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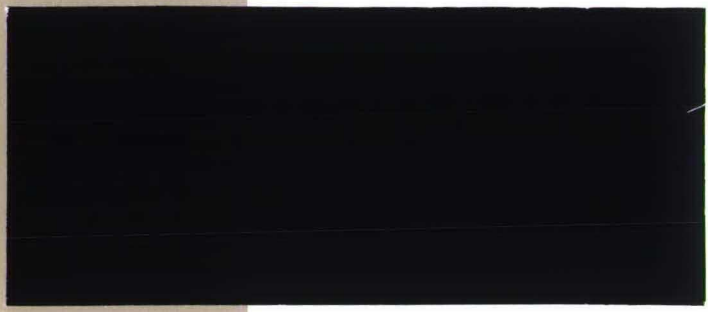

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MONTE CARLO SAMPLING AND VARIANCE REDUCTION TECHNIQUES

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Monte Carlo Sampling and Variance Reduction Techniques*

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MONTE CARLO SAMPLING AND VARIANCE REDUCTION TECHNIQUES

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Let $\ell(\boldsymbol{v})$ be the expected performance of a discrete event system (DES):

$$\ell(\boldsymbol{v}) = \boldsymbol{E}_{\boldsymbol{v}}\varphi\{L(\boldsymbol{Y})\} \tag{1}$$

where $L(\boldsymbol{Y})$ is the sample performance function (simulation model) driven by an input vector $\boldsymbol{Y}$ with probability distribution function (pdf) $f(\boldsymbol{y},\boldsymbol{v})$; the subscript $\boldsymbol{v}$ in $\boldsymbol{E}_{\boldsymbol{v}}$ means that the expectation is taken with respect to $f(\boldsymbol{y}, \boldsymbol{v})$; φ is a real valued function. To estimate $\ell(\boldsymbol{v})$ through simulation one generates a random sample $\boldsymbol{Y}_i$ with i = 1,..., N from $f(\boldsymbol{y}, \boldsymbol{v})$, computes the sample function $L(\boldsymbol{Y}_i)$, and the estimator

$$\bar{\ell}_N = \frac{1}{N}\sum_{i=1}^{N}\varphi[L(\boldsymbol{Y}_i)]. \tag{2}$$

This is called *Crude Monte Carlo (CMC)* sampling. *Variance reduction techniques (VRTs)* transform the underlying simulation model into a related one. Typically, the more one knows about the system, the more effective VRTs are. Well-known VRTs are antithetic and common random variables, control random variables, and importance sampling. Other VRTs are presented in Glynn and Iglehart (1988), Kleijnen (1974), and Wilson (1984).

There are good reasons for applying VRTs. (i) There may be negligible extra costs in terms of computer time and human effort. Examples are common and antithetic variables. (ii) The performance may represent the probability of a 'rare event'; for example, the failure probability of a highly reliable computer system may be 10^{-25}. Then the only practical alternative is importance sampling, which may make reliable estimation of the rare event probability feasible. In this paper we shall emphasize importance sampling.

Antithetic and Common Random Variables: Consider a simple example. X and Y are random variables (rv's) with known and fixed cumulative distribution functions (cdf's) F_1 and F_2. We seek a minimum variance estimator of $\boldsymbol{E}(X - Y)$. Since

$$Var(X - Y) = Var(X) + Var(Y) - 2Cov(X,Y) \tag{3}$$

$cov(X, Y)$ should be maximized. Assume that both X and Y are generated by the inverse trans-

formation method:

$$X = F_1^{-1}(U_1) = inf\{x: F_1(x) \geq U_1\}$$
$$Y = F_2^{-1}(U_2) = inf\{y: F_2(y) \geq U_2\} \quad (4)$$

where U_1 and U_2 are uniformly distributed on (0,1). We say that *common random variables (CRV)* are used if $U_1 = U_2 = U$. We say that *antithetic random variables (ARV)* are used if $U_2 = 1 - U_1$.

