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ON CONTROL VARIATE ESTIMATORS

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Scope and Purpose—Simulation is one method for analyzing models of systems whose behavior is affected by uncertain elements. If the uncertain elements are modeled as random variables with known distributions, then sample realizations of the system's behavior can be generated. Unfortunately, summary estimators derived from these realizations are themselves random variables, and thus are subject to sampling variability. The smaller this variance the more confidence we have in the estimate.

Variance reduction techniques (VRTs) are techniques designed to reduce the population variance of simulation based estimators. One example is called control variates (CVs). The purpose of this paper is to define a class of estimators that contains new CVs that have advantages over known CVs in special situations. Two examples are given along with some preliminary experimental results.

Abstract—Control variate (CV) estimators are a useful class of reduced variance estimators for simulation experiments. They correct the value of a crude estimator after the simulation outputs have been realized, and thus they do not alter the time path of the simulated stochastic process. In this paper, a broad characterization of CV estimators is proposed, the properties of this class of estimators are investigated, and the characterization is employed to derive new CV estimators that have advantageous properties in addition to reduced variance.

INTRODUCTION

Variance reduction techniques (VRTs) are techniques designed to reduce the population variance of estimators derived from simulation experiments on models of stochastic processes; they had their origins in survey sampling and Monte-Carlo estimation problems. By the term *control variate* (CV) we refer to statistics that attempt to correct the value of a crude estimator using the discrepancy between the value of a second estimator and its known expectation in a way made precise below. The appeal of control variates in simulation experiments is that the correction is applied after realizations of the stochastic process have been generated, and thus the CVs do not alter the time path of the stochastic process.

Several VRTs exploit auxiliary information present in a simulation experiment to achieve a variance reduction (see examples in Refs [1, 2]). Control variate estimators use the auxiliary information to adjust or correct the value of the estimator. The correction is usually in location or magnitude, where we use the term *location* to mean an additive shift, and *magnitude* to mean a multiplicative correction. The size of the correction is determined by the difference between a known quantity and an estimate of that quantity derived from the same simulation experiment. A different, but related technique is *poststratifying the sample*, in which a correction is made for disproportionate sampling; i.e. the discrepancy between a probabilistically proportionate sample and the sample that was actually realized is used. For a detailed comparison of control and poststratifying VRTs see Nelson and Schmeiser [2].

There is a well-established theory (see for instance Wilson [3]) and there are substantial experimental results (see, for example, Refs [4–6]) for CVs employing a linear correction of location. The only barriers to widespread application of linear CVs in practice are: (1) the difficulties in selecting an appropriate second estimator with known expectation that is also an effective CV, and (2) the necessity of using an experimental design prescribing independent replications. Selection of an inappropriate CV can result in increased variance rather than a variance reduction, and possibly an infeasible estimate (e.g. an estimate of a probability that is outside the interval [0, 1]). Using an

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experimental design based on replication analysis can be costly if the goal of the experiment is to estimate an infinite horizon ("steady-state") parameter of the stochastic process. In this paper we address the first problem by proposing the use of different (nonlinear) CVs when special aspects of the simulation experiment make them advantageous.

In the next section we propose a new general characterization of CV estimators. We then derive some basic properties of such estimators, and show how this general characterization leads to the discovery of new CV estimators. Since, to a first order approximation, the variance of nonlinear CVs is the same as linear CVs, the reason for exploring alternative forms cannot be only to enhance variance reduction. Rather, we seek to obtain advantageous properties such as reduced bias, bounds on estimators, or easy selection of an effective CV. A goal of this paper is to stimulate new directions in CV research, now that the basic theory of linear CVs is well established.

CONTROL VARIATE ESTIMATORS

Our notational convention is to use capital Roman letters to denote random variables, and their lower case counterparts to denote realizations. Lower case Greek letters denote constants.

The random variables in a simulation experiment can be partitioned into three sets: inputs (X), outputs (Y) and statistics (Z). *Inputs* are random variables defined by known probability distributions; *outputs* are functions of the inputs that are observed; *statistics* are functions of the outputs that are point estimators of the parameters of interest. For example, in a queueing simulation the inputs might include the interarrival time and service time random variables, the outputs might include customer sojourn times, and the statistics might include the fraction of time the server is idle, if the parameter of interest is the expected fraction of time the server is idle. These definitions are made precise in Nelson and Schmeiser [7], and are an essential part of a taxonomy of VRTs [2, 7]. In the present paper it is the outputs and the statistics that are of primary interest.

