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CORRELATION-INDUCTION TECHNIQUES FOR ESTIMATING QUANTILES IN SIMULATION EXPERIMENTS

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ABSTRACT

To estimate selected quantiles of the response of a finite-horizon simulation, we develop statistical methods based on correlation-induction techniques for variance reduction, with emphasis on antithetic variates and Latin hypercube sampling. The proposed multiple-sample quantile estimator is the average of negatively correlated quantile estimators computed from disjoint samples of the response, where negative correlation is induced between corresponding responses in different samples while mutual independence of responses is maintained within each sample. The proposed single-sample quantile estimator is computed from negatively correlated responses within one overall sample. We establish a central limit theorem for the single-sample estimator based on Latin hypercube sampling, showing that asymptotically this estimator is unbiased and has smaller variance than the comparable direct-simulation estimator based on independent replications. We also show that if the response is monotone in the simulation's random-number inputs and if the response satisfies some other regularity conditions, then asymptotically the multiple-sample estimator is unbiased and has smaller mean square error than the direct-simulation estimator.

1 INTRODUCTION

In this paper we formulate and analyze statistical methods for estimating selected quantiles of the response Y of a finite-horizon stochastic simulation experiment based on the variance reduction technique of correlation induction. Let $F(\cdot)$ denote the (unknown) cumulative distribution function (c.d.f.) of Y. For any r with $0 < r < 1$, the rth quantile ξ_r of the random variable Y is the smallest value t such that $F(t) \equiv \Pr\{Y \leq t\} \geq r$ (Serfling 1980). Most of the literature on simulation output analysis is concerned with estimating the mean (expected value) of the response Y or the mean of some appropriately chosen function of Y; unfortunately the problem of estimating quantiles is fundamentally different from the problem of estimating means (see Schmeiser 1990, p. 315). Quantiles provide additional information about the distribution of Y, and in certain cases they may be of more interest than the mean. For example, to meet the scheduled completion date δ of a large construction project with a specified degree of confidence (say, 95%), the project manager may use a simulation model of the project to obtain an estimator $\widehat{\xi}_{0.95}$ of the 95th percentile $\xi_{0.95}$ of the project duration Y; and then the required project starting time is estimated by $\delta - \widehat{\xi}_{0.95}$ (Wilson et al. 1982).

The direct-simulation method for estimating the rth quantile ξ_r of the response Y is based on the order statistics of a sample of independent identically distributed (i.i.d.) observations of Y. Variance reduction techniques seek to restructure the simulation experiment to improve the efficiency of the estimation procedure—that is, to reduce the estimation error for a fixed simulation budget. The problem of variance reduction for quantile estimation has received relatively little attention in the simulation literature. To address this problem, Lewis and Ressler (1989) extended the method of control variates to allow for nonlinear transformations of the control variable. Starting from an auxiliary response that is observed in the simulation experiment and that has known quantiles, Lewis and Ressler proposed using as a control variable the direct-simulation estimator of the rth quantile of the auxiliary response. However, these authors did not implement or test their method. Hsu and Nelson (1990) also used a control variable with known quantiles, although the estimators they developed are not classical linear control-variate estimators. Hsu and Nelson reported variance reductions of about 50%, but they considered very simple simulations in which analytical expressions can be obtained for the inverse c.d.f.'s of the control variables. In practice the main drawback of the above quantile-estimation methods seems to be the difficulty of identifying control variables with known quantiles (as opposed to identifying control variables with known means) that are strongly correlated with the response variable.

The objective of this work is to develop practical, effective variance reduction techniques for estimating selected quantiles of the response in large-scale, finite-horizon simulation experiments. The rest of this paper is organized as follows. In Section 2 we begin by discussing quantile estimation via direct simulation; and we establish some basic results on correlation-induction techniques for variance reduction, with emphasis on the methods of antithetic variates and Latin hypercube sampling. In Section 3 we formulate and analyze multiple-sample quantile estimators wherein negative correlation is induced between the corresponding simulation responses in disjoint samples while mutual independence of the responses is maintained within each sample. Section 4 treats quantile estimators resulting from correlation induction within a single sample. Finally in Section 5 we recapitulate our main findings, and we make recommendations for follow-up work. Although this paper is based on Avramidis (1993), precursors of the multiple-sample techniques discussed in Section 3 appeared in Avramidis (1992). See Avramidis and Wilson (1995b) for a detailed justification of the results presented in this paper together with a Monte Carlo study illustrating the application of these results to estimate quantiles of the completion time of a stochastic activity network.

2 BACKGROUND

2.1 Quantile Estimation via Direct Simulation

We consider finite-horizon simulation experiments in which the response has the form $Y \equiv y(\mathbf{U})$, where $\mathbf{U} \equiv (U_1, \ldots, U_d)$ is composed of d independent *random numbers*—i.e., random variables that are uniformly distributed on the unit interval (0, 1). The dimension d of the random-number input vector $\mathbf{U}$ is a finite constant. In terms of the (unknown) *inverse c.d.f.* of Y,

$$F^{-1}(u) \equiv \min\{t : F(t) \geq u\} \quad \text{for all} \quad u \in [0,\, 1]\,,$$

the quantile of order r of the distribution of Y is

$$\xi \equiv F^{-1}(r) \quad \text{for} \quad 0 < r < 1.$$

Throughout the rest of this paper, we assume that a single value of r is specified; and we suppress the dependence of ξ on r for notational simplicity.