Since both F_1^{-1} and F_2^{-2} are monotonic nondecreasing functions of U, it is readily seen that CRV imply a non-negative covariance in (3). It can be proved that $Cov(X,Y)$ is *maximized*, so that $Var(X-Y)$ is *minimized*. Similarly, $Var(X+Y)$ is minimized when ARV are used. See Glasserman and Yao (1992).

Consider now a more realistic case, namely minimum variance estimation of $\mathbf{E}\{L_1(\boldsymbol{X}) - L_2(\boldsymbol{Y})\}$ with n-dimensional random vectors $\boldsymbol{X}$ and $\boldsymbol{Y}$, and L_1 and L_2 real-valued monotone functions in each component of $\boldsymbol{X}$ and $\boldsymbol{Y}$. In practice, L_1 and L_2 may correspond with two comparable queueing systems; if there are (say) three servers in series, then n equals four (one U per customer arrival plus one U per service time). Rubinstein, Samorodnitsky and Shaked (1985) prove that if L_1 and L_2 are monotonic in the same direction in each component of the vectors $\boldsymbol{X}$ and $\boldsymbol{Y}$ respectively and the dependence is permitted only between the components $X^{(i)}$ and $Y^{(j)}$ having the same indices $(i=j)$, then the variance of $L_1(\boldsymbol{X}) - L_2(\boldsymbol{Y})$ is minimized when $\boldsymbol{U}_1 = \boldsymbol{U}_2 = \boldsymbol{U}$, componentwise.

Antithetics (ARV) means that in (2) pairs of *negatively* correlated samples are generated: $\boldsymbol{Y}_{2i-1}$ and $\boldsymbol{Y}_{2i}$ with $i=1,\ldots,N/2$ use $\boldsymbol{U}_{1,2i-1}$ and $\boldsymbol{U}_{2,2i} = \mathbf{1} - \boldsymbol{U}_{1,2i-1}$ respectively.

When comparing two or more systems ($L_1, L_2, \ldots, L_Q$ with $Q>1$), then both common and antithetic variates can be applied. Their optimal combination (in the context of metamodeling, using the blocking concept taken from experimental design theory) is studied in Schruben and Margolin (1978); also see Donohue, Houck, and Myers (1992).

Applications of common random variables are abundant in practice, since simulationists find it the natural way to run their experiments: compare alternative systems under 'the same circumstances' (same sampled traffic rate). Their analysis is often crude: a few runs with no formal statistical analysis. If the analysis is not neglected, then the only extra work involves the estimation of the correlations among the sample performances $L(\boldsymbol{Y})$. Applications of antithetics are rare, even though their implementation is very simple (as Kleijnen and Van Groenendaal, 1992, p. 199 show).

Control Random Variables: Suppose X is an unbiased estimator of μ. A random variable

C is called a *control variate* for X if it is correlated with X and its expectation γ is known. The *linear* control random variable $X(\alpha)$ is defined as

$$X(\alpha) = X - \alpha(C - \gamma) \tag{5}$$

where α is a scalar parameter. The variance of $X(\alpha)$ is minimized by

$$\alpha^* = Cov\{X, C\}/Var\{C\}. \tag{6}$$

The resulting minimal variance is

$$Var\{X(\alpha^*)\} = (1 - \rho_{XC}^2)Var\{X\} \tag{7}$$

where ρ_{XC} denotes the correlation coefficient between X and C. Because $Cov\{X, C\}$ is unknown, the optimal control coefficient α^* must be estimated from the simulation. Estimating both $Cov\{X, C\}$ and $Var\{C\}$ means that linear regression analysis is applied to estimate α^*. Estimation of α^* implies that the variance reduction becomes smaller than (7) suggests, and that the estimator may become biased. This VRT can be easily extended to multiple control variables (simulation input variables) and multiple response variables (simulation outputs). See Kleijnen and Van Groenendaal (1992, pp. 200-201); Lavenberg, Moeller and Welch (1982); Rubinstein and Marcus (1985); and Wilson (1984).

