this example, let us consider an analogous example, $\theta = \int_0^1 x^{-1/2} dx$. Notice that θ is finite ($\theta=2$) but $\mathrm{var}(\tau_C)$ is infinite (since $\int_0^1 dx/x$ does not converge).

Let $\theta' = \int_\delta^1 x^{-1/2}\, dx = 2-2\sqrt{\delta}$, for some $\delta > 0$ (see Figure 10.6). Then, $\theta-\theta' = \theta'' = \int_0^\delta x^{-1/2} dx = 2\sqrt{\delta}$. The MCSS procedure partitions [0,1), so that the final subinterval is $[0,\delta)$, where δ is small. The magnitude of δ depends directly on the size of the desired error-bound, ε. So that, since δ is small, θ'/θ is almost 1. Hence, the dominant contribution to θ comes from the region outside the point where the integrand is infinite. The estimator of θ' has a <u>finite</u> variance. Hence, it converges to θ' with probability one (see (1.3) and the sentence following). Furthermore, since the probability of choosing $\xi=0$ (which will yield theoretically an infinite function

value; computationally it yields an arithmetic overlow) is almost zero and since δ is small, the estimate for θ'' will be small. Note, too, that the probability of picking an $\xi=0$ is independent of the choice of δ.

11. PROSPECTUS FOR FURTHER RESEARCH

As we recall from the introduction, for a given θ, ε, and α, we are attempting to find an estimator $\hat{\theta}$ of θ, such that $\hat{\theta}$ is the solution of

$$\min\{L(\hat{\theta}):\hat{\theta} \in \underset{\sim}{\Theta}, \quad \mathrm{var}(\hat{\theta}) \leq (\varepsilon/t_\alpha)^2\} \tag{11.1}$$

where $L(\hat{\theta})$ is the total amount of labor required to calculate $\hat{\theta}$, and the minimum is taken over all estimators in the class $\underset{\sim}{\Theta}$.

In our experiments, so far, we have restricted the class of estimators to the ones discussed in Section 6. However, this class can be greatly expanded with the hope that a new minimum value can be found.

Some of the estimators which might be useful to further research are listed below.

(i) Antithetic Variate Techniques. Here, there exists a very large class of transformations which are variance-reducing. However, the number of points required for the more powerful ones increases exponentially with the dimension of the integrand.

Nevertheless, formulae which grow linearly, though not as powerful, should be explored.

These estimators are generally good when the integrand, f, is a multiple-differentiable function. On the other hand, there is little improvement when f varies rapidly in every direction.

(ii) Quasi-Random Formulae. These formulae could be generated from an initial random point so that the sample points will be spread (approximately equidistributed) throughout the region of integration. One possible approach is the following: let $\theta = \int_{U^k} f(\underline{x})\underline{dx}$, where U^k is the k dimensional hypercube. Choose $\underline{\xi} = (\xi_1,\ldots,\xi_k)$, where $\xi_i \sim U(0,1)$; then generate N samples from

$$\underline{\xi}_r = \left(\{\xi_1 + \frac{r}{N}\} \ ,\ldots, \ \{\xi_k + \frac{r}{N}\} \right) , \quad r=0,\ldots,N-1,$$

where $\{\cdot\}$ denotes the fractional part.

(iii) Stratification Procedures. Instead of bisection-type stratification, one could try trisection, partitions of unequal lengths, and partitions other than ones perpendicular to the axis. As an example of the last type, consider estimating $\theta = \int_0^1 \int_0^1 4xy \, dx \, dy$. The region of integration could be partitioned by the line $x+y=c$, where $0 \le c \le 2$.

The MCSS procedure could test, by sampling, some of the types of partitions and choose the estimator with the least

sample variance.

(iv) Regression Method. For each stratum, the idea is to fit, in the least squares norm, a multidimensional polynomial of a given degree to the samples drawn from that stratum. The decision rule to continue stratifying is based on an analysis-of-variance test. The procedure, otherwise, continues in the same manner as the MCSS procedure will. The estimate of the integral for the stratum is then the integral of the multidimensional polynomial.

(v) Control-Variate Regression Method. This method is the same as the last one except that the multidimensional polynomial fit, of a given degree, is used as a control variate.

In this study we have applied the sequential stratification technique only to the problems of estimating multidimensional integrals. However, there exist many other applications. One application is in the area of curve fitting. The classical numerical analysis techniques almost always use equidistanced partitions, but there may exist other partitions which would yield a better fit.

The sequential approach could first choose points (which may or may not be random) in the entire region where the fit is desired. Then that region is partitioned and the same number of points are chosen in each subregion. For each subregion, we fit polynomials of a given degree to the values of the data or function at the

points and apply a decision rule to determine if we should continue partitioning. The decision rule will depend on the type of norm used.

Remark: (iv) and (v) above, and the sequential curve-fitting technique here described are applications of the idea of fitting with spline-functions in which the choice of "knots" or "nodes" is sequentially determined and the data are randomly selected. The method (v) has been attempted with considerable success by M. Winston as an unpublished term-project in a Monte Carlo course at the University of Wisconsin, Madison (Spring 1970).

12. CONCLUSIONS

The Monte Carlo Sequential Stratification method opens up an avenue of attack in the design of optimum estimators for multiple integrals. The MCSS procedure frees the user from having to choose a partition of the region of integration, a priori. Instead, it programs the computer to search for an optimum placement of the strata. The effect of this search is to yield an estimator, chosen from a given class, and requiring close to a minimum amount of work for the given task.

