

APPROXIMATE ZERO-VARIANCE SIMULATION

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ABSTRACT

Monte Carlo simulation applies to a wide range of estimation problems, but converges rather slowly in general. Variance reduction techniques can lower the estimation error, sometimes by a large factor, but rarely change the convergence rate of the estimation error. This error usually decreases as the inverse square root of the computational effort, as dictated by the central limit theorem. In theory, there exist simulation estimators with zero variance, i.e., that always provide the exact value. The catch is that these estimators are usually much too difficult (or virtually impossible) to implement. However, there are situations, especially in the context of rare-event simulation, where the zero-variance simulation can be approximated well enough to provide huge efficiency gains. Adaptive versions can even yield a faster convergence rate, including exponential convergence in some cases. This paper gives a brief overview of these methods and discuss their practicality.

1 INTRODUCTION

1.1 Monte Carlo Estimation

Monte Carlo (MC) is the method of choice to estimate a mathematical expectation defined as a high-dimensional integral (Fishman 1996, Asmussen and Glynn 2007). To recall how it works, suppose we want to estimate  $\mu_0 = \mathbb{E}[X]$  for some random variable  $X$ . In its basic form, MC would generate  $n$  independent copies of  $X$ , say  $X_1, \dots, X_n$ , and estimate  $\mu_0$  by the sample average

$$\bar{X}_n = \frac{1}{n} \sum_{i=1}^n X_i.$$

The strong law of large numbers guarantees the almost sure convergence  $\bar{X}_n \rightarrow \mu_0$  when  $n \rightarrow \infty$ , and the accuracy of the MC method is described by the central limit theorem,

which tells us that the interval

$$\left( \bar{X}_n - \frac{z_{1-\alpha/2} S_n}{\sqrt{n}}, \bar{X}_n + \frac{z_{1-\alpha/2} S_n}{\sqrt{n}} \right)$$

is an asymptotically valid confidence interval for  $\mu_0$  with confidence level  $1 - \alpha$ , where  $z_{1-\alpha/2}$  is the  $(1 - \alpha/2)$ -quantile of the standard normal distribution; that is,  $\Phi(z_{1-\alpha/2}) = 1 - \alpha/2$  where  $\Phi$  is the standard normal distribution function, and

$$S_n^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X}_n)^2$$

is the sample variance, which is an unbiased estimator of  $\sigma^2 = \text{Var}[X]$ , assumed to be finite. The half-width of the confidence interval represents (in a probabilistic way) the estimation error. It converges to zero as  $n^{-1/2}$  when  $n \rightarrow \infty$ .

1.2 Markov Chain Model

A finite-horizon discrete-event simulation model can in general be viewed as a *discrete-time Markov chain* (DTMC)  $\{Y_j, j \geq 0\}$  that evolves in some general state space  $\mathcal{Y}$  until reaching a stopping time  $\tau$ . By putting enough information in the state  $Y_j$ , we can obtain that  $\{Y_j, j \geq 0\}$  is indeed a Markov chain and also that  $\tau$  is defined as the first time when the chain hits a given set of states,  $\Delta$ . That is,  $\tau = \inf\{j \geq 0 : Y_j \in \Delta\}$ . The Markov chain is assumed to have a transition kernel  $\{\mathbb{P}[\cdot | y], y \in \mathcal{Y}\}$  and initial distribution  $\pi_0$ , where  $\mathbb{P}[B | y] = \mathbb{P}[Y_j \in B | Y_{j-1} = y]$  and  $\pi_0(B) = \mathbb{P}[Y_0 \in B]$  for any measurable  $B \subset \mathcal{Y}$ . Suppose that each time we move from state  $y \in \mathcal{Y}$  to state  $z \in \mathcal{Y}$ , we incur a non-negative cost  $c(y, z)$ . The total cost is then the random variable

$$X = \sum_{j=1}^{\tau} c(Y_{j-1}, Y_j).$$

Let  $\mu(y) = \mathbb{E}_y[X]$  denote the expected value of  $X$  when  $Y_0 = y$ . We assume that  $\mu(y) < \infty$  for all  $y \in \mathcal{Y}$ . We want to estimate  $\mu_0 = \mathbb{E}[X] = \int_{\mathcal{Y}} \mu(y) \pi_0(dy)$ , the expected value of  $X$  for the initial distribution  $\pi_0$ .

We will exploit the fact that the function  $\mu : \mathcal{Y} \rightarrow \mathbb{R}$  satisfies the recurrence equation (or Poisson equation)

$$\begin{aligned} \mu(y) &= \mathbb{E}_y[c(y, Y_1) + \mu(Y_1)] \\ &= \int_{\mathcal{Y}} [c(y, z) + \mu(z)] d\mathbb{P}[dz | y] \end{aligned} \quad (1)$$

for  $y \notin \Delta$ , and  $\mu(y) = 0$  for  $y \in \Delta$ . This is a simplified form of the standard dynamic programming recurrence equation, without the minimization.

### 1.3 Variance Reduction

The usual way of improving accuracy is to change the estimator  $X$  to another estimator with the same expectation and smaller variance  $\sigma^2$ . Note that the bias (if any) and the computational cost are also important factors for the quality of an estimator. The computational cost is usually taken into account via a notion of efficiency, or work-normalized variance (Glynn and Whitt 1992, Glasserman 2004, Asmussen and Glynn 2007). In this paper, we concentrate on the variance only, and we assume that  $X$  has no bias.

We focus primarily on two families of variance reduction techniques, namely importance sampling and control variates. For each of them, we explain how zero-variance can be reached in principle, and we discuss situations where large gains can be obtained by approximating a zero-variance sampling scheme, in the DTMC setting discussed earlier. With adaptive schemes, it is possible to beat the  $O(n^{-1/2})$  convergence rate implied by the central limit theorem. There are even cases where one can obtain convergence at an exponential rate. We also discuss how convergence at a faster rate than  $O(n^{-1/2})$  can be achieved via generalized antithetic variates, or equivalently randomized quasi-Monte Carlo (L'Ecuyer 2008).

### 1.4 Rare Events

In the context of rare-event simulation, the system is often parameterized by a rarity parameter  $\varepsilon$  so that the important rare events become rarer (and accurate estimation becomes more difficult under naive simulation) when  $\varepsilon \rightarrow 0$ . In this type of setting, asymptotic approximations of  $\mu_0$ , valid when  $\varepsilon \rightarrow 0$ , can often be used to approximate a zero-variance sampling scheme. The quality and robustness of the estimators thus obtained can be characterized by asymptotic properties such as logarithmic efficiency (also called asymptotic optimality), bounded relative error (or relative variance), and vanishing relative error (L'Ecuyer

et al. 2008). We will briefly survey these properties and give examples.