In a direct-simulation experiment, we perform n independent replications that yield i.i.d. observations $\{Y_i : i = 1, \ldots, n\}$ of the target response. Sorting these observations in ascending order, we obtain the *order statistics*

$$Y_{1,n} \leq Y_{2,n} \leq \cdots \leq Y_{n,n}.$$

The *direct-simulation* estimator of ξ based on n independent replications is defined as

$$\widehat{\xi}_{\mathrm{DS}}(\psi, n) \equiv \psi(Y_{1,n}, Y_{2,n}, \ldots, Y_{n,n}),$$

where we will consider several choices for the function $\psi(\cdot)$. To express $\widehat{\xi}_{\mathrm{DS}}$ as a function of the unordered observations, we introduce the order functions

$$\Omega_{i,n}(t_1, \ldots, t_n) \equiv \text{the } i\text{th smallest number in } \{t_1, \ldots, t_n\}$$

for $i = 1, \ldots, n$; and the vector-valued function

$$\vec{\Omega}_n(t_1, \ldots, t_n) \equiv \left[\Omega_{1,n}(t_1, \ldots, t_n),\ \ldots,\ \Omega_{n,n}(t_1, \ldots, t_n)\right]$$

so that we can write

$$\widehat{\xi}_{\mathrm{DS}}(\psi, n) = \psi \circ \vec{\Omega}_n(Y_1, Y_2, \ldots, Y_n), \qquad (1)$$

where the symbol "$\circ$" denotes function composition.

The most natural choice for estimating ξ is to use $\widehat{\xi}_{\mathrm{DS}} = \min\{t : F_n(t) \geq r\}$, where $F_n(\cdot)$ is the empirical c.d.f. of Y. The usual definition of $F_n(\cdot)$ is

$$F_n(t) \equiv \begin{cases} 0, & \text{if } t < Y_{1,n}\,, \\ i/n, & \text{if } Y_{i,n} \leq t < Y_{i+1,n} \\ & \quad \text{and } 1 \leq i \leq n-1\,, \\ 1, & \text{if } Y_{n,n} \leq t\,; \end{cases}$$

and this choice for $F_n(\cdot)$ corresponds to taking $\psi(\cdot) = \psi_1(\cdot)$ in the general definition (1) of the direct-simulation quantile estimator, where

$$\psi_1(t_1, \ldots, t_n) \equiv t_{\lceil nr \rceil}$$

and $\lceil x \rceil$ denotes the smallest integer that is greater than or equal to x. See David (1981) for properties of $\widehat{\xi}_{\mathrm{DS}}(\psi_1, n)$.

A second quantile estimator that is used, for example, in the S statistical package (Becker and Chambers 1984) results from taking the empirical c.d.f. $F_n(t)$ to be a piecewise linear function in the range $Y_{1,n} \leq t \leq Y_{n,n}$ such that $F_n(Y_{i,n}) \equiv (i - 0.5)/n$ for

$i = 1, \ldots, n$ and such that $F_n(t) \equiv 0$ for $t < Y_{1,n}$ and $F_n(t) \equiv 1$ for $t > Y_{n,n}$. This choice for $F_n(\cdot)$ corresponds to taking $\psi(\cdot) = \psi_2(\cdot)$ in the general definition (1) of the direct-simulation quantile estimator, where

$$\psi_2(t_1, \ldots, t_n) \equiv \alpha_n t_{\lceil nr+0.5 \rceil - 1} + (1 - \alpha_n) t_{\lceil nr+0.5 \rceil}$$

with

$$\alpha_n \equiv \lceil nr + 0.5 \rceil - (nr + 0.5) \quad \text{for} \quad n = 1, 2, \ldots,$$

provided $0.5/n < r < (n - 0.5)/n$. To complete the definition of $\psi_2(\cdot)$, we add that

$$\psi_2(t_1, \ldots, t_n) \equiv \begin{cases} t_1, & \text{if } r \leq 0.5/n, \\ t_n, & \text{if } (n - 0.5)/n \leq r. \end{cases}$$

2.2 A General Scheme for Correlation Induction

To provide a general framework for correlation induction, we introduce the notion of negative quadrant dependence, which was defined by Lehmann (1966).

Definition 1 *The bivariate random vector* $(A_1, A_2)^{\mathrm{T}}$ *is negatively quadrant dependent (n.q.d.) if*

$$\Pr\{A_1 \leq a_1, A_2 \leq a_2\} \leq \Pr\{A_1 \leq a_1\} \cdot \Pr\{A_2 \leq a_2\}$$

for all a_1, a_2.

Equivalently, we will say that the distribution of $(A_1, A_2)^{\mathrm{T}}$ is n.q.d. We will exploit this concept in Result 2 below to provide the desired sufficient condition for negatively correlated simulation responses. Moreover, we use the concept of negative quadrant dependence to define a special class $\mathcal{G}$ of distributions for the random-number inputs. Every distribution $G \in \mathcal{G}$ must have the following correlation-induction properties:

CI_1 For some $k \geq 2$, G is a k-variate distribution with univariate marginals that are uniform on the unit interval (0, 1).

CI_2 Each bivariate marginal of G is n.q.d.

When it is desirable to indicate explicitly that a distribution in $\mathcal{G}$ is k-variate, we will write "$G^{(k)} \in \mathcal{G}$" rather than "$G \in \mathcal{G}$." Throughout this paper, we let $G_{\mathrm{IR}}^{(k)}$ denote the distribution of k independent random numbers. It is clear that $G_{\mathrm{IR}}^{(k)}$ satisfies conditions CI_1 and CI_2 so that $G_{\mathrm{IR}}^{(k)} \in \mathcal{G}$.

Using a k-variate distribution $G^{(k)}$ selected from the special class $\mathcal{G}$ of distributions, we induce negative quadrant dependence between k replications of Y as follows. Let $I_Y \equiv \{1, \ldots, d\}$ and let L_Y denote an arbitrary subset of I_Y consisting of the indices of the random-number inputs to the simulation response function $y(\cdot)$ that are used for correlation induction. We perform k dependent replications yielding outputs

$$Y^{(i)} = y\left(U_j^{(i)} : j \in I_Y\right) \quad \text{for } i = 1, \ldots, k \qquad (2)$$

by sampling the column vectors of input random numbers,

$$\mathcal{U}_j \equiv \left[U_j^{(1)}, \ldots, U_j^{(k)}\right]^{\mathrm{T}} \quad \text{for } j \in I_Y, \qquad (3)$$

according to a scheme satisfying the following conditions—

SC_1 For every index $j \in L_Y$, the random vector $\mathcal{U}_j$ has distribution $G^{(k)}$.

SC_2 For every index $j \in I_Y - L_Y$, the random vector $\mathcal{U}_j$ has the distribution $G_{\mathrm{IR}}^{(k)}$.