Importance Sampling: Let $g(y)$ be a pdf that dominates $f(y,v)$ in the absolutely continuous sense:

$$supp\{f(y, v)\} \subset supp\{g(y)\}. \tag{8}$$

Using g we can represent $\ell(v)$ in (1) as

$$\ell(v) = \int \varphi[L(z)]\frac{f(z,v)}{g(z)}g(z)\,dz = E_g\left\{\varphi[L(\mathbf{Z})]\frac{f(\mathbf{Z},v)}{g(\mathbf{Z})}\right\}, \tag{9}$$

where the subscript g means that the expectation is taken with respect to g. Hence, an unbiased estimator of $\ell(v)$ is

$$\bar{\ell}_N(v) = \frac{1}{N}\sum_{i=1}^{N}\varphi[L(\mathbf{Z}_i)]\,W(\mathbf{Z}_i) \tag{10}$$

where $W(z) = f(z,v)/g(z)$ is called the *likelihood ratio* (LR); Z_i is sampled from $g(z)$.

The choice of $g(y)$ is crucial. Consider the problem of minimizing the variance of $\bar{\ell}_N$ with respect to g:

$$\min_g Var_g\left\{\varphi[L(\mathbf{Z})]\frac{f(\mathbf{Z})}{g(\mathbf{Z})}\right\}. \tag{11}$$

It is well known (e.g. Kleijnen (1974)) that the solution of this problem requires knowledge of ℓ. But ℓ is precisely the quantity we want to estimate from the simulation!

However, in many applications one can obtain drastic variance reduction by choosing a $g(y)$ of the form $g(y) = f(y, v_0)$; in other words, $g(y)$ comes from the same parametric family as does the distribution $f(y)$. The parameter vector v_0 is called the *reference* parameter. In this case, the likelihood ratio W in (10) reduces to

$$W(\mathbf{Z}_i, v, v_0) = f(\mathbf{Z}_i, v)/f(\mathbf{Z}_i, v_0), \tag{12}$$

and, instead of the problem (11), one can consider the following *simpler* problem:

$$\min_{v_0} Var_{v_0}\{\varphi[L(\mathbf{Z})]W(\mathbf{Z}, v, v_0)\}. \tag{13}$$

Rubinstein and Shapiro (1993) discuss variance reduction, emphasizing the case $v_0 = v_0^*$ where v_0^* is the optimal solution of (13).

Unlike the crude estimator, (10) allows us to estimate the response surface $\ell(v)$ essentially at *any* point v from a *single* simulation run (that is, from N replicates of a single factor combination). Moreover the *gradient* $\nabla\ell(v)$ and higher order derivatives (such as Hessians) can be estimated simultaneously with $\ell(v)$ (see Rubinstein and Shapiro 1993).

Until now we considered importance sampling for static models. Assume now that $\{L_t\}$ is a discrete time *regenerative* process with a renewal cycle length τ. An example is the waiting time process in a stable $GI/G/1$ queue with FIFO discipline. The expected steady-state performance can then be written as

$$\ell(v) = \frac{\mathbf{E}_v X}{\mathbf{E}_v \tau} \tag{14}$$

where $X = \sum_1^\tau L_t$. Note that when $\{L_t\}$ is a continuous time process, then the sum in $X = \sum_1^\tau L_t$ is replaced by the corresponding integral.

Assume again that $g(z)$ dominates $f(z, v)$ in the absolutely continuous sense (see (8)). It can be shown that

$$\ell(v) = \mathbf{E}_g\{\sum_1^\tau L_t \tilde{W}_t\}/\mathbf{E}_g\{\sum_1^\tau \tilde{W}_t\} \tag{15}$$

where

$$\tilde{W}_t = \prod_1^t W_j, \quad W_j = f(\mathbf{Z}_j, v)/g(\mathbf{Z}_j),$$

and $\mathbf{Z}_j$ is distributed according to $g(z)$; see Rubinstein and Shapiro (1993).