### 1.5 Outline

The remainder of the paper is organized as follows. Some of the main asymptotic robustness properties of estimators in a rare event setting are summarized in Section 2. In Section 3, we recall how to simulate a Markov chain with importance sampling, define a zero-variance estimator in that context, and give examples where this zero-variance estimator can be well approximated. In Section 4, we provide a similar discussion on how zero-variance can be approximated via control variates. Section 5 discusses adaptive learning algorithms to approach the zero-variance estimator, for the two families of variance reduction techniques discussed earlier. Difficulties and potential remedies are highlighted. Generalized antithetic variates are discussed in Section 6. Section 7 summarizes the important facts concerning zero-variance estimation and discusses some directions of research we believe are worthy to push forward.

## 2 ASYMPTOTICS FOR RARE-EVENT SIMULATION

In rare-event simulation, asymptotic analysis of estimators is usually done under the following type of framework. The quantity  $\mu_0 = \mu_0(\varepsilon) > 0$  to be estimated is parameterized by a rarity parameter  $\varepsilon > 0$ , in a way that  $\lim_{\varepsilon \rightarrow 0^+} \mu_0(\varepsilon) = 0$ . We have a family of estimators  $X = X(\varepsilon)$  taking their values in  $[0, \infty)$ , such that  $\mathbb{E}[X(\varepsilon)] = \mu_0(\varepsilon)$  and  $\text{Var}[X(\varepsilon)] = \sigma_0^2(\varepsilon)$  for each  $\varepsilon > 0$ . For a given model, different parameterizations may specify different asymptotic regimes (Heidelberger 1995, Juneja and Shahabuddin 2006). For example, in a queueing system with buffer size  $B$  and  $s$  servers, we can take  $\varepsilon = 1/B$  if we are interested in very large values of  $B$ , and  $\varepsilon = 1/s$  if we are interested in what happens when there is a large number of servers. In reliability models, some of the failure rates are often taken as polynomial functions of  $\varepsilon$  (Shahabuddin 1994, Nakayama 1996).

In this type of setting, we would like to be able to estimate  $\mu_0(\varepsilon)$  to a given relative accuracy with a computing budget that does not increase with  $\varepsilon$ . This corresponds to the notion of an estimator with *bounded relative error* (BRE), defined below. There are situations, however, where the best available estimators do not have BRE, but require a computing budget that increases only very slowly with  $\varepsilon$  for a given relative accuracy. These estimators often enjoy the slightly weaker property of *logarithmic efficiency* (LE), also known as *asymptotic optimality*. Importance sampling estimators constructed via the theory of large deviations often have this property (Heidelberger 1995, Juneja and Shahabuddin 2006, Asmussen and Glynn 2007). A third property, also defined below, is that of *vanishing relative*

error (VRE). It means that the relative error converges to zero when  $\varepsilon \rightarrow 0$ , for a given computing budget.

**Definition 1** (a) The estimator  $X(\varepsilon)$  has *bounded relative error* (BRE) (Heidelberger 1995), or equivalently *bounded relative variance*, if

$$\limsup_{\varepsilon \rightarrow 0} \frac{\sigma_0(\varepsilon)}{\mu_0(\varepsilon)} < \infty. \quad (2)$$

(b) It is *logarithmically efficient* (LE) (Heidelberger 1995, Asmussen and Glynn 2007) if

$$\lim_{\varepsilon \rightarrow 0} \frac{\ln \mathbb{E}[X^2(\varepsilon)]}{2 \ln \mu_0(\varepsilon)} = 1. \quad (3)$$

(c) It has *vanishing relative error* (VRE) (L'Ecuyer et al. 2008) if

$$\limsup_{\varepsilon \rightarrow 0} \frac{\sigma_0(\varepsilon)}{\mu_0(\varepsilon)} = 0, \quad (4)$$

or equivalently if

$$\limsup_{\varepsilon \rightarrow 0} \frac{\mathbb{E}[X^2(\varepsilon)]}{\mu_0^2(\varepsilon)} = 1. \quad (5)$$

The VRE property is obviously stronger than BRE, which is itself stronger than LE. VRE is strongly related to zero-variance simulation in the sense that VRE implies that  $X(\varepsilon)$  is generated from a probability law that converges in the  $L_\infty$  norm to a zero-variance measure (L'Ecuyer et al. 2008). We will see examples where this property holds.

Dupuis and Wang (2004) give a Lyapunov (sufficient) condition for LE, interpreting the Lyapunov function as a *subsolution* to the recurrence equation of a stochastic game in which we select a change of measure for importance sampling, and then an adversary selects a set of sample paths with the worst possible variance contribution. Other sets of Lyapunov conditions for the BRE, LE, and VRE properties can be found in Blanchet and Glynn (2007) and L'Ecuyer et al. (2008). These conditions are often convenient to verify the BRE, LE, and VRE properties, and can also be used to design importance sampling schemes that satisfy these properties.

### 3 ZERO VARIANCE VIA IMPORTANCE SAMPLING

Suppose that the estimator  $X$  of interest can be written as  $X = h(\omega)$  for some (measurable) function  $h : \Omega \rightarrow \mathbb{R}$ , where  $\omega$  obeys a probability measure  $\mathbb{P}$  defined over a measurable space  $(\Omega, \mathcal{F})$ , where  $\Omega$  is the sample space and  $\mathcal{F}$  is a  $\sigma$ -field. In *importance sampling* (IS), we replace  $\mathbb{P}$  by another probability measure  $\tilde{\mathbb{P}}$  over the same measurable space and for which  $d\tilde{\mathbb{P}}(\omega) \neq 0$  whenever  $h(\omega)d\mathbb{P}(\omega) \neq 0$ .