SC_3 The column vectors $\mathcal{U}_1, \ldots, \mathcal{U}_d$ are mutually independent.

Sampling condition SC_1 specifies that we induce dependence between the outputs $\left\{Y^{(i)} : i = 1, \ldots, k\right\}$ by arranging a negative quadrant dependence between the jth random numbers sampled on each pair of replications, provided $j \in L_Y$. Sampling condition SC_2 specifies that for each $j \notin L_Y$, the jth random number should be sampled independently on different replications. Finally sampling condition SC_3 requires mutual independence of the random numbers used within the ith replication to generate the output $Y^{(i)}$; and together with property CI_1, this guarantees that each $Y^{(i)}$ has the correct distribution.

Definition 2 *The sample* $\left\{Y^{(i)} : i = 1, \ldots, k\right\}$ *is called a* (G, L_Y)*-sample of* Y *if it is generated as in* (2) *and* (3) *subject to conditions* SC_1–SC_3.

The next two results provide the justification for using correlation-induction techniques to reduce the variance of simulation-generated statistics.

Result 1 *If* G *satisfies condition* CI_2, *if* $\left\{Y^{(i)} : i = 1, \ldots, k\right\}$ *is a* (G, L_Y)*-sample of* Y, *and if* $y(\cdot)$ *is a monotone function of each argument with index in* L_Y, *then* $\left[Y^{(i)}, Y^{(\ell)}\right]^{\mathrm{T}}$ *is n.q.d. for* $i \neq \ell$.

Result 1 is essentially Theorem 1(ii) of Lehmann (1966).

Result 2 *If the bivariate random vector* $(A_1, A_2)^{\mathrm{T}}$ *is n.q.d., then* $\mathrm{Cov}(A_1, A_2) \leq 0$, *with equality holding if and only if* A_1 *and* A_2 *are independent.*

Result 2 is Lemma 3 of Lehmann (1966).

For an elaboration of the general framework for correlation induction presented in this section, see Avramidis and Wilson (1995a). In the next subsection we give examples of correlation-induction techniques that are special cases of the general scheme described above, and in each case we prove that the relevant distribution G belongs to the class $\mathcal{G}$.

2.3 Special Cases of Correlation Induction

2.3.1 Antithetic Variates (AV)

To generate two correlated replications by the method of antithetic variates, we sample the random numbers $\{U_j^\star : j = 1, \ldots, d\}$ independently and compute the column vectors of (3) according to the relation

$$\mathcal{U}_j = (U_j^\star, 1 - U_j^\star)^{\mathrm{T}} \quad \text{for } j = 1, 2, \ldots, d.$$

We let $G_{\mathrm{AV}}^{(2)}$ denote the distribution of $\mathcal{U}_j$. It is straightforward to check that $G_{\mathrm{AV}}^{(2)}$ satisfies conditions CI_1 and CI_2 so that $G_{\mathrm{AV}}^{(2)} \in \mathcal{G}$. The method of antithetic variates is clearly a special case of the general correlation-induction scheme described by (2) and (3) with $L_Y = I_Y$.

2.3.2 Latin Hypercube Sampling (LHS)

To generate k correlated replications via Latin Hypercube Sampling (LHS), we compute the input random numbers according to the relation

$$U_j^{(i)} = \frac{\pi_j(i) - 1 + U_{ij}^\star}{k} \quad \text{for } \left\{ \begin{array}{l} i = 1, \ldots, k, \\ j = 1, \ldots, d, \end{array} \right. \qquad (4)$$

where

(a) $\pi_1(\cdot), \ldots, \pi_d(\cdot)$ are permutations of the integers $\{1, \ldots, k\}$ that are randomly sampled with replacement from the set of $k!$ such permutations, with $\pi_j(i)$ denoting the ith element in the jth randomly sampled permutation; and

(b) $\{U_{ij}^\star : j = 1, \ldots, d,\ i = 1, \ldots, k\}$ are random numbers sampled independently of each other and of the permutations $\pi_1(\cdot), \ldots, \pi_d(\cdot)$.

We let $G_{\mathrm{LH}}^{(k)}$ denote the distribution of each k-dimensional column vector of input random numbers generated in this way so that

$$\mathcal{U}_j \sim G_{\mathrm{LH}}^{(k)} \ \text{ if } \left\{ \begin{array}{c} \mathcal{U}_j = \left[U_j^{(1)}, \ldots, U_j^{(k)}\right]^{\mathrm{T}} \text{ is} \\ \text{generated according to (4)} \end{array} \right\}. \qquad (5)$$

The key property of LHS is that for each j ($j = 1, \ldots, d$), the components of the column vector $\mathcal{U}_j$ form a stratified sample of size k from the uniform distribution on the unit interval (0, 1) such that there is a single observation in each stratum and the observations within the sample are negatively quadrant dependent; moreover, different stratified samples of size k are independent. Since $\pi_j(\cdot)$ is a random permutation of the integers $\{1, \ldots, k\}$, each element $\pi_j(i)$ for $i = 1, \ldots, k$ has the discrete uniform distribution on the set $\{1, \ldots, k\}$; and thus in the definition (4), the variate $\pi_j(i)$ randomly indexes a subinterval (stratum) of the form $\left((\ell - 1)/k,\ \ell/k\right]$ for some $\ell \in \{1, \ldots, k\}$. Since $U_{ij}^\star$ is a random number sampled independently of $\pi_j(i)$, we see that $U_j^{(i)}$ is uniformly distributed in the subinterval indexed by $\pi_j(i)$; and it follows that $U_j^{(i)}$ is uniformly distributed on the unit interval (0, 1). Moreover, since $\pi_j(\cdot)$ is a permutation of $\{1, \ldots, k\}$, every subinterval (stratum) of the form $\left((\ell - 1)/k,\ \ell/k\right]$ for $\ell = 1, \ldots, k$ contains exactly one of the negatively quadrant dependent random numbers $\left\{U_j^{(i)} : i = 1, \ldots, k\right\}$ so that the components of $\mathcal{U}_j$ constitute a stratified sample of the uniform distribution on (0, 1). Finally, we notice that the column vectors $\mathcal{U}_1, \ldots, \mathcal{U}_d$ are independent since the random permutations $\{\pi_j(\cdot) : j = 1, \ldots, d\}$ and the random numbers $\{U_{ij}^\star : i = 1, \ldots, k; j = 1, \ldots, d\}$ are all generated independently. We formalize this discussion in the following result.