The MCSS algorithm was programmed and tested for a wide variety of integration problems. The result in every case tested produced an estimate which was better than the corresponding direct sampling estimate. The amount of improvement depended upon the integrand and the region of integration.

In comparing the MCSS technique with Haber's MMC and Taverini's NIMDQD multiple numerical quadrature algorithms, we found that the MCSS procedure was superior when the dimension of the integral was ten or greater, and was comparable between seven and ten dimensions.

Basic to the field of sequential stratification is that it enables us to get away from the overworked and outmoded notions of equidistant grids, fixed-length intervals, and equal-sized partitions. Instead, the computer, together with the appropriate

decision rule, can determine the grid size according to the behavior of the data. However, as the remarks made in the previous section indicate, much more research needs to be done in the field of sequential stratification.

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A P P E N D I X

The FORTRAN Program Listing

```
'RUN ZEIDMAN,8002,3273676662,10,300
'FOR7D,ISZ ,MAIN
      DOUBLE PRECISION  F,ESAVE,VSAVE,E1,E2,SS1,SS2,VOL,XI
      COMMON/B1/NPTTOT,NDIR(50),TA,NOSTOP,NCA
      COMMON/B3/MCRUDE/B5/TIMAX,NPTMIN
      COMMON/BLK2/K0,KINC,KMAX,NCYCLE,FC
      DIMENSION A (20), B (20),  XI(20),AASAVE(20,25),BBSAVE(20,25)
     1ESAVE(25),VSAVE(25),E1(20),E2(20),SS1(20),SS2(20)
      EXTERNAL F
C*************************************************************************
C     IF CRUDE MONTE CARLO IS DESIRED SET MCRUDE=1
C     IF ANTITHETIC VARIATE IS DESIRED SET MCRUDE=0
C     NOSTOP=DON'T USE STOPPING RULE UNTIL VOLRU/VOLR .LT. 2**(-NO.
C     IF NCA=0,THENPICK CO-ORDINATE DIRECTIONS IN RANDOM FASHION OF
C     NCYCLE=K PICK ALL CO-ORDINATE DIRECTIONS
C     IF NCA=1,THEN PICK CO-ORDINATE DIRECTIONS IN CYCLIC ORDER
C     NPTMIN=MINIMUM NUMBER OF POINTS TO BE USED WHEN SAMPLING DIRI
C     TIMAX=MAXIMUM TIME TO BE USED IN SAMPLING DIRECTLY
C*************************************************************************
      TIMEON=TIMEF(1.0)
      READ 101,K,K0,KINC,KMAX,NCYCLE,MCRUDE,NOSTOP,NCA,NPTMIN
101   FORMAT(9I5)
      READ 102,ERROR,TA,FC,TIMAX,A1,B1
102   FORMAT(E10.3,5F10.0)
      IF(A1 .EQ. 0.0  .AND. B1 .EQ. 0.0) B1=1.0
      DO 10 I=1,K
      A(I)=0.0
10    B(I)=1.0
      PRINT 3
3     FORMAT(30H1 THE REGION OF INTEGRATION IS/)
      PRINT 1,(A(I),I=1,K)
      PRINT 1,(B(I),I=1,K)
1     FORMAT(1H ,10(F10.5,3X))
      PRINT 103
103   FORMAT('0     K      K0     KINC    KMAX NCYCLE MCRUDE NOSTOP
     1NPTMIN    ERROR         TA           FC          TIMAX')
      PRINT 104,K,K0,KINC,KMAX,NCYCLE,MCRUDE,NOSTOP,NCA,NPTMIN,ERR
     1TA,FC,TIMAX
104   FORMAT(9(2X,I5),1X,E10.3,3(1X,F10.2))
C*************************************************************************
C     PLACE CONTROL VARIATE BELOW
C     PHI = 0.0 INDICATES THAT NO CONTROL VARIATE IS DESIRED
C*************************************************************************
      PHI = 0.
      PRINT 14,PHI
14    FORMAT('0THE INTEGRAL OF THE CONTROL VARIATE PHI = ',E14.8//
```

```
      NPTTOT=0
      CALL MCSS  (A,B,XI,AASAVE,BBSAVE,ESAVE,VSAVE,K,25,F,ERROR,VOL,
     1ERRBD,E1,E2,SS1,SS2)
      VOL=VOL+PHI
      TIMTOT=(TIMEF(1.0)-TIMEON)/1000.
      PRINT 2, VOL,NPTTOT,ERROR,TA,ERRBD
2     FORMAT(6H0 VOL=D20.11,25X,12HTOTAL NPTS.=I10/ 7H ERROR=E12.5,1
     115HERROR BOUND OF F5.2,11H STD. DEV.=E17.10)
      PRINT 16,TIMTOT
16    FORMAT(13HOTOTAL TIME =F10.3,8H SECONDS/)
      STOP
      END
```

```
'FOR7D,ISZ ,MCSS