Under this condition, we have

$$\begin{aligned} \mathbb{E}[X] &= \int h(\omega) d\mathbb{P}(\omega) \\ &= \int h(\omega) \frac{d\mathbb{P}(\omega)}{d\tilde{\mathbb{P}}(\omega)} d\tilde{\mathbb{P}}(\omega) \\ &= \tilde{\mathbb{E}}[h(\omega)L(\omega)], \end{aligned}$$

where  $L = d\mathbb{P}/d\tilde{\mathbb{P}}$  is the likelihood ratio (or Radon-Nikodým derivative) between the two measures and  $\tilde{\mathbb{E}}$  is the expectation associated with  $\tilde{\mathbb{P}}$ . Then we can generate  $n$  independent realizations of  $\omega$  from  $\tilde{\mathbb{P}}$ , say  $\omega_1, \dots, \omega_n$ , and use the average

$$\bar{X}_{\text{is},n} = \frac{1}{n} \sum_{i=1}^n h(\omega_i)L(\omega_i)$$

as an unbiased estimator of  $\mu_0$ . The aim is to select  $\tilde{\mathbb{P}}$  so that

$$\widetilde{\text{Var}}[h(\omega)L(\omega)] \stackrel{\text{def}}{=} \tilde{\mathbb{E}}[(h(\omega)L(\omega))^2] - \mu_0^2$$

is as small as possible, and preferably much smaller than  $\text{Var}[X] = \mathbb{E}[h(\omega)] - \mu_0^2$ . If  $h$  is non-negative, one can check that  $d\tilde{\mathbb{P}}(\omega) = (h(\omega)/\mathbb{E}[h(\omega)])d\mathbb{P}(\omega)$  yields variance zero. In the case where  $\mathbb{P}$  and  $\tilde{\mathbb{P}}$  are (possibly multivariate) continuous probability distributions with densities with respect to the Lebesgue measure,  $L$  is the ratio of these densities. If they are discrete distributions, then  $L$  is the ratio of probabilities.

We shall concentrate on the case where the system is modeled by a DTMC  $\{Y_j, j \geq 0\}$  as in Section 1.2. Here,  $\omega$  represents the sample path  $Y_0, Y_1, \dots, Y_\tau$  and we have  $X = h(Y_0, \dots, Y_\tau) = \sum_{j=1}^\tau c(Y_{j-1}, Y_j)$ . To estimate  $\mu_0 = \mathbb{E}[X]$  by IS, we restrict ourselves to changes of measure that replace  $\mathbb{P}$  and  $\pi_0$  by a different kernel and (possibly) a modified initial distribution, so the model remains a Markov chain under IS. It turns out that a zero-variance change of measure can be found within this class.

We replace the transition kernel  $\{\mathbb{P}[\cdot | y], y \in \mathcal{Y}\}$  by a new kernel  $\{\tilde{\mathbb{P}}[\cdot | y], y \in \mathcal{Y}\}$ , and the initial distribution  $\pi_0$  by  $\tilde{\pi}_0$ , chosen so that for all  $B \in \mathcal{F}$ ,  $\tilde{\mathbb{P}}[B | y] > 0$  whenever  $\int_B \mu(y')\mathbb{P}[dy' | y] > 0$ ,  $\tilde{\pi}[B] > 0$  whenever  $\int_B \mu(y')\pi[dy'] > 0$ , and

$$\tilde{\mathbb{E}}[\tau] < \infty. \quad (6)$$

We should emphasize that the latter is a nontrivial condition. We then have  $\mu_0 = \tilde{\mathbb{E}}[X_{\text{is}}]$  where

$$X_{\text{is}} = \sum_{j=1}^\tau c(Y_{j-1}, Y_j)L(Y_0, \dots, Y_j) \quad (7)$$

and

$$L(Y_0, \dots, Y_j) = \frac{d\pi_0}{d\tilde{\pi}_0}(Y_0) \prod_{i=1}^j \frac{d\mathbb{P}}{d\tilde{\mathbb{P}}}(Y_i | Y_{i-1})$$

is the likelihood ratio associated with the choice of initial state and the first  $j$  transitions.

For more concreteness and simplicity, suppose that the state space  $\mathcal{Y}$  is discrete, so the transition kernel is determined by a matrix of transition probabilities  $p(y, z) = \mathbb{P}[Y_j = z | Y_{j-1} = y]$  for  $x, z \in \mathcal{Y}$ , and initial probabilities  $\pi_0(y) = \mathbb{P}[Y_0 = y]$  for  $y \in \mathcal{Y}$ . We replace the probabilities  $p(y, z)$  and  $\pi_0(y)$  by new probabilities  $\tilde{p}(y, z)$  and  $\tilde{\pi}_0(y)$ . Then,

$$\mathbb{P}[\tau = n, (Y_0, \dots, Y_\tau) = (y_0, \dots, y_n)] = \pi_0(y_0) \prod_{j=1}^n p(y_{j-1}, y_j)$$

and the likelihood ratio for the initial state and the first  $j$  transitions becomes

$$L(Y_0, \dots, Y_j) = \frac{\pi_0(Y_0)}{\tilde{\pi}_0(Y_0)} \prod_{i=1}^j \frac{p(Y_{i-1}, Y_i)}{\tilde{p}(Y_{i-1}, Y_i)}.$$

In the case of a continuous state space, the transition probabilities are replaced by densities and the likelihood ratio has the same form.

Suppose now that we change the probabilities so that

$$\tilde{\pi}(y) = \pi(y)\mu(y)/\mu_0, \quad (8)$$

$$\tilde{p}(y, z) = p(y, z)[c(y, z) + \mu(z)]/\mu(y) \text{ if } \mu(y) > 0, \quad (9)$$

$$\tilde{p}(y, z) = p(y, z) \text{ if } \mu(y) = 0, \quad (10)$$

where  $p$  represents a probability in the discrete case and a density in the continuous case. Suppose also that condition (6) holds under these new probabilities. Then, one can verify that the IS estimator  $X_{\text{is}}$  in (7) equals  $\mu_0$  with probability one under  $\tilde{\mathbb{P}}$ , so it has zero variance (Booth 1987, Kuruganti and Strickland 1996, Kollman et al. 1999, L'Ecuyer and Tuffin 2007). Indeed, we have

$$\begin{aligned} X_{\text{is}} &= \sum_{j=1}^{\tau} c(Y_{j-1}, Y_j) L(Y_0, \dots, Y_j) \\ &= \sum_{j=1}^{\tau} c(Y_{j-1}, Y_j) \frac{\pi_0(Y_0)}{\tilde{\pi}_0(Y_0)} \prod_{i=1}^j \frac{p(Y_{i-1}, Y_i)}{\tilde{p}(Y_{i-1}, Y_i)} \\ &= \sum_{j=1}^{\tau} c(Y_{j-1}, Y_j) \frac{\mu_0}{\mu(Y_0)} \prod_{i=1}^j \frac{\mu(Y_{i-1})}{c(Y_{i-1}, Y_i) + \mu(Y_i)} \\ &= \mu_0, \end{aligned}$$

where the last equality is obtained by induction on the value taken by  $\tau$ , using the fact that  $\mu(Y_\tau) = 0$ . These zero-variance modified probabilities are also unique in the

sense that no other probabilities  $\tilde{\pi}(y)$  and  $\tilde{p}(y, z)$  give a Markov chain whose IS estimator has zero variance.