Proposition 1 *For any $k \geq 2$, the distribution $G_{\mathrm{LH}}^{(k)}$ defined in (5) is in the class $\mathcal{G}$.*

In view of Proposition 1, we can take $G^{(k)} = G_{\mathrm{LH}}^{(k)}$ and $L_Y = \{1, \ldots, d\}$ in (2) and (3); and thus we see that LHS is a special case of correlation induction. First devised by McKay, Beckman, and Conover (1979), LHS was subsequently studied by Stein (1987) and Owen (1992a, b).

3 CORRELATION INDUCTION ACROSS SAMPLES

Motivated by the need to obtain an estimate of the variance of a quantile estimator, Schafer (1974) suggested using k independent samples, each consisting of $m = n/k$ independent observations. To simplify the exposition, we assume throughout this paper that n is an integral multiple of k. Letting $\widehat{\xi}_{\mathrm{DS}}^{(i)}(\psi, m)$ denote the direct-simulation estimator of ξ based on the ith sample ($i = 1, \ldots, k$), we define the *direct simulation-multiple sample* estimator of ξ based on k

samples and a total of n observations to be the average of the direct-simulation estimators based on the k samples of size $m = n/k$,

$$\widehat{\xi}_{\text{DS-MS}}(\psi, k, n) \equiv k^{-1} \sum_{i=1}^{k} \widehat{\xi}_{\text{DS}}^{(i)}(\psi, n/k), \qquad (6)$$

where we have substituted n/k for m on the right-hand side of (6) to show the exact dependence of $\widehat{\xi}_{\text{DS-MS}}(\psi, k, n)$ on the function $\psi(\cdot)$, the parameter k, and the total sample size n. Although the direct simulation–multiple sample estimator does not use any variance reduction techniques, we introduce it because it will simplify the statement of some of our results.

At the expense of having a variance estimator associated with the quantile estimator, we can improve upon the direct simulation–multiple sample quantile estimator by inducing negative correlation between the direct-simulation estimators computed from the k disjoint samples each of size $m = n/k$ that constitute the overall n-run experiment. Consider the following scheme for generating dependent replications $\left\{\widehat{\xi}_{\text{DS}}^{(i)}(\psi, n/k) : i = 1, \ldots, k\right\}$. Let $G^{(k)}$ be a k-variate distribution selected from $\mathcal{G}$. Let L_Y denote an arbitrary subset of $\{1, \ldots, d\}$ consisting of the indices of the random-number inputs to $y(\cdot)$ that are used for correlation induction. Generate m "column" samples $\{\mathcal{C}_j : j = 1, \ldots, m\}$ with the following properties:

CI–MS$_1$ The column sample

$$\mathcal{C}_j \equiv \left[Y_j^{(1)}, \ldots, Y_j^{(k)}\right]^{\mathrm{T}}$$

is a $(G^{(k)}, L_Y)$-sample of Y for each $j = 1, \ldots, m$; and

CI–MS$_2$ The column samples $\{\mathcal{C}_j : j = 1, \ldots, m\}$ are mutually independent.

The total set of Y-observations can be arranged in k "row" samples,

$$\mathcal{R}_i \equiv \left[Y_1^{(i)}, \ldots, Y_m^{(i)}\right] \quad \text{for} \quad i = 1, \ldots, k.$$

Condition CI–MS$_2$ guarantees that each row sample consists of m independent observations of Y, and condition CI–MS$_1$ suggests that we have induced dependence between the row vectors $\{\mathcal{R}_i : i = 1, \ldots, k\}$. From this sampling scheme we can compute $\widehat{\xi}_{\text{CI-MS}}(\psi, G^{(k)}, n)$, the *correlation induction–multiple sample* estimator of ξ based on the k-variate distribution $G^{(k)}$. Specifically, $\widehat{\xi}_{\text{CI-MS}}(\psi, G^{(k)}, n)$ is obtained by choosing $L_Y = \{1, \ldots, d\}$, computing the direct-simulation estimator of ξ from each row sample

$$\widehat{\xi}_{\text{DS}}^{(i)}(\psi, m) = \psi \circ \vec{\Omega}_m\left(Y_1^{(i)}, \ldots, Y_m^{(i)}\right) \quad \text{for} \quad i = 1, \ldots, k,$$

and then averaging these k (dependent) estimators to obtain

$$\widehat{\xi}_{\text{CI-MS}}\left(\psi, G^{(k)}, n\right) \equiv k^{-1} \sum_{i=1}^{k} \widehat{\xi}_{\text{DS}}^{(i)}(\psi, n/k). \qquad (7)$$

We have substituted n/k for m in the right-hand side of (7) to show the exact dependence of $\widehat{\xi}_{\text{CI-MS}}(\psi, G^{(k)}, n)$ on the function $\psi(\cdot)$, the distribution $G^{(k)}$, the parameter k, and the total sample size n. We will occasionally suppress the dependence of $\widehat{\xi}_{\text{CI-MS}}$ on some or all of its three arguments when no confusion can result from this usage.

We have opted to take $L_Y = \{1, \ldots, d\}$, meaning that we use all d random-number inputs to induce dependence between the observations in each of the column samples. This was done to simplify the notation and to eliminate extra parameters when formulating $\widehat{\xi}_{\text{CI-MS}}$. We also remark that the direct-simulation estimator $\widehat{\xi}_{\text{DS}}(\psi, n)$ is a special case of $\widehat{\xi}_{\text{CI-MS}}(\psi, G^{(k)}, n)$ in which we take $G^{(k)} = U(0, 1)$, the uniform distribution on the one-dimensional space $(0, 1)$ so that $k = 1$. In this case each column sample reduces to a single observation of Y, and the row sample becomes a sample of n i.i.d. observations of Y.