Let Y_1 and Y_2 be two sequences of scalar output random variables, and let s_1 and s_2 be two scalar valued functions such that

$$E[s_1(Y_1)] = \theta \quad \text{and} \quad E[s_2(Y_2)] \cong \alpha \tag{1}$$

where θ is the parameter of interest and α is known. We are interested in estimators of the form

$$Z_c = h(s_1, s_2) \tag{2}$$

where s_1 is the original or "crude" estimator of θ and s_2 is the control variate; CV estimators use the difference between α and the realized value of s_2 to correct the estimate of θ provided by s_1. As shown below, s_1 and s_2 must be correlated for the combined estimator h to be effective. In the taxonomy of Nelson and Schmeiser [2, 7] the CV estimator (2) uses *auxiliary information* (Y_2) and *equivalent information* (the combined estimator h) to form the CV estimator, and possibly *dependence induction* to force s_1 and s_2 to be correlated. When s_1 and s_2 are functions of outputs from the same real or conceptual system the technique is sometimes called *internal* CV, and when s_2 is a function of outputs from a similar real or conceptual system, the VRT is sometimes called *external* CV. A new hybrid CV that blurs these distinctions is proposed later.

The most well-known control variate estimators are the *linear* CV

$$Z_c = s_1 - \beta(s_2 - \alpha) \tag{3}$$

where β is a constant or is estimated from the simulation outputs, and the *ratio* CV

$$Z_c = s_1 s_2^{-1} \alpha. \tag{4}$$

See, for instance, Cochran [8] or Kleijnen [9]. Both (3) and (4) extend naturally to multivariate control variates (see Refs [10, 11], respectively). Because of the new direction taken here we concentrate on univariate CVs, but extension to multivariate controls is straightforward.

The linear and ratio CVs are special cases of (2) that have proven useful. We now propose a new, general characterization of CVs in terms of five required properties. Although this is a more restrictive characterization than (2), any estimator that satisfies these five properties is still not guaranteed to be effective. Instead, these five properties establish a much smaller class of estimators in which to search for new CVs. In the next section we examine the statistical implications of these properties.

(P1) $E[s_1(Y_1)] = \theta$ and $E[s_2(Y_2)] \cong \alpha$

(P2) $E[Z_c] \cong \theta$

(P3) $h(\theta, \alpha) = \theta$

(P4) $h(s_1, \alpha) = s_1$

(P5) $|h(s_1, \eta) - s_1|$ is nondecreasing in $\eta - \alpha$ for $\eta > \alpha$, and $\alpha - \eta$ for $\eta < \alpha$.

Property (P1) establishes that s_1 and s_2 are estimators of their respective estimands (θ and α), while (P2) establishes that Z_c is a useful estimator of θ (we leave the "$\cong$" vague for now, but usually interpret it to mean at least a consistent estimator). We make use of (P3) below to examine the bias of such estimators. Property (P4) implies that no correction occurs if s_2 is equal to its expectation, and (P5) establishes that the correction is greater as the discrepancy between s_2 and α increases. CV estimators (3) and (4) possess these properties.

VARIANCE OF CV ESTIMATORS

The class of estimators characterized by (P1)–(P5) is still quite large and diverse. However, some statistical properties of the class as a whole can still be derived. The following results are helpful, but not conclusive, for evaluating potential new CVs. Additional analysis of specific cases will usually be required, as illustrated in the next section.

Suppose that h is analytic at (θ, α), so that we can expand it in a Taylor series about that point. Then

$$Z_c = h(\theta, \alpha) + \frac{\partial h(\theta, \alpha)}{\partial s_1}(s_1 - \theta) + \frac{\partial h(\theta, \alpha)}{\partial s_2}(s_2 - \alpha) + R_2 \tag{5}$$

where R_2 is the remainder term in the Taylor series expansion. Dropping the remainder term we can use the expansion to show that

$$\mathrm{Var}(Z_c) \cong \left[\frac{\partial h}{\partial s_1}\right]^2 \mathrm{Var}(s_1) + \left[\frac{\partial h}{\partial s_2}\right]^2 \mathrm{Var}(s_2) + 2\frac{\partial h}{\partial s_1}\frac{\partial h}{\partial s_2}\mathrm{Cov}(s_1, s_2) \tag{6}$$

where the partial derivatives are evaluated at (θ, α). Cramèr [12] showed that if s_1 and s_2 are sample central moments, then the remainder term needed to make (6) an equality is $O(n^{-3/2})$, where n is the sample size. Frequently s_1 and s_2 are sample means of the sequences Y_1 and Y_2, respectively; see Wilson and Pritsker [5] for an argument against using sample means.