It is important to recognize that condition (6) may fail to hold under the zero-variance probabilities, as illustrated by the next example where  $\tau$  becomes infinite with probability 1.

**Example 1** Consider a DTMC with  $\mathcal{Y} = \{0, 1, 2\}$ ,  $\Delta = \{2\}$ ,  $\pi_0(0) = 1$ ,  $p(0, 0) = p(0, 1) = 1/2$ , and  $p(1, 0) = p(1, 1) = p(1, 2) = 1/3$ . We define  $\mu(y)$  as the expected number of transitions before reaching state 2, given that we are in state  $y$ . We then have  $\mu(2) = 0$ ,  $c(y, 2) = 0$  for any  $y$ , and  $c(y, z) = 1$  for  $z \neq 2$ . Then, (9) gives  $\tilde{p}(y, 2) = 0$  for  $y = 0, 1$ , which implies that the chain will never reach the stopping time  $\tau$  under these new probabilities!  $\square$

This example unveils the fact that whenever all the transitions leading directly to  $\Delta$  have zero cost, these transitions will be assigned zero probability and we will never reach  $\Delta$  under the new probabilities. Fortunately, there is a simple trick to resolve this difficulty: Just add a cost  $\delta$  to any transition that enters  $\Delta$ , where  $\delta > 0$  is a constant, and run the simulation with the zero-variance probabilities thus obtained. With this trick, under the additional assumptions that  $\sup_{y \in \mathcal{Y}, z \in \Delta} c(y, z) < \infty$  and  $\inf_{y \in \mathcal{Y}} \mathbb{P}[\tau \leq m | Y_0 = y] > 0$  for some constant  $m$ , one can show that (6) is satisfied under the probabilities (9) (Baggerly, Cox, and Picard 2000). Afterward, we subtract  $\delta$  to the final (zero-variance) estimator.

Of course, we cannot implement (9) and (8) exactly, because the function  $\mu : \mathcal{Y} \rightarrow \mathbb{R}$  is unknown, but we can approximate this zero-variance change of measure if we can replace  $\mu$  in these equations by a good proxy (or good approximation) chosen so that it is not too difficult to generate variates from the corresponding IS distributions.

**Example 2** We give a simple academic example where zero variance can be reached exactly. Of course, simulation is not needed in this case; this is just an illustrative example. Consider a DTMC with state-space  $\mathcal{Y} = \{0, 1, \dots, B\}$ , for which  $p(y, y+1) = p_y$  and  $p(y, y-1) = 1 - p_y$ , for  $y = 1, \dots, B-1$ , and take  $\Delta = \{0, B\}$  (so the probabilities from 0 and from  $B$  are irrelevant). We want to compute the probability of reaching  $B$  before reaching 0, starting from a given  $y$ , i.e.,  $\mu(y) = \mathbb{P}[Y_\tau = B | Y_0 = y]$ . This is a stylized version of a problem that arises in telecommunications, where one is interested in how frequently a router becomes congested. Here, the recurrence equation (1) becomes

$$\mu(y) = p_y \mu(y+1) + (1 - p_y) \mu(y-1)$$

for  $y = 1, \dots, B-1$ , with the boundary conditions  $\mu(0) = 0$  and  $\mu(B) = 1$ . Assuming that we start from a fixed state  $Y_0 = y_0$ , the zero-variance change of measure is defined by

$$\tilde{p}_y = \frac{p_y \mu(y+1)}{\mu(y)}.$$

Because  $\mu(0) = 0$ , we see that  $\tilde{p}_1 = 1$  and that no sample path will ever return to 0 under zero-variance IS.

When  $p_y = p < 1$  for  $y = 1, \dots, B-1$ , this problem is known as the gambler's ruin problem. Its solution is  $\mu(y) = (1 - \rho^{-y}) / (1 - \rho^{-B})$  if  $\rho = p / (1 - p) \neq 1/2$ , and  $\mu(y) = y/B$  if  $\rho = 1/2$ . This gives

$$\tilde{p}_y = \frac{1 - \rho^{-y-1}}{1 - \rho^{-y}} p.$$

Note that the new probabilities  $\tilde{p}_y$  do not depend on  $B$ , but they depend on the distance from 0. Moreover, one can verify that  $(p_{y-1} / \tilde{p}_{y-1})(1 - p_y) / (1 - \tilde{p}_y) = 1$ , which means that any cycle (subpath going from one state to the same state) in a sample path does not contribute to the likelihood ratio. In other words, all paths leading to  $B$  are essentially the same path and have the same likelihood ratio. If  $p < 1/2$ , we have  $\rho < 1$  and  $\tilde{p}_y > 1/2$  for all  $y$ , so the system is attracted toward  $B$  under IS. If  $p > 1/2$ , we also have  $\tilde{p}_y > p > 1/2$ .

For large  $B$ , we can use the approximation  $\mu(y) = (\rho^{B-y} - \rho^B) / (1 - \rho^B) \approx \rho^{B-y}$ , which corresponds to the probability of the sample path that goes directly from  $y$  to  $B$ . This path is the *dominating* path when  $\rho$  is small, in the sense that it has a much larger probability than the other paths leading to  $B$ , and it is easy to see that using this approximation in (9) leads to an estimator with VRE for  $p \rightarrow 0$ , or  $B \rightarrow \infty$  with  $p < 1/2$ , because then  $\rho^{B-y} / \mu(y) \rightarrow 1$ .  $\square$

In the previous example, there is essentially a single path leading to  $B$ . For more complex Markov chains, the number of distinct paths to the target set can be much larger, and this can greatly complicate the computation of the zero-variance IS. Yet, good approximations are sometimes possible, based on asymptotic analysis, as shown by the next example, taken from L'Ecuyer et al. (2008).

**Example 3** Suppose that our Markov chain has finite state space  $\mathcal{Y} = \{0, \dots, M-1\}$ , a fixed initial state  $y_0$ , and that we want to estimate the probability  $\mu_0$  that the chain hits a given set  $B \subset \mathcal{Y}$  before returning to  $y_0$ . We have  $\Delta = B \cup \{y_0\}$ . Suppose that the transition probabilities are parameterized as

$$p(y, z) = p(y, z, \varepsilon) = \mathbb{P}[Y_j = z \mid Y_{j-1} = y] = a(y, z) \varepsilon^{b(y, z)},$$

where  $a(y, z)$  and  $b(y, z)$  are non-negative constants for each pair  $(y, z)$ . We can then write  $\mu_0 = \mu_0(\varepsilon)$ .