      SUBROUTINE  MCSS (AA,BB,XI,AASAVE,BBSAVE,ESAVE,VSAVE,KDIM,MAX
     1F,ERROR,TOTAR,ERRBD,E1,E2,SS1,SS2)
C*******************************************************************
C  PROGRAM TO FIND ESTIMATE OF THE INTEGRAL USING A SEQENTIAL BISEC
C      STRATIFICATION SCHEME.
C*******************************************************************
      IMPLICIT DOUBLE PRECISION (E,S,T,V)
      DOUBLE PRECISION F,Q,AREA,AREA0,AREAP,ACTERR,RHSMAX,XI
      REAL TOTDIF,TRTTI,ERROR,ERRBD,TA,TOLI,TIMAX,VOLR,VOLRJ,VOL,LR
      DIMENSION AA(KDIM),BB(KDIM),XI(KDIM),AASAVE(KDIM,MAXLEV),
     1BBSAVE(KDIM,MAXLEV),ESAVE(MAXLEV),VSAVE(MAXLEV),E1(KDIM),E2(K
     2SS1(KDIM),SS2(KDIM)
      DIMENSION KSAVE(25),SS(100)
      COMMON/B1/NPTTOT,NDIR(50),TA,NOSTOP,NCA
      COMMON/B2/VARSS,NN
      COMMON/B3/MCRUDE/B4/TOLI,VOLRJ/B5/TIMAX,NPTMIN,C
      COMMON/BLK1/K,JDIR,VOL
      COMMON/BLK2/K0,KINC,KMAX,NCYCLE,FC
      COMMON/ANTI/ Q(100)
      DIMENSION ERAW(10),NRAW(10),KTRAW(10),VRAW(10)
      EQUIVALENCE (XI),(E1),(E2),(SS1),(SS2)
      EXTERNAL F
C*******************************************************************
C      ((AA(I),BB(I)),I=1,...,KDIM) = REGION OF INTEGRATION
C      F= FUNCTION WHICH IS TO BE INTEGRATED
C      ERROR =TA * STANDARD ERROR.  WHERE STD. ERR. SQRTF(SAMPLE MEA
C      TA=THE NUMBER OF STD. DEV. DESIRED BY THE USER
C      SO THAT THE TRUE VALUE OF THE INTEGRAL WILL BE IN (RNAREA-ERR
C      K= NUMBER OF POINTS PER INTERVAL PER ITERATION
C      TOL=TOLERANCE OR ERROR BOUNDS ON SAMPLE MEAN VARIANCE
C      LR=LABOR RATIO=LABOR FOR STRATF./ LABOR FOR CRUDE M.C.
C*******************************************************************
      DO 60 I=1,KDIM
      IF(AA(I).GE.BB(I)) GO TO 901
60    CONTINUE
C*****DATA CHECK*****************************************************
      IF( NCYCLE .LT. 1) NCYCLE=K
      IF( KMAX.LT. 1) KMAX=50
      IF(K0 .LT. 1)  K0=20
      IF(KINC .LT. 1) KINC=10
      IF(NPTMIN.LT. 0) NPTMIN=K0*NCYCLE
      IF(MCRUDE .NE. 0 .AND. MCRUDE .NE. 1) MCRUDE=0
      IF(MCRUDE  .EQ.  1) GO TO  66
      IF(K0/2.0-K0/2 .GT. .001) K0=K0+1
      IF(KINC/2.0- KINC/2 .GT. .001) KINC=KINC+1
66    IF(NCA .NE. 0.AND. NCA.NE. 1) NCA=0
```

```
C*****INITIALIZE**********************************INITIALIZE**********
      RDF=4.0*KDIM+FC+4.0
      RLS1=20.3*NCYCLE+0.3
      RLS2=134.0*NCYCLE+20.0
      NPTMAX=TIMAX*5000
      IF(NPTMAX .LE. 0) NPTMAX=100
      C=1.0
      CA=0.25
      IF(MCRUDE .EQ. 1) GO TO 67
      C=0.5
      CA=0.125
67    REGION=0.0
      TOTAR=0.0
      ACTERR=0.0
      TOTHET =0.
      TOTDIF =0.0
      TRTTI=0.0
      TOTSIG=0.0
      LEVEL=0
      NUSED=0
      NST=0
      LEV=1
      AREA0=0.0
      NN0=0
      VAR0=0.0
      DO 210 I=1,10
      ERAW(I)=0.0
      VRAW(I)=0.
      NRAW(I)=0
210   KTRAW(I)=0
      ELAST=0.
      SMVL=0.
      NLAST=0
      TOLI=(ERROR/TA)**2
      CALL VOLTOL(AA,BB,KDIM,VOLRJ,TOLI,1)
      VOLR=VOLRJ
C*************************************************************************
CALCULATE APPROXIMATIONS FOR MEAN AND VARIANCE IN REGION R0
C*************************************************************************
  9   IF(NCYCLE .EQ. KDIM)GO TO 81
C*************************************************************************
C
C     FIND DIRECTIONS IN CYLIC ORDER
C
C*************************************************************************
      IF(NCA .EQ. 0) GO TO 85
      DO 190 I=1,NCYCLE
      NCAM1=NCA-1
      NDIR(I)=MOD(NCAM1,KDIM)+1
190   NCA=NCA+1
      GO TO 81
```

```
C*******************************************************************
C      FIND RANDOM DIRECTIONS WITH NO REPETITIONS.