Expression (6) is exact for the linear CV estimator (3), and permits determination of the multiplier β^* that minimizes the variance of (3) by taking the derivative of (6) with respect to β. The result is [13]:

$$\beta^* = \frac{\mathrm{Cov}(s_1, s_2)}{\mathrm{Var}(s_2)}.$$

Using β^*, the variance of Z_c is $(1 - \rho^2)\mathrm{Var}(s_1)$, where ρ is the correlation coefficient of s_1 and s_2. Of course, β^* is not usually known, but it may be estimable from the simulation outputs (see Ref. [9]). In the case of the ratio CV (4), it is well-known that Z_c will have smaller variance than s_1 if

$$\rho > \frac{1}{2}\frac{\theta}{\alpha}\sqrt{\frac{\mathrm{Var}(s_2)}{\mathrm{Var}(s_1)}}$$

when $\theta\alpha^{-1} > 0$ [8].

In general, (6) shows that $\mathrm{Var}(Z_c)$ will be less than $\mathrm{Var}(s_1)$, to the order of the approximation, if

$$\rho < \frac{-1}{2}\frac{\partial h}{\partial s_2}\sqrt{\frac{\mathrm{Var}(s_2)}{\mathrm{Var}(s_1)}} \quad \text{when } \frac{\partial h(\theta,\alpha)}{\partial s_2} > 0$$
$$\rho > \frac{-1}{2}\frac{\partial h}{\partial s_2}\sqrt{\frac{\mathrm{Var}(s_2)}{\mathrm{Var}(s_1)}} \quad \text{when } \frac{\partial h(\theta,\alpha)}{\partial s_2} < 0 \tag{7}$$

since by (P4), $\partial h/\partial s_1$ evaluated at (θ, α) is one. Thus, the correlation between s_1 and s_2 must be large enough to counteract the variance introduced by incorporating s_2 into Z_c for the CV estimator to be effective.

Note that, since the expectation operator is linear, (3) is unbiased by (P1) when β is a constant. On the other hand, (4) is not unbiased in general, and neither is (3) when β^* is estimated from the same outputs that are arguments for s_1 and s_2. However, from (5), (P1) and (P3), when s_1 and s_2 are sample central moments $E(Z_c)$ can be written as

$$E(Z_c) = \theta + \sum_{k=2}^{\infty} a_k$$

where the a_k terms go to zero as k goes to infinity. In particular, if s_1 and s_2 are sample means, then $a_k = b_k n^{-k}$ for some constants b_k. Techniques such as Jackknifing [14] may be employed to reduce the bias when it takes this form, although frequently at the cost of increased variance.

Using the results of this section, is there any reason for using the ratio CV (4) instead of the linear CV (3), since the linear CV has smaller variance? First, β^* usually must be estimated, which introduces bias and decreases the potential variance reduction [15]. However, suppose we set $\beta = 1$ in (3), which is not an unreasonable choice when s_1 and s_2 are commensurate. Then from (6) and (7) we note that the variance of (4) will be less than the variance of (3) if $0 < \theta\alpha^{-1} < 1$; in other words, large, positive α is beneficial for the ratio CV, but the magnitude of α has no effect on the variance of the linear CV. While the optimal multiplier β^* is usually unknown, the relative ordering of θ and α may be known. Although this is not an overwhelming argument in favor of (4), it demonstrates how other functional forms may have advantageous properties. In the next section we give some more compelling illustrations.

FINDING NEW CV ESTIMATORS

Any estimator with properties (P1)–(P5) can be considered a CV, but its usefulness must be evaluated with respect to several criteria, including variance, bias, bounds, and ease of selection. In this section we search for estimators with properties (P1)–(P5) that also have characteristics giving them advantages over the linear CV, at least in special situations. Some experimental results for one new CV are also reported.

Extensions of the linear and ratio CV are suggested by (P1)–(P5). A first possibility is to extend the linear CV (3) to one that is polynomial in $(s_2 - \alpha)$, i.e.

$$Z_c = s_1 - \beta_1(s_2 - \alpha) + \beta_2(s_2 - \alpha)^2 + \ldots.$$

Kleijnen [9] discusses this extension and reports only marginally improved results. An extension of the ratio CV (4) that includes a "multiplier" β is

$$Z_c = s_1\left[\frac{\alpha}{s_2}\right]^{1/\beta}. \tag{8}$$

However, the logarithm of (8) is of the same form as (3), and thus will usually offer little improvement over using the linear CV directly.