Models of highly reliable Markovian systems considered in Shahabuddin (1994), Nakayama (1996), L'Ecuyer and Tuffin (2007), for example, fit this framework. In these models,  $B$  represents the set of state where the system is failed and  $y_0$  is the state of a new system. Each transition corresponds either to a failure of one or more components (it brings the system closer to  $B$ ) or to a repair (it brings

the system farther from  $B$ ). Typically,  $b(y, z) > 0$  for the failure transitions and  $b(y, z) = 0$  for the repair transitions, so  $\mu_0(\varepsilon) \rightarrow 0$  when  $\varepsilon \rightarrow 0$ .

For  $y \notin \Delta$ , let  $\Pi_B(y)$  be the set of all sample paths  $\pi = (y, y_1, \dots, y_\tau)$  where  $y_\tau \in B$  and  $y_j \notin \Delta$  for  $j < \tau$ . Let  $\Pi_B = \Pi_B(y_0)$ . Suppose that there is a set  $\Pi_1 \subset \Pi_B$  such that

$$p(\pi, \varepsilon) = \prod_{j=1}^{\tau} p(y_{j-1}, y_j, \varepsilon) = a(\pi) \varepsilon^b + o(\varepsilon^b)$$

for all  $\pi \in \Pi_1$ , for some constants  $a(\pi) > 0$  and  $b > 0$ , and  $p(\pi, \varepsilon) = o(\varepsilon^b)$  for all  $\pi \notin \Pi_1$ . We also assume that all cycles that belong to some path  $\pi \in \Pi_B$  have probability  $O(\varepsilon^\delta)$ , for some constant  $\delta > 0$ . This implies that  $\Pi_1$  must be finite, because it cannot contain paths having a cycle. When  $\varepsilon \rightarrow 0$ ,  $\Pi_1$  is the set of dominant paths of  $\Pi_B$ , in the sense that

$$\lim_{\varepsilon \rightarrow 0} \frac{1}{\mu_0(\varepsilon)} \sum_{\pi \in \Pi_1} p(\pi, \varepsilon) = 1.$$

We now apply IS with modified probabilities for which

$$\tilde{p}(\pi, \varepsilon) = \prod_{j=1}^{\tau} \tilde{p}(y_{j-1}, y_j, \varepsilon) = \frac{a(\pi)}{a} + o(1) \quad (11)$$

when  $\varepsilon \rightarrow 0$ , for all  $\pi \in \Pi_1$ , where  $a = \sum_{\pi \in \Pi_1} a(\pi)$ . We assume that for each path  $\pi \in \Pi_B \setminus \Pi_1$  for which  $p(\pi, \varepsilon) = \Theta(\varepsilon^{b(\pi)})$  for  $b(\pi) > b$ , we have  $\tilde{p}(\pi, \varepsilon) = \Theta(\varepsilon^{c(\pi)})$  for some constant  $c(\pi)$  that satisfies

$$2[b(\pi) - b] > c(\pi) > 0. \quad (12)$$

We also assume that for any state  $y \notin \Delta$  that belongs to a path  $\pi \in \Pi_B$ , the probability of returning to  $y$  before hitting  $\Delta$  under IS is strictly less than 1, and the likelihood ratio associated with any such cycle does not exceed 1 if  $\varepsilon$  is small enough.

Under these conditions, the IS estimator is  $X_{\text{is}}(\varepsilon) = p(\pi, \varepsilon) / \tilde{p}(\pi, \varepsilon) = a \varepsilon^b + o(\varepsilon^b)$  if we reach  $B$  via a path  $\pi \in \Pi_1$ , which happens with probability  $1 + o(1)$ , and all other paths have  $o(1)$  contribution (L'Ecuyer et al. 2008).

L'Ecuyer and Tuffin (2007) propose heuristic methods to approximate zero-variance IS in this setting and illustrate the effectiveness of their proposals by numerical examples of highly reliable Markovian systems. After observing that

$$\mu(y) = \sum_{\pi \in \Pi_B(y)} p(\pi, \varepsilon),$$

they start with the simple idea of replacing  $\mu(y)$  in (9) by its crude lower bound

$$v_0(y) = \max_{\pi \in \Pi_B(y)} p(\pi, \varepsilon),$$

which is usually easy to compute from any state  $y$  by solving a shortest path problem. This estimate is fine when a single path dominates the sum, but otherwise it may underestimate  $\mu(y)$  significantly. Typically, this underestimation becomes worse when we are farther away from  $B$ . L'Ecuyer and Tuffin (2007) suggest refinements to this crude lower bound. A first improvement is to sum the probabilities of a set of disjoint dominant paths leading to  $B$  instead of just a single one. This gives a tighter lower bound,  $\bar{v}_0(y)$ . In another refinement, they estimate  $\mu(y_0)$  in preliminary runs with a crude IS strategy, then approximate  $\mu(y)$  by a function  $v_1(\cdot)$  that interpolates this estimate of  $\mu_0$  at  $y_0$  and on the set  $B$  (where  $\mu(y) = 1$ ) by raising  $v_1(\cdot)$  to some power. They also propose further refinements.

In their numerical experiments, IS with these types of approximations performs much better than the popular heuristics such as simple failure biasing (SFB), balanced failure biasing (BFB), and balanced likelihood ratios, proposed earlier for these types of models (L'Ecuyer and Tuffin 2007). L'Ecuyer et al. (2008) show that if  $\mu(y)$  in (9) is replaced by  $v(y)$  where  $v(y)$  is the sum of probabilities of all the dominant paths from  $y$  (those with the smallest power of  $\varepsilon$ ), then we have VRE. In this sense, the method performs increasingly better when  $\varepsilon$  gets smaller. If we just take  $v(y)$  as the probability of the most probable path to failure from  $y$ , then we have BRE but not VRE in general. With SFB or BFB, one can achieve BRE (under some conditions), but never VRE.  $\square$

In the previous examples, we have a DTMC model with a stopping time naturally defined by a subset of states. In other situations, the model might have to be reformulated appropriately so it fits our DTMC framework. This can always be done by including enough information in the state. For example, if we consider a continuous time Markov chain (CTMC) in which the cost depends on the holding time at each step, or for which the time horizon is fixed (instead of being the time when the CTMC hits a given set of states), then it suffices to include the current time (or the time that remains before reaching the horizon) in the state of the DTMC. Likewise, if we have a DTMC model with a fixed number of steps, then we must include the current step number (or the number of steps that remain) in the state.