C*******************************************************************
85     DO 90 JJ=1,NCYCLE
       NDIR(JJ)=RANUN(R)*KDIM+1.0
83     DO 80 JK=1,JJ
       IF(JJ .EQ. JK) GO TO 80
       IF(NDIR(JK) .NE. NDIR(JJ)) GO TO 80
       NDIR(JJ)=RANUN(R)*KDIM+1.0
       GO TO 83
80     CONTINUE
90     CONTINUE
C*******************************************************************
81     KMAXI=KMAX
       IF(LEVEL .EQ. 0) KMAXI=2*KMAX
       NN=0
       VARSS=0.
C*******************************************************************
       DO 70 K=K0,KMAXI,KINC
       TOTSS0=0.0
       N0=2*K
C*******************************************************************
       DO 20 JJJ=1,NCYCLE
       IF(NCYCLE .EQ. KDIM) JDIR=JJJ
       IF(NCYCLE .LT. KDIM) JDIR=NDIR(JJJ)
       CALL MEANVR(AA,BB,XI,KDIM,F,E1(JDIR),E2(JDIR),SS1(JDIR),SS2(
       SS(JDIR)=( CA/(K-1)+ CA/K)*(SS1(JDIR)+SS2(JDIR))+((E1(JDIR)-E
      1R))/N0)**2+Q(JDIR)/N0
       TOTSS0=TOTSS0 + SS(JDIR)
20     CONTINUE
       SS0=TOTSS0/NCYCLE
C*******************************************************************
C
C      PERFORM TEST TO SEE IF ADDITONAL SAMPLES ARE NECESSARY TO ACH
C      BETTER ESTIMATE OF THE VARIANCE
C
C*******************************************************************
       TEST=TOLI/4.
       IF (LEVEL .EQ. 0) TEST=TOLI/9.
       IF(VARSS*(C/NN)**2 .LE. TEST) GO TO 51
C
70     KLAS=K
C*******************************************************************
       K=KLAS
51     NPTTOT=NPTTOT + NN
```

```
C*************************************************************************
C      FIND DEL MAX AND THE DIRECTION
C*************************************************************************
       TOTE0=0.0
       VOL=0.5*VOLRJ
       VOL2=VOL**2
       VOLRJ2=VOL2*4.0
       VOK=VOL/K
       V2OK=VOL2/(K-1)
       DO 100 JJJ=1,NCYCLE
       IF(NCYCLE .EQ. KDIM) JDIR=JJJ
       IF(NCYCLE .LT. KDIM) JDIR=NDIR(JJJ)
       E1(JDIR)=E1(JDIR)*VOK
       E2(JDIR)=E2(JDIR)*VOK
       SS1(JDIR)=SS1(JDIR)*V2OK*C
       SS2(JDIR)=SS2(JDIR)*V2OK*C
       SS(JDIR)=SS(JDIR)*VOLRJ2
       TOTE0=TOTE0+E1(JDIR)+E2(JDIR)
       S1=DSQRT(SS1(JDIR))
       S2=DSQRT(SS2(JDIR))
       IF(MCRUDE .EQ. 0) Q(JDIR)=Q(JDIR)*VOLRJ2/N0
       DEL=SS(JDIR)/(S1+S2)**2
       IF(JJJ .EQ. 1) GO TO 52
       IF(DEL .LE.DELMAX)  GO TO 100
52     DELMAX=DEL
       MAXDIR = JDIR
       E1MAX=E1(JDIR)
       E2MAX=E2(JDIR)
       SS1MAX=SS1(JDIR)
       SS2MAX=SS2(JDIR)
100    CONTINUE
       IF(SS0 .LT. 0)  SS0=0.0
       SS0=SS0*VOLRJ2
       SMV=SS0/(C*NN)
       VOL4=VOLRJ2**2
       VARSS=VARSS*VOL4*(C/NN)**2
       SMVUP=SMV+4.0*DSQRT(VARSS)/(NN*C)
       IF(LEVEL.EQ.0)SMVUP=SMV+9.0*DSQRT(VARSS)/(NN*C)
       EN=TOTE0/NCYCLE
       PRINT 33,EN,NN,ELAST,NLAST,SMVL
33     FORMAT(' EN=',D16.10,4X,'NN=',I5,5X,'ELAST=',D16.10,4X,'NLAST=
      1,5X,'SMVL=',D15.8)
       EN=(EN*NN+ELAST*NLAST)/(NN+NLAST)
       SMVUP=(SMVUP*NN+SMVL*NLAST)/(NN+NLAST)
       SS0UP=SMVUP*(NN+NLAST)*C
C*************************************************************************
C      PRINT RESULTS OF TEST FOR ACCURACY OF SAMPLE VARIANCES
C      PRINT ESTIMATES OF MEAN AND VARIANCE.
C*************************************************************************
       DO 110 IAB=1,KDIM
110    PRINT 27,IAB,AA(IAB),IAB,BB(IAB)
```

```
27     FORMAT(4H AA(I2,2H)=F14.9,5X,3HBB(I2,2H)=F14.9)
       PRINT 123,VOLRJ
123    FORMAT(1H+,80X,'VOLRJ=',E14.8)
       TEST=TEST*VOL4
       PRINT 61,VARSS,TEST
61     FORMAT(1H ,20X,6HVARSS=D20.10,10X,5HTEST=D20.10)
       PRINT 21,LEVEL
21     FORMAT(7HOLEVEL=I4)
       DO 130 ND=1,NCYCLE
       IF(NCYCLE .LT. KDIM) JD=NDIR(ND)
       IF(NCYCLE .EQ. KDIM) JD=ND