For completeness, we present a modification of the linear CV (3) suggested by Kaur [16].

$$Z_c = \delta s_1 + b^*(s_2 - \alpha) \tag{9}$$

where δ is a constant and b^* is the estimated value of β^*. Kaur shows that if $2\rho^2 - 1 < \delta < 1$ then the mean squared error of (9) is less than (3) using b^*. Thus, knowledge of ρ can be used to produce an improved estimator. However, (9) does not strictly satisfy (P4), and we will restrict attention to estimators that satisfy all five properties.

To find new CV estimators, we seek estimators such as (3) and (4) that satisfy (P1)–(P5). An example of a new CV discovered in this way is given below

$$Z_c = S_1^{s_2/\alpha}. \tag{10}$$

If θ is a probability, or any quantity between 0 and 1, then (10) satisfies (P1)–(P5). In addition, Z_c is guaranteed to be between 0 and 1, which is not true of (3) or (4). Of course, if s_1 and s_2 are negatively correlated the numerator and denominator in the exponent of (10) should be reversed. We call (10) the *power* CV.

From (6) the variance of (10) is approximately

$$\mathrm{Var}(s_1) + \left[\frac{\theta}{\alpha}\ln\theta\right]^2 \mathrm{Var}(s_2) - 2\frac{\theta}{\alpha}\ln\theta\,\mathrm{Cov}(s_1, s_2)$$

and, by (7), will have smaller variance than s_1 if

$$\rho > \frac{-\theta\ln\theta}{2\alpha}\sqrt{\frac{\mathrm{Var}(s_2)}{\mathrm{Var}(s_1)}} \tag{11}$$

provided α is positive; in fact, (11) shows that large α and θ close to 1 are advantageous. However, the power CV is not unbiased. Carrying the Taylor series expansion in (5) out to one more order, some tedious algebra shows that

$$E(Z_c) \cong \theta + \frac{(\ln\theta + 1)}{\alpha}\mathrm{Cov}(s_1, s_2) + \frac{\theta}{2}\left[\frac{\ln\theta}{\alpha}\right]^2 \mathrm{Var}(s_2).$$

Thus, when $0 < \theta < e^{-1}$ ($\cong 0.3679$) the power CV will be biased high, and when $e^{-1} < \theta < 1$ the bias terms will tend to cancel since $\mathrm{Cov}(s_1, s_2)$ is positive. Of course, this result could also be used to correct for the bias by estimating it.

As a preliminary experimental evaluation of the power CV, we performed a simulation experiment to estimate the steady-state probability of finding no customers in an $M/M/1$ queue with arrival rate λ and service rate μ. Since $\theta = Pr(\text{empty}) = 1 - \lambda\mu^{-1}$ is known, we can evaluate not only the variance of (10), but also the bias. One continuous run was divided into large batches by time which were assumed to be approximately independent, and an estimate of Pr(empty) was derived from each of 15 batches by a simple time average; note that this is one way to apply CVs in infinite horizon experiments, the second barrier to application of CVs mentioned earlier. The estimated variances in Table 1 are the variances of these batch mean estimates of Pr(empty) derived from 25 replications of

Table 1. Simulation results for power CV

θ	λ/μ	Batch size	Estimated variance: Crude	Linear	Power	Estimated bias
0.9	0.1	500	0.294E − 5	0.167E − 5	0.135E − 5	0.01E − 2
0.5	0.5	1000	0.353E − 4	0.201E − 4	0.189E − 4	0.03E − 2
0.1	0.9	5000	0.412E − 4	0.428E − 4	0.398E − 4	1.62E − 2

the entire procedure. The simulation was started with the steady-state expected number of customers present in the queue.

For the control variate we chose the sample mean of the time between customer arrivals in each batch, which has asymptotic expectation λ^{-1} (as the batch size grows); λ was fixed at 1 for the experiment. The two estimators should be positively correlated since long interarrival times lead to more time when the queue is empty. For comparison, we also constructed the linear CV estimate (3) with estimated optimal β^* from the same experiments. The estimated bias for the power CV is reported, but in all cases the estimated bias for the linear CV was at least as large.

While the variance reductions are modest, there is almost no additional computational effort required to compute the power CV since it has no multiplier to estimate. The poorer performance of the linear CV is partially due to the variability of the estimator of β^*. However, setting $\beta = 1$ seriously degraded its performance. The bias is negligible until $\lambda\mu^{-1} = 0.9$, and would undoubtedly decrease for both estimators with longer batches. These results do not show that the power CV dominates the linear CV for estimating probabilities, since the linear CV might perform better with other choices of the control estimator, but they do demonstrate that other forms are worth considering for special problems.