**Example 4** This example is adapted from De Boer et al. (2007). In Example 3, suppose that we have a CTMC  $\{X(t), t \geq 0\}$  with state space  $\mathcal{X}$  and that the transition probabilities are transition rates instead. Thus, the time until the next transition is always an exponential random variable with state-dependent rate. There is a fixed time

horizon  $t_*$  and we want to estimate the probability  $\mu_0$  of reaching the set of states  $\tilde{B}$  before time  $t_*$ , from a given initial state  $y_0$ .

Let  $\{X_j, j \geq 0\}$  be the embedded DTMC (the sequence of visited states). We can easily reformulate this process as a DTMC by redefining the state at step  $j$  (just after the  $j$ th transition) as  $Y_j = (X_j, R_j)$ , where  $R_j$  is the remaining clock time before reaching  $t_*$ ,  $B = \{(X_j, R_j) : X_j \in \tilde{B} \text{ and } R_j > 0\}$  and  $\Delta = B \cup \{(X_j, R_j) : R_j \leq 0\}$ . The zero-variance change of measure is defined as usual, based on  $Y_j$ . Let  $\mu(y) = \mu(x, t)$  be the probability of reaching  $\tilde{B}$  before the time limit if the DTMC is in state  $y = (x, t)$ . We have

$$\mu(x, t) = \begin{cases} 1 & \text{if } x \in \tilde{B} \text{ and } t > 0, \\ 0 & \text{if } t \leq 0, \\ \mathbb{E}_{(x,t)}[\mu(X_1, R_1)] & \text{otherwise.} \end{cases}$$

In the latter case, we have

$$\begin{aligned} & \mathbb{E}_{(x,t)}[\mu(X_1, R_1)] \\ &= \int_0^t \sum_{x' \in \mathcal{X}} \mu(x', t - \delta) p(x, x') \lambda_x \exp[-\lambda_x \delta] d\delta, \end{aligned}$$

where  $\lambda_x$  is the total jump rate when the CTMC is in state  $x$ , and  $p(x, x')$  is the probability that this jump is to state  $x'$ . Here,  $p(x', t - \delta | x, t) = p(x, x') \lambda_x \exp[-\lambda_x \delta]$ , for  $\delta > 0$ , is the density of the next state at  $(x', t - \delta)$  when the current state is  $(x, t)$  for the DTMC.

To obtain a zero-variance IS estimator, we change the density  $p$  to a density  $\tilde{p}$  defined by

$$\tilde{p}(x', t - \delta | x, t) = \frac{\mu(x', t - \delta)}{\mu(x, t)} p(x', t - \delta | x, t)$$

for  $x' \in \mathcal{X}$  and  $0 < \delta < t$ , and 0 elsewhere, if  $\mu(x, t) > 0$  (De Boer et al. 2007). Under this new density, the time until the next jump is no longer exponential, so we no longer have a CTMC. This time is nonzero only over the interval  $(0, t)$ , and it is not a truncated exponential either; in fact, since  $\mu(x', t - \delta)$  is decreasing in  $\delta$ , the right “tail” of the new distribution of the time to the next jump (before truncation) decreases faster than for the exponential distribution. When  $\mu(x, t) = 0$ , the density is unchanged:  $\tilde{p}(x', t - \delta | x, t) = p(x', t - \delta | x, t)$ .

De Boer et al. (2007) observe that sampling from this zero-variance IS is unpractical and propose a simple approximation, similar to those of the previous example, valid for the case where the expected number of transitions within the time horizon  $t_*$  is small. The idea is to approximate  $\mu(y)$  by the sum of probabilities of a few dominant paths (those having the largest probability) among those leading to the rare set  $B$ . They give numerical examples where this approach performs well. In these examples, they consider

a single dominant path, namely the “shortest path” leading to  $B$ . They also perform an asymptotic analysis in which the jump rates are parameterized by  $\varepsilon$  in the same way as the transition rates in Example 3. They show that their approach provides an IS estimator with BRE in general, and VRE under additional conditions similar to the VRE conditions in Example 3.  $\square$

#### 4 ZERO VARIANCE VIA CONTROL VARIATES

A zero-variance estimator can also be defined via *control variates* (CV), as follows (Henderson and Glynn 2002, Henderson and Simon 2004, Kim and Henderson 2006). We again assume the same DTMC model as in Section 1.2. The idea is to replace the estimator  $X = \sum_{j=1}^{\tau} c(Y_{j-1}, Y_j)$  by

$$X_{\text{cv}} = X - M_{\tau}$$

where

$$\begin{aligned} M_{\tau} &= \sum_{j=1}^{\tau} (c(Y_{j-1}, Y_j) + \mu(Y_j) - \mu(Y_{j-1})) \\ &= \sum_{j=1}^{\tau} (c(Y_{j-1}, Y_j) + \mu(Y_j) \\ &\quad - \mathbb{E}[c(Y_{j-1}, Y_j) + \mu(Y_j) \mid Y_{j-1}]). \end{aligned}$$

One can easily verify that  $\mathbb{E}[M_{\tau}] = 0$ , so  $\mathbb{E}[X_{\text{cv}}] = \mathbb{E}[X]$  (unbiasedness), and that  $X_{\text{cv}} = \mu(y_0)$ , a constant, because  $\mu(Y_{\tau}) = 0$ . Thus, we have a zero-variance estimator.

Of course, the function  $\mu$  is unknown, but we still have  $\mathbb{E}[M_{\tau}] = 0$  if we define

$$M_{\tau} = \sum_{j=1}^{\tau} (c(Y_{j-1}, Y_j) + v(Y_j) - \mathbb{E}[c(Y_{j-1}, Y_j) + v(Y_j) \mid Y_{j-1}]), \quad (13)$$

where  $v$  is an approximation of the function  $\mu$  such that  $v(y) = 0$  for  $y \in \Delta$ . This  $M_{\tau}$  is a martingale, regardless of the choice of  $v$ . With a reasonably good approximation, the variance can sometimes be reduced significantly. Adaptive learning methods to find a good  $v$  are discussed in Section 5. Note that this methodology is usually not appropriate for rare-event simulation, because it does not make the rare events occur more frequently.

Kim and Henderson (2007) extends the method to regenerative simulation for the estimation of steady-state performance measure. Henderson and Glynn (2002) consider applications to infinite-horizon models with discounting and to stochastic differential equations.

#### 5 APPROXIMATIONS AND ADAPTIVE LEARNING

For both IS and CV, the zero-variance schemes described earlier require the knowledge or a good approximation of the function  $\mu$ . In previous examples, such approximations were obtained *a priori* by the sum of probabilities of a few dominating sample paths. More generally, in the rare event setting of Section 2, one can do well in some cases by replacing  $\mu$  by an approximation obtained from a priori knowledge of the asymptotic behavior of the system, e.g., from large deviation’s theory (Dupuis and Wang 2004, Juneja and Shahabuddin 2006, Asmussen and Glynn 2007, Blanchet and Glynn 2007).