130    PRINT 22,JD,AA(JD),BB(JD),NO,E1(JD),E2(JD),SS(JD),SS1(JD),SS2
      1,Q(JD)
22     FORMAT(5H DIR=I2,3H A=F14.9,3X,3H B=F14.9,3H N=I5,3X,3HE1=D20
      15X,3HE2=D20.11/5H SSO=D20.11,5X,4HSS1=D20.11,5X,4HSS2=D20.11,
      12HQ=D16.9/)
       PRINT 41,SMV,SMVUP,TOLI,NN,SSOUP,EN
41     FORMAT( 1X,'SMV=',D14.8, 5X,'SMVUP=',D14.8, 5X,'TOLI=',E14.8,
      1        5X,3HNN=I6,5X,6HSSOUP=D14.8,5X,3HEN=D14.8)
       RHSMAX=SS(MAXDIR)/DELMAX
       PRINT 24,SSO,RHSMAX,DELMAX,MAXDIR
24     FORMAT(5H SSO=D20.10,10X,14H   (S1+S2)**2=D20.10,5X,
      17HDELMAX=E20.10,5X,7HMAXDIR=I5/)
C*******************************************************************
C
C       STOPPING RULE
C
C*******************************************************************
64     SMV=SMVUP
       IF(VOLRJ*(2**NOSTOP) .GT. VOLR) GO TO 2
       IF (SMV .GT. TOLI) GO TO 2
C*******************************************************************
C
C            VARIANCE IN I-TH STRATA WITHIN THE TOLERANCE
C
C*******************************************************************
       NPT=NN
       GO TO 19
C*******************************************************************
C      NO ADDITION PTS NEEDED ADD NEW ESTIMATE TO PREVIOUS ONE.
C*******************************************************************
3      TOTAR=TOTAR+AREA
       ACTERR=ACTERR + SMV
C*******************************************************************
C      PRINT INTERMEDIATE RESULTS FOR CALCULATION OF INTEGRAL
C*******************************************************************
       DO 120 IAB=1,KDIM
120    PRINT 27,IAB,AA(IAB),IAB,BB(IAB)
       REGION=REGION + VOLRJ
       NUSED=NUSED+NPT
```

```
      NST=NST+1
      PRINT 29,VOLRJ ,REGION,NUSED,NST
29    FORMAT(8H0 VOLRJ=E14.8,,10X,10HSUM VOLRJ=,E14.8,10X,6HNUSED=I1(
     110X,11HNO. STRATA=I5)
      PRINT 23,AREA,TOTAR,SMV,ACTERR,NPTTOT
23    FORMAT(7H   EST=D14.8,5X,8HSUM EST=D14.8,5X,4HSMV=D12.6,5X,
     18HSUM SMV=D14.8,3X,10HTOTAL NPT=I7/)
 65   IF(LEVEL   .EQ.  0)  GO TO 999
C*************************************************************************
C     YES--DONE WITH STRATIFICATION PART .
C     NO--NOT DONE MUST TEST ANOTHER STRATA
C     RETRIEVE THE LAST ELEMENT ON INFO LIST AND POP LIST BY 1
C*************************************************************************
      DO 40 I=1,KDIM
      AA(I)=AASAVE(I,LEVEL)
40    BB(I)=BBSAVE(I,LEVEL)
      E1MAX=ESAVE(LEVEL)
      SS1MAX=VSAVE(LEVEL)
      K=KSAVE(LEVEL)
      LEVEL = LEVEL - 1
      CALL VOLTOL(AA,BB,KDIM,VOLRJ,TOLI,2)
      GO TO 16
C*************************************************************************
C     NO--VARIANCE IN I TH STRATA NOT WITHIN TOLERANCE
C
C      DECISION RULE          STRATIFICATION TEST
C
CALCULATE THE NUMBER OF PTS TO GET THE DESIRED VARIANCE
C*************************************************************************
2     SUP=1.0+2.0*DSQRT(VARSS)/(SS1MAX+SS2MAX)
      SS1MAX=SS1MAX*SUP
      SS2MAX=SS2MAX*SUP
       NPT=SSOUP/TOLI-NN
      IF( NPT .LT. 0 )  NPT=0
       N12=(DSQRT(SS1MAX)+DSQRT(SS2MAX))**2/TOLI
      RMON=FLOAT(N0)/N12
      LR=1.0+RMON*(2.*NCYCLE-1)+(RMON*RLS1+RLS2/N12)/
     1(RDF+(KDIM+10.0)/NPT)
      PRINT 109,LR,K,KMAXI,NPT,N12
109   FORMAT(13H LABOR RATIO=F10.5,20X,2HK=I5,5X,6HKMAXI=I5,5X,4HNPT=
     1,5X,'N1+N2=',I10)
      IF(DELMAX .GT.  LR )  GO TO 7
      IF(VOLRJ*(2**NOSTOP) .GT. VOLR) GO TO 7
C*************************************************************************
C
C     DON'T STRATIFY.  CALCULATE AREA USING CRUDE M.C.
C
C*************************************************************************
      IF(NPT .LE.NPTMAX) GO TO 19
      PRINT 111,NPTMAX