We compare the mean square error (MSE) of the correlation induction–multiple sample estimator $\widehat{\xi}_{\text{CI-MS}}(\psi, G^{(k)}, n)$ versus the MSE of the direct simulation–multiple sample estimator $\widehat{\xi}_{\text{DS-MS}}(\psi, k, n)$.

Theorem 1 *If $y(\cdot)$ and $\psi(\cdot)$ are monotone functions of each of their arguments, then*

$$\text{MSE}\left[\widehat{\xi}_{\text{CI-MS}}\left(\psi, G^{(k)}, n\right)\right] \leq \text{MSE}\left[\widehat{\xi}_{\text{DS-MS}}(\psi, k, n)\right]$$

for any k-variate distribution $G^{(k)} \in \mathcal{G}$ and any sample size n.

Remark 1. Typically the function $\psi(\cdot)$ satisfies the monotonicity requirement in Theorem 1. We observe that $\psi_1(\cdot)$ and $\psi_2(\cdot)$ satisfy this requirement.

Remark 2. If $y(\cdot)$ is only a monotone function of the arguments with index in a proper subset M_Y of $\{1, \ldots, d\}$, then the conclusion of Theorem 1 remains true if we use $L_Y = M_Y$ to generate the column samples as in property CI–MS$_1$.

Next we wish to compare $\widehat{\xi}_{\text{CI-MS}}(\psi, G^{(k)}, n)$ with the direct-simulation estimator $\widehat{\xi}_{\text{DS}}(\psi, n)$. Without any assumptions about the distribution of Y, it is difficult to compare the bias, variance, and MSE of these two estimators for finite n because there are no closed-form expressions for the bias and variance of the relevant order statistics. However, under some regularity conditions on the inverse c.d.f. of Y, the asymptotic behavior of the bias and variance of the order statistics can be characterized by the next result.

Lemma 1 *Let $\{Y_{1,n}, \ldots, Y_{n,n}\}$ denote the order statistics of a random sample of size n from a distribution having inverse c.d.f. $Q(\cdot)$. Let $\{i_n\}$ and $\{j_n\}$ denote sequences of positive integers such that $i_n/n = r_1 + O(1/n)$ and $j_n/n = r_2 + O(1/n)$, where r_1 and r_2 are constants such that $0 < r_1 \le r_2 < 1$. Suppose that the following regularity conditions hold:*

- RC_1 *There exist nonnegative integers a and b such that $Q(u)u^a(1-u)^b$ is bounded for $0 \le u \le 1$.*
- RC_2 *There exists a set $\mathcal{S} \subset [0, 1]$ such that: (i) $\mathcal{S}$ contains all except a finite number of points in $[0, 1]$; (ii) the constants r_1, r_2 belong to $\mathcal{S}$; (iii) the inverse c.d.f. $Q(\cdot)$ and its first and second derivatives $Q'(\cdot)$ and $Q''(\cdot)$ are bounded and continuous in $\mathcal{S}$; and (iv) the third derivative $Q'''(\cdot)$ exists and is bounded in $\mathcal{S}$.*

Then

$$\mathrm{E}[Y_{i_n,n}] = Q(r_1) + O(1/n)$$

and

$$\begin{aligned}&\mathrm{Cov}(Y_{i_n,n}, Y_{j_n,n})\\ &= \frac{1}{n} r_1(1-r_2)Q'(r_1)Q'(r_2) + O(1/n^2).\end{aligned}$$

Asymptotic expressions for the bias and variance of the quantile estimators $\widehat{\xi}_{\text{DS}}(\psi_1, n)$ and $\widehat{\xi}_{\text{DS}}(\psi_2, n)$ are readily obtained via Lemma 1. If conditions RC_1 and RC_2 hold with $Q(\cdot) = F^{-1}(\cdot)$ and $r_1 = r_2 = r$, then applying Lemma 1 for $i_n = \lceil nr \rceil$ and $j_n = \lceil nr \rceil$, we have

$$\mathrm{Bias}\left[\widehat{\xi}_{\text{DS}}(\psi_1, n)\right] = O(1/n) \tag{8}$$

and

$$\mathrm{Var}\left[\widehat{\xi}_{\text{DS}}(\psi_1, n)\right] = \frac{r(1-r)}{n[F'(\xi)]^2} + O(1/n^2); \tag{9}$$

and applying Lemma 1 to the order statistics $Y_{\lceil nr+0.5\rceil-1,n}$ and $Y_{\lceil nr+0.5\rceil,n}$ upon which $\widehat{\xi}_{\text{DS}}(\psi_2, n)$ depends, we have

$$\mathrm{Bias}\left[\widehat{\xi}_{\text{DS}}(\psi_2, n)\right] = O(1/n) \tag{10}$$

and

$$\mathrm{Var}\left[\widehat{\xi}_{\text{DS}}(\psi_2, n)\right] = \frac{r(1-r)}{n[F'(\xi)]^2} + O(1/n^2). \tag{11}$$

Now we are able to make an asymptotic comparison of the MSEs of the single- and multiple-sample direct-simulation quantile estimators. Let k be fixed. Combining (8) and (9) (respectively, (10) and (11)), we see that for $\psi(\cdot) = \psi_1(\cdot)$ (respectively, $\psi(\cdot) = \psi_2(\cdot)$),

$$\begin{aligned}&\lim_{n\to\infty} n\mathrm{MSE}\left[\widehat{\xi}_{\text{DS-MS}}(\psi, k, n)\right]\\ &= \lim_{n\to\infty} n\mathrm{Bias}^2\left[\widehat{\xi}_{\text{DS-MS}}(\psi, k, n)\right]\\ &\qquad + \lim_{n\to\infty} n\mathrm{Var}\left[\widehat{\xi}_{\text{DS-MS}}(\psi, k, n)\right]\\ &= 0 + \frac{r(1-r)}{[F'(\xi)]^2}\\ &= \lim_{n\to\infty} n\mathrm{MSE}\left[\widehat{\xi}_{\text{DS}}(\psi, n)\right].\end{aligned}$$

This result is of some intrinsic interest—it states that, in an asymptotic MSE sense, the direct estimator $\widehat{\xi}_{\text{DS}}$ and the multiple-sample estimator $\widehat{\xi}_{\text{DS-MS}}$ are equivalent. Zelterman (1987) has pointed out this property.