Most practical approaches to approximate  $\mu$  work by first selecting a parametric class of functions  $\mathcal{V} = \{v(\cdot; \theta) : \mathcal{Y} \rightarrow \mathbb{R}, \theta \in \Theta\}$ , where  $\Theta \subseteq \mathbb{R}^m$ , and  $\theta = (\theta_1, \dots, \theta_m)$  is a vector of parameters that we try to optimize so that  $v = v(\cdot; \theta)$  is close to  $\mu$  in some sense.

One natural and convenient way of doing this is to select a fixed set of basis functions  $v_1, \dots, v_m$ , independent over  $\mathbb{R}$ , and define  $\mathcal{V}$  as the space of all linear combinations of these functions, i.e., the linear space

$$\mathcal{V} = \left\{ v = v(\cdot; \theta) = \sum_{i=1}^m \theta_i v_i(\cdot) \right\} \quad (14)$$

where  $\theta = (\theta_1, \dots, \theta_m) \in \mathbb{R}^m$ . In this setting, the vector  $\theta$  is usually found by least-squares approximation: an estimate  $\hat{\mu}(y)$  of  $\mu(y)$  is obtained at a finite number of initial states  $y$ , say  $y_1, \dots, y_r \in \mathcal{Y}$ , and then we compute

$$\theta = \arg \min_{\theta \in \Theta} \sum_{\ell=1}^r |v(y_{\ell}; \theta) - \hat{\mu}(y_{\ell})|^2$$

via standard least-squares linear regression, assuming that the design points  $y_1, \dots, y_r$  have been selected so that the regression coefficients are identifiable.

More generally, the parameterization can be nonlinear, in which case the optimal  $\theta$  can be much more difficult to find. It can be approximated by statistical adaptive learning (Juneja and Shahabuddin 2006), using techniques such as stochastic approximation and (iterative) sample average approximation, for example (Kim and Henderson 2006). This can work even if no explicit characterization of  $\mu$  is available a priori.

All these methods can converge to the zero-variance sampling only if the parameterized class  $\mathcal{V}$  contains the function  $\mu$ . Otherwise, the distance between  $\mu$  and its closest approximation in  $\mathcal{V}$  imposes a positive lower bound on the variance per simulation run. This means that if  $\mathcal{V}$  is fixed and  $\mu \notin \mathcal{V}$ , the central-limit theorem will eventually kick in when the computing budget increases toward  $\infty$ ,

so the convergence rate is asymptotically  $O(n^{-1/2})$  (in the probabilistic sense) in terms of the number  $n$  of simulation runs. But if  $\mu \in \mathcal{V}$ , we can do better. One simple case where  $\mu \in \mathcal{V}$  is if the state space  $\mathcal{Y}$  is finite, say  $\mathcal{Y} = \{y_1, \dots, y_m\}$ , and we take the vector  $\theta$  equal to the vector  $\mu$ ; that is,  $\theta_i = \mu(y_i)$  for  $i = 1, \dots, m$ . Kollman et al. (1999) and Baggerly et al. (2000) consider a slightly more general case where  $\mathcal{V}$  is a linear space of the form (14) that contains  $\mu$ .

In general, the most difficult task is to select a good parameterized space  $\mathcal{V}$ , so that  $\mu$  can be well approximated by at least one function from that space. In the linear case, this means a good set of basis functions  $v_1, \dots, v_m$ . In the case of IS, another key issue is that an efficient method must be available to generate random variates from the transformed probabilities or densities. If we replace  $\mu$  in (9) by an arbitrary approximation  $v$ , this would typically give a probability distribution for which no efficient random variate generation is available. This is an important limitation.

For IS, instead of parameterizing  $v$ , we can directly parameterize the IS distribution, and then minimize the variance of  $X_{is}$  with respect to these IS parameters. This type of approach has been the most popular in the past (Rubinstein and Shapiro 1993, Rubinstein 1999). It includes the cross-entropy method, for example. A major advantage is that we can restrict ourselves a priori to a parameterized class of distributions from which random variate generation is easy.

### 5.1 Adaptive Learning of Zero-Variance IS

Several algorithms have been proposed to approximate zero-variance IS by statistical learning of the function  $\mu$ , or of the IS distribution (or Markov chain transition kernel) that minimizes the variance within some class of distributions (Juneja and Shahabuddin 2006). Under certain conditions, the function  $\mu$  and the zero-variance transition kernel can be learned adaptively at an exponential rate and this provides an estimator with exponential convergence, in the sense that the error converges as  $O(e^{-\kappa n})$  for some constant  $\kappa > 0$  instead of the usual  $O(n^{-1/2})$  (Booth 1985, Booth 1987, Kollman et al. 1999, Baggerly et al. 2000).

Kollman et al. (1999) have proposed an *adaptive importance sampling* method, also called *adaptive Monte Carlo* (AMC), which proceeds iteratively as follows. At step  $i$ , it uses an approximation  $\mu^{(i)}$  of  $\mu$  (or a guess of  $\mu$ , at the first step), and performs  $r_i$  independent simulation replications using the probabilities (in the case of a discrete state space)

$$\tilde{P}^{(i)}(y, z) = \frac{P(y, z)(c(y, z) + \mu^{(i)}(z))}{\sum_{w \in \mathcal{Y}} P(y, w)(c(y, w) + \mu^{(i)}(w))}, \quad (15)$$

obtained by replacing  $\mu$  by  $\mu^{(i)}$  in the zero-variance expression (9). For  $\mu^{(i+1)}$ , these authors use a linear model, which they fit to the simulation data at step  $i$  by least-squares

regression. Under the assumptions that the linear model is exact (which is typically not quite realistic unless the model contains as many parameters as the number of states), and that the  $r_i$ 's are large enough, they prove that  $\mu^{(i)}$  converges to  $\mu$  at an exponential rate when  $i \rightarrow \infty$ . This result also applies to variants of their algorithm, including one in which  $\mu^{(i+1)}$  is defined as a convex combination of  $\mu^{(i)}$  and the least-squares fit. Baggerly, Cox, and Picard (2000) extend these results to general (continuous) state spaces. Note that this algorithm can be represented by a large Markov chain, whose state contains the current vector  $\mu^{(i)}$ . Desai and Glynn (2001) show that proving convergence to the zero-variance IS cannot be done in general with the standard techniques for analyzing geometric convergence of Harris-recurrent Markov chains, and requires specific methods of proof.