A modification of (10) (suggested to the author by Bruce Schmeiser of Purdue University) is to raise the exponent of s_1 to the power β, and use a judicious choice of β to enhance the effectiveness of the power CV in a manner similar to the linear CV. The optimal value of β is

$$\beta^* = \frac{-\alpha}{\theta \ln \theta} \frac{\operatorname{Cov}(s_1, s_2)}{\operatorname{Var}(s_2)}. \tag{12}$$

Using β^*, the population variance of (10) is approx. $(1-\rho^2)\operatorname{Var}(s_1)$, as it was for (3). However, an estimate of (12) also involves an estimate of θ, and experimental results for the same model showed that the modified power CV with estimated β^* had a larger variance than (10). The primary advantage of the power CV seems to be the guarantee of estimates in $[0, 1]$ without the need to determine an adjusting multiplier.

Although frequently mentioned in textbook discussions of control variates, applications of external CVs have seldom appeared in the literature; an exception is Gaver and Shedler [17]. The idea behind external CVs is to simulate the system of interest and also a second, analytically tractable system using common random numbers (an example of dependence induction [2]) so that the corresponding outputs from the two systems should be positively correlated. The difference between a statistic computed from the second simulation and its known expectation is then used as a control. For example, if the parameter of interest is expected customer delay in a queue, then the delay in a Markovian queue with the same service rate and arrival rate might be used as the control system. The appeal of this form of CV is that the control for the parameter of interest can be the corresponding parameter for the second system. It is hoped that the corresponding statistics will be strongly positively correlated, and it may be that $\beta = 1$ is reasonable for the linear CV since the quantities are commensurate. However, an important disadvantage is that, even though only one set of random numbers must be generated, a second simulation must be executed. The variance reduction must be substantial to offset the extra computational effort.

Based on (P1)–(P5) another idea has been developed. Let v be a (possibly vector) of parameters of the input distributions for the analytically tractable control system, so that we can write $\alpha = c(v)$ and the function c is known. It is assumed that the system of interest has the same set of input parameters v, but differs in other respects. Instead of simulating the second system, we do the following: (1) simulate the system of interest, (2) compute s_1 and $\hat{v}$, an estimate of v, and (3) use the CV estimator $Z_c = s_1 - \beta[c(\hat{v}) - \alpha]$. Here $s_2 = c(\hat{v})$, which may not be unbiased for α but should be made to be consistent to satisfy (P1). We call CVs of this type *analytic* control variates. Note that the control system is not simulated, but rather the control variate is derived as a function of the realized input parameters of the system of interest.

In the particular example currently under investigation [18] the system of interest is an open queueing network and the control system is a similar Jackson network [19]. Thus, the parameter v includes the external arrival rates, the service rates of the servers at each queue, and the customer routing probabilities. In preliminary experimentation, the analytic CV outperformed the standard external CV for estimation of expected server utilization and customer waiting times, but neither CV produced satisfactory results for expected waiting time in all cases considered (no numerical results are given here to avoid preempting Sharon's report). Unfortunately, setting $\beta = 1$ did not prove satisfactory, as was originally hoped.

The primary advantage of the analytic control comes if effective versions can be developed for broad classes of models (such as queueing networks or certain inventory systems), so that selection of a CV is easy if it is determined that the simulation model is in that class. And of course, there is no inherent reason for using the analytic controls in the linear CV form.

CONCLUSIONS

The origin of the broader characterization of CVs presented here is a new taxonomy of VRTs [2, 7], which decomposes VRTs into basic classes of transformations. This taxonomy suggests broader definitions of a number of VRTs and facilitates comparisons between VRTs.

The power CV (10) is a natural functional form suggested by the new characterization of CVs. We suspect that there are many other useful forms, and (P1)–(P5) define a class of estimators in which to search for them. In special situations, these CVs offer advantages over the linear CV in terms of reduced bias, bounds on their values, and ease of selection given knowledge of the special situation.

The analytic CVs could potentially allow a host of tractable models to be employed as CVs for similar, but intractable models without having to simulate the tractable system. Ease of selection is the primary benefit of these estimators, since recognition of the existence of the approximate, tractable model is all that is required. The potential for exploiting such CVs seems great, but is still an open area of research. While VRTs are still not widely used by practitioners, this kind of research may eventually lead to wider use through automated application of VRTs in simulation languages; see Anonuevo and Nelson [20] for a prototype.

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