Finally we compare, in an asymptotic MSE sense, the correlation induction–multiple sample estimator $\widehat{\xi}_{\text{CI-MS}}(\psi, G^{(k)}, n)$ with the direct estimator $\widehat{\xi}_{\text{DS}}(\psi, n)$.

Theorem 2 *If $y(\cdot)$ is a monotone function of each of its arguments and if conditions RC_1 and RC_2 of Lemma 1 are satisfied for $Q(\cdot) = F^{-1}(\cdot)$ and $r_1 = r_2 = r$, then*

$$\begin{aligned}&\limsup_{n\to\infty} n\mathrm{MSE}\left[\widehat{\xi}_{\text{CI-MS}}\left(\psi, G^{(k)}, n\right)\right]\\ &\le \lim_{n\to\infty} n\mathrm{MSE}\left[\widehat{\xi}_{\text{DS}}(\psi, n)\right]\\ &= \frac{r(1-r)}{[F'(\xi)]^2}\end{aligned}$$

for any distribution $G^{(k)} \in \mathcal{G}$ and for both $\psi(\cdot) = \psi_1(\cdot)$ and $\psi(\cdot) = \psi_2(\cdot)$.

4 CORRELATION INDUCTION WITHIN A SAMPLE

Multiple-sample estimators are more prone to suffer from bias than single-sample estimators. If the bias component of MSE is expected to be dominant (see Avramidis and Wilson (1995b) for a discussion of such situations), then using a multiple-sample estimator might actually increase MSE by increasing bias, even if it reduces variance. This is the motivation for considering correlation induction within a sample—we use a single-sample estimator based on a sample of dependent observations. In Subsection 4.1 we discuss the general estimator based on correlation induction within a sample; and in Subsection 4.2 we study a special case of this estimator based on Latin hypercube sampling.

4.1 Correlation Induction–Single Sample Estimators

Consider the following scheme for generating n (dependent) replications of the simulation. We select an n-variate distribution $G^{(n)} \in \mathcal{G}$, and we let $L_Y \subseteq \{1,\ldots,d\}$ denote the set of indices of the random-number inputs to the response function $y(\cdot)$ that are used for correlation induction. We compute $\widehat{\xi}_{\text{CI-SS}}(\psi, G^{(n)})$, the *correlation induction–single sample* estimator of ξ based on the function $\psi(\cdot)$ and the n-variate distribution $G^{(n)}$, by choosing $L_Y = \{1,\ldots,d\}$, generating a $(G^{(n)}, L_Y)$-sample of Y, and taking the usual quantile estimator based on this sample,

$$\widehat{\xi}_{\text{CI-SS}}\left(\psi, G^{(n)}\right) \equiv \psi \circ \vec{\Omega}_n\left(Y^{(1)},\ldots,Y^{(n)}\right),$$

where

$$\{Y^{(1)},\ldots,Y^{(n)}\} \text{ is a } (G^{(n)},\{1,\ldots,d\})\text{-sample of } Y.$$

The dependence of $\widehat{\xi}_{\text{CI-SS}}$ on the sample size n is implicit in the distribution $G^{(n)}$.

We emphasize the requirement that the distribution $G^{(n)}$ used for inducing dependence must have dimension equal to the sample size n. Thus, in order for $\widehat{\xi}_{\text{CI-SS}}$ to be well-defined for all sample sizes, we must use subclasses of distributions in $\mathcal{G}$ that are defined for any given dimension. This is not the case for the distribution $G^{(2)}_{\text{AV}}$, which is defined as a two-dimensional distribution and cannot be extended to higher dimensions. On the other hand, the distribution $G^{(n)}_{\text{LH}}$ is defined for all n and thus is appropriate for use with $\widehat{\xi}_{\text{CI-SS}}$. For other examples of distributions that are suitable for use with $\widehat{\xi}_{\text{CI-SS}}$, see Avramidis and Wilson (1995b).

The estimator $\widehat{\xi}_{\text{CI-SS}}$ is fundamentally different from the estimators discussed previously—it is computed as a function $\psi(\cdot)$ of the order statistics of a sample of *dependent* observations, while the estimators $\widehat{\xi}_{\text{DS-MS}}$ and $\widehat{\xi}_{\text{CI-MS}}$ discussed in Section 3 are computed by applying the function $\psi(\cdot)$ to the order statistics of a sample of *independent* observations. Intuitively, we expect that if we induce negative correlation between each pair of Y-observations, then we should obtain a beneficial compensating effect: if one observation of the pair falls in the upper tail of $F(\cdot)$, then the other observation of the pair will tend to fall in the lower tail of $F(\cdot)$; and thus the tails of $F(\cdot)$ should be estimated more precisely than with i.i.d. sampling. More generally we show that for each cutoff value t, the estimator $F_n(t)$ has smaller variance if we induce negative quadrant dependence (and hence negative correlation) between each pair of observations in the sample $\{Y^{(i)} : i = 1,\ldots,n\}$. We have

$$\begin{aligned}\operatorname{Var}[F_n(t)] &= \operatorname{Var}\left[n^{-1}\sum_{i=1}^{n}\mathbf{1}\left\{Y^{(i)} \le t\right\}\right] \\ &= n^{-1}F(t)[1-F(t)] \qquad (12) \\ &\quad + \frac{2}{n^2}\sum_{\substack{i,\ell=1\\ i<\ell}}^{n}\operatorname{Cov}\left[\mathbf{1}\{Y^{(i)} \le t\},\, \mathbf{1}\{Y^{(\ell)} \le t\}\right];\end{aligned}$$

and since $\mathbf{1}\{Y^{(i)} \le t\}$ is a monotone function of $Y^{(i)}$ for each fixed t and for $i = 1,\ldots,n$, we can apply Results 1 and 2 of Subsection 2.2 to conclude that each covariance on the right-hand side of (12) is nonpositive if each pair of Y-observations is n.q.d. Now when the Y-observations are i.i.d., the variance of $F_n(t)$ is given by the first term on the right-hand side of (12); and thus we see that inducing a negative quadrant dependence (and hence a negative correlation) between each pair of observations in a single sample will yield an empirical c.d.f. $F_n(\cdot)$ that is everywhere a more accurate estimator of the underlying theoretical c.d.f. $F(\cdot)$ than could be obtained with random sampling. Since all of the quantile estimators discussed here are ultimately based on the inverse of the empirical c.d.f. (or a piecewise-linear approximation to the inverse of the empirical c.d.f.), it is plausible that inducing negative correlation between the observations in a single sample will yield a more accurate quantile estimator than a single- or multiple-sample estimator based on a comparable number of independent observations.