111   FORMAT(' ***** NPT .GT. NPTMAX STRATIFY      NPTMAX = ',I10,' *
```

```
     1******')
      GO TO 7
19    IF(NPT .GT. 2*KMAXI*NCYCLE) NPT=2*KMAXI*NCYCLE
      IF( NPT .LT. 0 )  NPT=0
      NN=NN+NLAST
      CALL CRUDMC(AA,BB,XI,KDIM,F,NPT,NN,SSOUP,AREA,SMV)
      AREA=(AREA*VOLRJ+TOTEO*NO+ELAST*NLAST)/(NPT+NN)
      NPTTOT=NPTTOT+NPT
      NPT=NPT+NN
      GO TO 3
C*************************************************************
C
C     STRATIFICATION RECOMMENDED
C     BEGIN STRATIFICATION PROCEDURE
C
C*************************************************************
7     IF(LEVEL.LT.MAXLEV) GO TO 13
      PRINT 8,MAXLEV
8     FORMAT(15HOLEVEL IS OVER I3)
      GO TO 18
C*************************************************************
C     IS REGION   TOO SMALL TO CONTINUE SUBDIVIDING.      -
C*************************************************************
13    IF(VOLRJ/VOLR.GT. 1.0E-08) GO TO 12
      PRINT 102,VOLRJ
102    FORMAT(22HOVOLRJ/ /OLR.LT.1.0E-10,10X,6HVOLRJ=E17.10/)
18    NPT=SSOUP/TOLI
      PRINT 112
112   FORMAT(1H+,60X,'*****DIRECT SAMPLING WILL BE USED FOR THIS ST
     1*****'/)
      GO TO 19
C*************************************************************
C     IF THE REGION TO BE STRATIFIED ADDS UP TO THE ORIGINAL REGION
C     THEIR ESTIMATES TO THE ORIGINAL ONE
C*************************************************************
12    IF(NN-NO+NLAST .EQ. 0) GO TO 56
      DO 200 L=LEV,10
      IF(VOLRJ .LE. 2.0**(-L)*VOLR) GO TO 200
      ERAW(L)=ERAW(L)+((TOTEO-E1MAX-E2MAX)*NO+ELAST*NLAST)/(NN-NO+N
      NRAW(L)=NRAW(L)+NN-NO+NLAST
      VRAW(L)=VRAW(L)+SSOUP
      KTRAW(L)=KTRAW(L)+1
      IF(KTRAW(L) .LT. 2**(L-1) )  GO TO 56
      AREAO=AREAO +ERAW(L)*NRAW(L)
      VARO=VARO+VRAW(L)*NRAW(L)
      NNO=NNO+NRAW(L)
      AREAP=AREAO/NNO
      VARP=VARO/NNO**2
      PRINT 205,LEV,L,ERAW(L),AREAP,NNO,VARP
205   FORMAT(5H LEV=I2,5X,5HERAW(I2,2H)=D11.5,10X,6HAREAP=D11.5,5X,
```

```
     15H NNO=I6,5X,5HVARP=D11.5)
      LEV=L+1
      GO TO 56
200   CONTINUE
C*****************************************************************
C*****************************************************************
C
C     SAVE INFORMATION OF THE REGION WHERE SAMPLE VARIANCE IS THE LAR
C     AND SET UP NEW RC REGION
C
C*****************************************************************
56    LEVEL = LEVEL + 1
      DO 50 I=1,KDIM
      AASAVE(I,LEVEL)=AA(I)
      BBSAVE(I,LEVEL)=BB(I)
      IF ( I.NE.MAXDIR) GO TO 50
      IF(SS1(MAXDIR) .GT. SS2(MAXDIR)) GO TO 53
      AASAVE(MAXDIR,LEVEL)=0.5*(AA(MAXDIR)+BB(MAXDIR))
      ESAVE(LEVEL)=E2MAX
      VSAVE(LEVEL)=SS2MAX
      BB(MAXDIR)=AASAVE(MAXDIR,LEVEL)
      GO TO 50
53    BBSAVE(MAXDIR,LEVEL)=0.5*(AA(MAXDIR)+BB(MAXDIR))
      ESAVE(LEVEL)=E1MAX
      VSAVE(LEVEL)=SS1MAX
      AA(MAXDIR)=BBSAVE(MAXDIR,LEVEL)
      E1MAX=E2MAX
      SS1MAX=SS2MAX
50    CONTINUE
      KSAVE(LEVEL)=K
      CALL VOLTOL(AA,BB,KDIM,VOLRJ,TOLI,3)
C*****************************************************************
C
C     IS THE NEW STRATUM WITHIN DESIRED ACCURACY.
C
C*****************************************************************
16    SMV=SS1MAX/(K*C)
      ELAST=E1MAX
      SMVL=SMV
      NLAST=K
      IF(VOLRJ*(2**NOSTOP) .GT. VOLR) GO TO 9
      IF(SMV.GT.    TOLI    ) GO TO 9
      PRINT 26,SMV,TOLI
26    FORMAT(' NEW STRATUM WITHIN DESIRED ACCURACY',5X,'SMV=',D14.8,
     15X,'TOLI=',E13.8)
C
C     USING CRUDE M.C. TAKE MORE SAMPLES AND CALCULATE  VOLUME FOR N
C
       NPT=2*K*NCYCLE-K
```

```
      CALL CRUDMC(AA,BB,XI,KDIM,F,NPT,K,SS1MAX,AREA,SMV)
      AREA=(AREA*VOLRJ+E1MAX*K)/(NPT+K)
      NPTTOT=NPTTOT+NPT
C     INCREASE NPT FOR NUSED COUNTER