Let $\mathbf{Z}_{11},\ldots,\mathbf{Z}_{\tau_1 1},\ldots,\mathbf{Z}_{1N},\ldots,\mathbf{Z}_{\tau_N N}$ be a sample of N regenerative cycles generated from $g(z)$. Then a consistent estimator of $\ell(v)$ is

$$\bar{\ell}_N(v) = \sum_1^N \sum_1^{\tau_i} L_{ti}\tilde{W}_{ti}/\sum_1^N \sum_1^{\tau_i} \tilde{W}_{ti}. \tag{16}$$

Note that (as in the static case) the response surface $\ell(v)$ can be estimated from a single

simulation run, and so can derivatives of arbitrary order. Assuming again that $g(\mathbf{y}) = f(\mathbf{y}, \nu_0)$, Rubinstein and Shapiro (1993) discuss how to choose the reference parameter vector ν_0 in order to obtain variance reduction.

Finally we briefly discuss *rare events*. Assume that one wants to estimate the probability $\ell(x, \nu) = P_\nu\{L > x\} = \mathbf{E}_\nu\{\varphi(L)\}$ with $\varphi(L) = I_{\{L>x\}}$ and $I_{\{L>x\}}$ the indicator of the event $\{L > x\}$. If x is large, then $\ell(x, \nu)$ is small, for example, 10^{-25}.

Asmussen, Rubinstein and Wong (1993) discuss how to choose a 'good' reference parameter ν_0 in (16). Consider the following modification of $\tilde{W}_t$:

$$\tilde{W}_t = \begin{cases} \prod_{j=1}^{t} W(\mathbf{Z}_j, \nu_0) & \text{if } t \le \varsigma, \\ \prod_{j=1}^{\varsigma} W(\mathbf{Z}_j, \nu_0) & \text{if } \varsigma < t \le \tau \end{cases} \tag{17}$$

where ς is the random stopping time defined as $\varsigma = inf\ \{t: L_t = x\}$ with fixed integer x. For example, L_t may be the queue length just prior to customer arrivals and $x = b$ the buffer size in the $GI/G/1/b$ queue. The basic idea is to introduce more congestion at the beginning of the cycle, by making the queue unstable (choosing $\rho(\nu_0) > 1$), until the level x is crossed; then the cycle is finished by switching back to the original traffic intensity. Heidelberger (1993) demonstrates that this estimator yields high accuracy, provided ν_0 is properly chosen: say, chose ν_0 according to *large deviation theory* (see Buklew, Ney and Sadovsky (1991)), or select ν_0 such that it minimizes the estimated variance of $\bar{\ell}_N(x, \nu)$ with respect to ν.

Kriman and Rubinstein (1993) introduce the notion of *complexity* of estimators, as follows. An estimator $\bar{\ell}_N(x) = \bar{\ell}_N(x, \nu)$ of ℓ is called ϵ,δ *accurate* if

$$Pr\left\{ \left| \frac{\bar{\ell}_N(x)}{\ell(x)} \right| < 1 - \epsilon \right\} > 1 - \delta. \tag{18}$$

If this inequality is guaranteed by a sample size $N = O(p(x))$ for some polynomial function p, then the estimator $\bar{\ell}_N(x)$ is called ϵ,δ *polynomial*. They show that in order for an estimator to be polynomial, it suffices that the squared coefficient of variation of $\bar{\ell}_N(x)$ is bounded in x by a polynomial function $p(x)$. Furthermore, with a "properly" chosen reference parameter vector ν_0, the estimator defined by (16) and (17) is a *polynomial* one, whereas the crude estimator is an *exponential* one, meaning that the required sample size grows exponentially with x.

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