4.2 Latin Hypercube–Single Sample Estimators

We define the *Latin hypercube–single sample* estimator of ξ as

$$\widehat{\xi}_{\text{LH-SS}}(\psi, n) \equiv \widehat{\xi}_{\text{CI-SS}}\left(\psi, G^{(n)}_{\text{LH}}\right).$$

Thus $\widehat{\xi}_{\text{LH-SS}}(\psi, n)$ is a function $\psi(\cdot)$ of the order statistics of a $\left(G^{(n)}_{\text{LH}}, \{1,\ldots,d\}\right)$-sample of Y; and we will refer to such a sample as a *Latin hypercube sample of size* n. By Proposition 1 in Subsection 2.3.2 and by Results 1 and 2 in Subsection 2.2, any pair of Y-observations in a Latin hypercube sample of any size is n.q.d. and hence negatively correlated if $y(\cdot)$ is a monotone function of each of its arguments; and in such a case, the intuitive motivation discussed in the last paragraph of the previous subsection applies. However, we will see that monotonicity of $y(\cdot)$ is not necessary to guarantee improvement, at least for the special case of Latin hypercube sampling. We will derive the asymptotic distribution of $\widehat{\xi}_{\text{LH-SS}}(\psi_1, n)$ under appropriate conditions on the response Y; and as a by-product, we will see that $\widehat{\xi}_{\text{LH-SS}}(\psi_1, n)$ is asymptotically more efficient than $\widehat{\xi}_{\text{DS}}(\psi_1, n)$ and $\widehat{\xi}_{\text{DS}}(\psi_2, n)$.

We start with some preliminary notation and definitions. Let $\mathbf{U} \equiv (U_1, \ldots, U_d)$ denote the vector of random-number inputs to the simulation and let $\mathbf{u} \equiv (u_1, \ldots, u_d)$ denote a realization of $\mathbf{U}$. Given an arbitrary real-valued, square-integrable function $\varphi(\cdot)$ defined on the d-dimensional unit cube $[0,1]^d$, we decompose $\varphi(\cdot)$ as in Stein (1987). We define the following functionals of $\varphi(\cdot)$: (a) the *mean* of $\varphi(\cdot)$,

$$\mu_\varphi \equiv \mathrm{E}[\varphi(\mathbf{U})] = \int_{[0,1]^d} \varphi(\mathbf{u})\, d\mathbf{u};$$

(b) the jth *main effect* of $\varphi(\cdot)$,

$$\begin{aligned}\varphi_j(u_j) &\equiv \mathrm{E}[\varphi(\mathbf{U})|U_j = u_j] \\ &= \int_{[0,1]^{d-1}} \varphi(u_1, \ldots, u_j, \ldots, u_d) \prod_{\substack{\tau=1 \\ \tau \neq j}}^{d} du_\tau\end{aligned}$$

for $u_j \in [0, 1]$ and $j = 1, \ldots, d$; (c) the *additive part* of $\varphi(\cdot)$,

$$\varphi_{\text{add}}(\mathbf{u}) \equiv \sum_{j=1}^{d} \varphi_j(u_j) - (d-1)\mu_\varphi \quad \text{for} \quad \mathbf{u} \in [0, 1]^d;$$

and (d) the *residual from additivity* of φ,

$$\varphi_{\text{res}}(\mathbf{u}) \equiv \varphi(\mathbf{u}) - \varphi_{\text{add}}(\mathbf{u}) \quad \text{for} \quad \mathbf{u} \in [0, 1]^d.$$

We observe that $\mathrm{E}[\varphi_j(U_j)] = \mathrm{E}[\varphi_{\text{add}}(\mathbf{U})] = \mu_\varphi$ for each j, and $\mathrm{E}[\varphi_{\text{res}}(\mathbf{U})] = 0$. Moreover,

$$\begin{aligned}\mathrm{E}\big[\varphi^2_{\text{res}}(\mathbf{U})\big] &= \mathrm{Var}[\varphi_{\text{res}}(\mathbf{U})] \qquad (13) \\ &= \mathrm{Var}[\varphi(\mathbf{U})] - \sum_{j=1}^{d} \mathrm{Var}[\varphi_j(U_j)],\end{aligned}$$

where the last equality follows by observing that $\mathrm{Cov}[\varphi(\mathbf{U}), \varphi_j(U_j)] = \mathrm{Var}[\varphi_j(U_j)]$ for each j.

Recalling the representation of the simulation response $Y = y(\mathbf{U})$ as a function of the input random vector $\mathbf{U}$, we define

$$\chi(\mathbf{u}) \equiv \mathbf{1}\{y(\mathbf{u}) \leq \xi\} = \begin{cases} 1, & \text{if } y(\mathbf{u}) \leq \xi, \\ 0, & \text{otherwise,} \end{cases}$$

and we let $\chi_j(\cdot)$, $\chi_{\text{add}}(\cdot)$, and $\chi_{\text{res}}(\cdot)$ respectively denote the jth main effect, the additive part, and the residual from additivity of $\chi(\cdot)$. The asymptotic distribution of $\widehat{\xi}_{\text{LH-SS}}(\psi_1, n)$ is given by the following limit theorem in which $\xrightarrow{\mathcal{D}}$ denotes convergence in distribution (Billingsley 1986, pp. 338–339) and $N(\mu, \sigma^2)$ denotes a normal random variable with mean μ and variance σ^2.