      NPT=NPT+K
      ELAST=0.
      SMVL=0.
      NLAST=0
      GO TO 3
C*****************************************************************
C     ERROR RETURN
901   PRINT 101,I
101   FORMAT(25H0***** A    .GT.  B *****,8H ON THE I2,8H-TH AXIS)
C     NORMAL RETURN
999   ERRBD=TA*DSQRT(ACTERR)
      IF(LEV .LE. 1) RETURN
      AREA0=AREA0/NN0
      VAR0=VAR0/NN0**2
      LEV=LEV-1
      ACTERR=(VAR0*ACTERR)/(ACTERR+VAR0)
      PRINT 206,AREA0,VAR0,NN0,LEV,ACTERR
206   FORMAT(7H0AREA0=D14.8,5X,5HVAR0=D14.8,5X,4HNN0=I7,5X,4HLEV=I2
     1'ACTERR*=',D14.8/)
      IF(VAR0 .LT.  1.0D-150   .OR.   ACTERR  .LT.  1.0D-150) RETUR
      TOTAR=(VAR0*TOTAR+ACTERR*AREA0)/(VAR0+ACTERR)
      RETURN
      END
```

```
'FOR7D,ISZ ,MEANVR
      SUBROUTINE MEANVR(AA,BB,XI,KDIM,F,E1,E2,SS1,SS2)
      IMPLICIT DOUBLE PRECISION (E,S,V,Y)
      DOUBLE PRECISION  F,Q,XI
      REAL VOL
      DIMENSION AA(KDIM),BB(KDIM),XI(KDIM)
      COMMON/B2/VARSS,NN
      COMMON/B3/MCRUDE
      COMMON/BLK1/K,JDIR,VOL
      COMMON/BLK2/KO,KINC,KMAX,NCYCLE,FC
      COMMON/ANTI/ Q(100)
      EQUIVALENCE (AA),(BB),(XI)
      EXTERNAL F
C*************************************************************************
CALCULATE MEAN AND VARIANCE  FOR LEFT AND RIGHT STRATA
CALCULATION OF VARIANCE BY USING THE HELMHERT TRANSFORMATION.
C*************************************************************************
      CJ=0.5*(AA(JDIR)+BB(JDIR))
      HALF=CJ-AA(JDIR)
      IF( K.GT. KO) GO TO 1
      E1=0.
      E2=0.
      SS1=0.
      SS2=0.
      Q(JDIR)=0.0
      KK=KO
      KL=0
      GO TO 2
1     KK=KINC
      KL=K-KINC
      IF(MCRUDE .EQ. 0) KL=KL/2
C*************************************************************************
C
C     SELECT K RANDOM POINTS EACH FROM REGIONS R1 AND R2
C     BY USING ANTITHETIC VARIATES IF DESIRED
C
C*************************************************************************
 2    IF(MCRUDE .EQ. 0) KK=KK/2
      DO 10 J=1,KK
      CALL RANPT(AA,BB,JDIR,1,HALF,CJ,KDIM,XI)
      Y1=F(XI,KDIM)
      IF(MCRUDE .EQ. 1) GO TO 11
      CALL ANTHET   (AA,BB,JDIR,1,HALF,CJ,KDIM,XI)
      YA1=F(XI,KDIM)
11    CALL RANPT(AA,BB,JDIR,2,HALF,CJ,KDIM,XI)
      Y2=F(XI,KDIM)
      IF(MCRUDE .EQ. 1) GO TO 12
      CALL ANTHET   (AA,BB,JDIR,2,HALF,CJ,KDIM,XI)
      YA2=F(XI,KDIM)
```

```
C*************CALCULATE ESTIMATE OF Q NEEDED TO CALCULATE SSO*****
      Q(JDIR)=(Y1-Y2)*(YA2-YA1) + Q(JDIR)
      Y1=Y1+YA1
      Y2=Y2+YA2
C*****************************************************************
C
CALCULATE THE VARIANCE OF SSO
C
C*****************************************************************
12    NN=NN+2
      IF(J .EQ. 1) GO TO 4
      IF(KM1 .LE. 0) GO TO 4
      KP=KM1+1
      VARSS=VARSS+(KM1*(Y1-E1/KP)**2-SS1)**2/(KM1*KP)
      VARSS=VARSS+(KM1*(Y2-E2/KP)**2-SS2)**2/(KM1*KP)
4     IF(MCRUDE .EQ. 0) NN=NN+2
C*****************************************************************
C
CALCULATE THE VARIANCE OF E1 AND E2.
C
C*****************************************************************
      KM1=KL+J-1
      IF(KM1 .EQ. 0 )  GO TO 3
      SS1=SS1+(KM1*Y1-E1)**2/(KM1*(KM1+1))
      SS2=SS2+(KM1*Y2-E2)**2/(KM1*(KM1+1))
3     E1=E1 + Y1
10    E2=E2+Y2
C
CALCULATE VARSS FOR THE LAST ITERATION THRU THE DO LOOP
C
      KP=KM1+1
      VARSS=VARSS+(KM1*(Y1-E1/KP)**2-SS1)**2/(KM1*KP)
      VARSS=VARSS+(KM1*(Y2-E2/KP)**2-SS2)**2/(KM1*KP)
      RETURN
      END
```

```
'FOR7D,ISZ ,VOLTOL
      SUBROUTINE VOLTOL(A,B,KDIM,VOLRJ,TOLI,IGOTO)
      DIMENSION A(KDIM),B(KDIM)
      EQUIVALENCE (A),(B)
C*****************************************************************
C     CALCULATE VOLUME AND TOLERANCE FOR REGION R(I)
C*****************************************************************
      IF(IGOTO .EQ. 3) GO TO 3
      VOLRJ=1.0
      DO 10 I=1,KDIM
10    VOLRJ=VOLRJ*(B(I)-A(I))
      GO TO 11
3     VOLRJ=0.5*VOLRJ
      GO TO 2
11    GO TO (1,2),IGOTO
C   WHEN IGOTO=1,THEN BEFORE CALLING THIS SUBROUTINE,SET TOLI=(ERROR
1     TOL=TOLI
      VOLR=VOLRJ
      RETURN
2     VIOV=VOLRJ/VOLR
      IF(VIOV .GT. .001) TOLI=TOL*VIOV
      IF(VIOV .LE. .001) TOLI=.001 *TOL
      RETURN
      END
```

```
'FOR7D,ISZ ,RANPT
      SUBROUTINE RANPT(AA,BB,JDIR,LOR,HALF,CJ,KDIM,XI)
      EQUIVALENCE (AA),(BB)
      DOUBLE PRECISION  XI,XS
      COMMON/B3/MCRUDE
      DIMENSION AA(KDIM),BB(KDIM),XI(KDIM),XS(100)
C*************************************************************************
C     GENERATE UNIFORM SAMPLE
C*************************************************************************
      AC=AA(JDIR)
      IF(LOR .EQ. 2  .AND.  MCRUDE .EQ.  0) GO TO 11
      IF(LOR .EQ. 2) AC=CJ
      DO 10 I=1,KDIM
      IF(I .EQ. JDIR) GOTO 1
      XI(I)=RANUN(R)*(BB(I)-AA(I))+AA(I)
      GO TO 10
1     XI(I)=RANUN(R)*HALF+ AC
10    XS(I)=XI(I)
      RETURN
11    DO 30 I=1,KDIM
30    XI(I)=XS(I)
      XI(JDIR)=XS(JDIR)+CJ-AA(JDIR)
      RETURN
C*************************************************************************
C*****
      ENTRY ANTHET  (AA,BB,JDIR,LOR,HALF,CJ,KDIM,XI)
C*****
C*************************************************************************
      DO 20 I=1,KDIM
      IF(I .EQ. JDIR   .AND.  LOR  .EQ.  1 ) GO TO 2
      XI(I)=AA(I)+BB(I) - XS(I)
      GO TO 20
2     IF(LOR .EQ. 1 )  XI(I)=AA(I)+CJ-XS(I)
      IF(LOR .EQ. 2 )  XI(I)=CJ+BB(I)-XS(I)
20    CONTINUE
      RETURN
      END
```

```
'FOR7D,ISZ ,CRUDMC
      SUBROUTINE CRUDMC(AA,BB,XI,KDIM,F,NPT,NN,SS,AREA,SMV)
C*************************************************************************
CALULATE APPROXIMATION TO INTEGRAL BY SAMPLING DIRECTLY FROM THE GIV
C     AND BY USING A SEQUENTIAL SAMPLING SCHEME
C*************************************************************************
      DOUBLE PRECISION  AREA,SSQ,Y,YA,SS,SMV
      DOUBLE PRECISION  F,XI
      DIMENSION AA(KDIM),BB(KDIM),XI(KDIM)
      COMMON/B3/MCRUDE/B4/TOLI,VOLRJ
      COMMON/B5/TIMAX,NPTMIN,C
      EQUIVALENCE (AA),(BB),(XI)
      TIMEON=TIMEF(1.0)
      AREA=0.
      SSQ=0.0
      NTIMES=0
      IF (NPT .LE. 1)  RETURN
      NPTO2=NPT/2
      IF(MCRUDE .EQ. 1) NPTO2=NPT
      IF(NPTO2 .GT. 10000) NPTO2=10000
4     DO 10 I=1,NPTO2
      CALL RANPT(AA,BB,0,0,0.,0.,KDIM,XI)
      Y=F(XI,KDIM)
      IF(MCRUDE .EQ. 1) GO TO 1
      CALL ANTHET  (AA,BB,0,0,0.,0.,KDIM,XI)
      YA=F(XI,KDIM)
      Y=Y+YA
1     NM1=I-1 + NTIMES*NPTO2
      N=NM1+1
      IF(NM1 .EQ. 0) GO TO 10
      SSQ=SSQ+(NM1*Y-AREA)**2/(NM1*N)
10    AREA=AREA + Y
      NTIMES=NTIMES+1
      IF(NPT*NTIMES .LT. NPTMIN) GO TO 4
      SMV=(SS*(NN/C)+SSQ*VOLRJ**2)/(NPT*NTIMES+NN)**2
      TIMTOT=(TIMEF(1.0)-TIMEON)/1000.
      IF(SMV .LE. TOLI) GO TO 3
      IF(TIMTOT .LT. TIMAX) GO TO 4
      PRINT 5, TIMAX
5     FORMAT(' **** MAXIMUM TIME LIMIT OF ',F5.1, ' SECONDS PER STRA
     1EXCEEDED AND SMV .GT. TOLI **********')
3     NPT=NTIMES*NPT
      Y=AREA*VOLRJ/NPT
      PRINT 28,NPT,TIMTOT,Y
28    FORMAT(20X,4HNPT=I7,10X,5HTIME=F10.3,8H SECONDS,10X,5HEST0=D14
      RETURN
      END
```

```
'FOR,IS `,F
      DOUBLE PRECISION FUNCTION F(X,KDIM)
      DOUBLE PRECISION  X
      DIMENSION X(KDIM)
      EQUIVALENCE (X)
C*************************************************************************
C     USER SUPPLIED FUCTION
C*************************************************************************



      RETURN
      END
'FIN
```