Theorem 3 *Suppose that the following continuity conditions hold:*

CC_1 *The function $y(\cdot)$ has a finite set of discontinuities $\mathcal{D}$, with $\mathcal{D}_j$ denoting the set of jth coordinates of points in $\mathcal{D}$ for $j = 1, \ldots, d$.*

CC_2 *There exists a neighborhood $\mathcal{N}(\xi)$ of ξ such that given $U_j = u_j \in [0, 1] - \mathcal{D}_j$ for any $j = 1, \ldots, d$, the response $Y = y(\mathbf{U})$ has a density in $\mathcal{N}(\xi)$.*

If $F(\cdot)$ has a bounded second derivative in a neighborhood of ξ, and if $F'(\xi) \neq 0$, then

$$n^{1/2}\Big[\widehat{\xi}_{\text{LH-SS}}(\psi_1, n) - \xi\Big] \xrightarrow{\mathcal{D}} N\big(0, \sigma^2_{\text{LH-SS}}\big)$$

as $n \to \infty$, where

$$\sigma^2_{\text{LH-SS}} = \frac{\mathrm{Var}[\chi_{\text{res}}(\mathbf{U})]}{[F'(\xi)]^2}.$$

To facilitate a comparison of $\widehat{\xi}_{\text{LH-SS}}(\psi_1, n)$, the Latin hypercube–single sample quantile estimator, with the direct-simulation single-sample estimators $\widehat{\xi}_{\text{DS}}(\psi_1, n)$ and $\widehat{\xi}_{\text{DS}}(\psi_2, n)$, we establish results analogous to Theorem 3 for the direct-simulation estimators. If $F(\cdot)$ is differentiable at ξ with $F'(\xi) \neq 0$, then $\widehat{\xi}_{\text{DS}}(\psi_1, n)$ is asymptotically Normal:

$$n^{1/2}\Big[\widehat{\xi}_{\text{DS}}(\psi_1, n) - \xi\Big] \xrightarrow{\mathcal{D}} N\big(0, \sigma^2_{\text{DS}}\big) \quad \text{as } n \to \infty, \qquad (14)$$

where

$$\sigma^2_{\text{DS}} = \frac{r(1-r)}{[F'(\xi)]^2} = \frac{\mathrm{Var}[\chi(\mathbf{U})]}{[F'(\xi)]^2}$$

(Corollary 2.3.3.A of Serfling 1980). A similar result, proved in Avramidis and Wilson (1995), holds for $\widehat{\xi}_{\text{DS}}(\psi_2, n)$.

Proposition 2 *If $F(\cdot)$ has a probability density function (p.d.f.) $f(\cdot)$ that is continuous and nonzero at ξ, then*

$$n^{1/2}\left[\widehat{\xi}_{\text{DS}}(\psi_2, n) - \xi\right] \xrightarrow{\mathcal{D}} N(0, \sigma^2_{\text{DS}}) \quad \text{as} \quad n \to \infty. \tag{15}$$

It follows immediately from (13) applied to the function $\chi(\cdot)$ that

$$\sigma^2_{\text{LH-SS}} \leq \sigma^2_{\text{DS}}.$$

Hence Theorem 3 and results (14) and (15) tell us that $\widehat{\xi}_{\text{LH-SS}}(\psi_1, n)$ is asymptotically more efficient than $\widehat{\xi}_{\text{DS}}(\psi_1, n)$ and $\widehat{\xi}_{\text{DS}}(\psi_2, n)$. In Avramidis and Wilson (1995b) we quantify the efficiency increases that are achievable with the various single- and multiple-sample quantile estimators based on Latin hypercube sampling and antithetic variates.

5 CONCLUSIONS AND RECOMMENDATIONS

The theoretical results presented in this paper provide substantial evidence that some of the proposed correlation-induction techniques for estimating quantiles can yield worthwhile improvements in estimator accuracy relative to direct simulation. Avramidis and Wilson (1995b) also provide experimental evidence supporting this conclusion. In particular, the Latin hypercube–single sample estimator appears to be effective for estimating the upper extreme quantiles of the network completion time of a stochastic activity network.

Although several issues require follow-up investigation, perhaps the most urgent need is for a more extensive experimental evaluation of the proposed quantile estimators. An important unresolved issue is the performance of these quantile estimators when the assumptions underlying the main theoretical results (namely, Theorems 1, 2, and 3) are violated. Moreover, it is unclear whether the efficiency improvements observed for the Latin hypercube–single sample quantile estimator are typical of the gains that can be anticipated in practice. In the spirit of Nelson (1990) and Avramidis, Bauer, and Wilson (1991), a comprehensive experimental evaluation is required for the correlation-induction quantile estimators developed in this paper.

Follow-up work is also required to extend the theoretical development to cover a larger class of simulation experiments. Although our development is limited to simulations for which the dimension d of the vector of random-number inputs is fixed, we believe that much of this development can ultimately be extended to simulations where d is random. Such a complication naturally arises in the following situations: (a) a finite-horizon simulation involving, for example, the acceptance-rejection method for generating random variates; and (b) an infinite-horizon simulation potentially involving the generation of an unlimited number of random variates. Moreover, we believe that all of our results can be extended to multiresponse simulations.

In light of the demonstrated effectiveness of Latin hypercube sampling (LHS), we believe that emphasis should be given to this technique in future research. Theorem 3 should be extended to apply to the single-sample estimator $\widehat{\xi}_{\text{LH-SS}}(\psi_2, n)$ and to the multiple-sample estimator $\widehat{\xi}_{\text{CI-MS}}\left(\psi_\ell, G^{(k)}_{\text{LH}}, n\right)$ for $\ell = 1, 2$. It would also be highly desirable to have an analogue of LHS for infinite-horizon simulations. Another direction along which LHS can be generalized is to stratify the marginal distributions of subvectors of the vector of input random numbers, where the dimension of the subvectors is higher than one (Owen 1992b). Finally, practical methods should be developed for constructing asymptotically valid confidence regions for a vector of selected quantiles under Latin hypercube sampling.

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