Ahamed, Borkar, and Juneja (2006) proposed another iterative learning algorithm that approximates  $\mu$  by *adaptive stochastic approximation* (ASA), in the case where  $\mathcal{Y}$  is finite. It starts with a given distribution of the initial state  $Y_0$ , an initial transition matrix  $\tilde{P}^{(0)}$ , and an initial guess  $\mu^{(0)}$  of the function  $\mu$ . The ASA algorithm runs a single sample path. At step  $j$  of the path, if the current state is  $y_j \notin \Delta$ , the current transition matrix  $\tilde{P}^{(j)}$  is used to generate the next state  $y_{j+1}$ . From this new state, we update the estimate of  $\mu(y_j)$  by the look-ahead rule:

$$\begin{aligned} \mu^{(j+1)}(y_j) &= (1 - a_j(y_j))\mu^{(j)}(y_j) \\ &+ a_j(y_j) \left[ c(y_j, y_{j+1}) + \mu^{(j)}(y_{j+1}) \frac{P(y_j, y_{j+1})}{\tilde{P}^{(j)}(y_j, y_{j+1})} \right], \end{aligned}$$

where  $\{a_j(y), j \geq 0\}$ , is a sequence of *step sizes* that satisfies  $\sum_{j=1}^{\infty} a_j(y) = \infty$  and  $\sum_{j=1}^{\infty} a_j^2(y) < \infty$  for each state  $y$ . The probability matrix is then updated as

$$\begin{aligned} \tilde{P}^{(j+1)}(y_j, y_{j+1}) &= \max \left( \delta, \right. \\ &\left. P(y_j, y_{j+1}) \frac{c(y_j, y_{j+1}) + \mu^{(j+1)}(y_{j+1})}{\mu^{(j+1)}(y_j)} \right) \end{aligned}$$

where  $\delta > 0$  is a constant whose role is to ensure that the likelihood ratio remains bounded (to rule out the possibility that it takes huge values). For the other states, we leave  $\mu^{(j+1)}(y) = \mu^{(j)}(y)$  and  $\tilde{P}^{(j+1)}(y, z) = \tilde{P}^{(j)}(y, z)$ . We then normalize via

$$\tilde{P}^{(j+1)}(y_j, y) = \frac{\tilde{P}^{(j+1)}(y_j, y)}{\sum_{z \in \mathcal{Y}} \tilde{P}^{(j+1)}(y_j, z)}$$

for all  $y \in \mathcal{Y}$ . When  $y_j \in \Delta$ , i.e., if the stopping time is reached at step  $j$ ,  $y_{j+1}$  is generated again from the initial distribution, and the current probability matrix and estimate

of  $\mu$  are left unchanged. This method makes sense only if the state space is finite and not too large, because of the need to store the vector  $\mu^{(j)}$  explicitly.

For larger state spaces, we can restrict ourselves a priori to a linear space as in (14), and use adaptive learning to optimize the parameter vector  $\theta$  instead of learning  $\mu(y)$  directly for each state  $y$ .

**Example 5** [Bolia, Juneja, and Glasserman \(2004\)](#) use least-squares regression with a given set of basis functions to approximate the value function in the context of pricing an American option, as in the least-square Monte Carlo method ([Glasserman 2004](#)), and also approximate the zero-variance IS by plugging in (9) a least-squares approximation of the *continuation* value function (the value of the option conditional on not exercising it at the current step). In a first-stage, they learn good vectors of weights  $\theta$  for each of these two value functions, and use them to approximate both the zero-variance IS and the optimal stopping rule. In a second stage, they use these approximations to estimate the value function more accurately. A key ingredient of their proposal is their choice of basis functions of the form  $v_i(y) = \exp[a_i \log^2 y + b_i \log y]$ , where the  $a_i$  and  $b_i$  are constants. With this particular choice, the IS densities at each step turn out to be mixtures of lognormal distributions, from which random variates are easy to generate. In their numerical illustrations, the variance is reduced by factors ranging from about 5 to 15, which is far from spectacular but still significant. The main factor limiting further variance reduction seems to be the lack of fit between the true value function and the best approximation with their selected basis functions.  $\square$

## 5.2 Adaptive Learning for Control Variates

For control variates, it is also natural to approximate  $\mu$  via (14) and least-squares regression. If we denote the control variate (13) by  $M_\tau(v)$ , this gives

$$M_\tau(v(\cdot; \theta)) = \sum_{i=1}^m \theta_i M_\tau(v_i).$$

In other words, we have a linear combination of  $m$  control variates  $M_\tau(v_i)$ , so the optimal  $\theta_i$  can be estimated via the standard least-squares regression procedure used for linear control variates ([Glasserman 2004](#), [Asmussen and Glynn 2007](#)). Of course, the key issue again is the choice of basis functions  $v_1, \dots, v_m$ . This is highly problem-dependent.

In the case where the parameterization of  $v(y; \theta)$  is nonlinear, optimizing  $\theta$  is more complicated. [Kim and Henderson \(2006\)](#) study and compare two stochastic optimization methods for that context, one based on stochastic approximation and the other based on sample average approximation. They demonstrate the feasibility of these methods by a numerical experiment with the pricing of barrier

options. In their experiment, sample average approximation is the best performer.

## 6 ZERO VARIANCE VIA GENERALIZED ANTITHETIC VARIATES AND QUASI-MONTE CARLO

With *generalized antithetic variates* (GAV), we estimate  $\mu_0 = \mathbb{E}[X]$  by the average of  $k$  dependent realizations of  $X$ , say  $X^{(1)}, \dots, X^{(k)}$ :

$$X_a = \frac{1}{k} \sum_{i=1}^k X^{(i)}$$

([Wilson 1979](#), [Ben-Ameur et al. 2004](#), [L'Ecuyer 2008](#)).

The variance of  $X_a$  is

$$\begin{aligned} \text{Var}[X_a] &= \frac{1}{k^2} \sum_{j=1}^k \sum_{\ell=1}^k \text{Cov}[X^{(j)}, X^{(\ell)}] \\ &= \frac{\text{Var}[X]}{k} + \frac{2}{k^2} \sum_{j < \ell} \text{Cov}[X^{(j)}, X^{(\ell)}]. \end{aligned}$$

We have  $\text{Var}[X_a] < \text{Var}[X]/k$  if and only if the sum of covariances is negative. It does not seem obvious a priori how zero variance can be achieved with the GAV scheme.

The classical *antithetic variates* (AV) scheme takes  $k = 2$ ,  $X^{(1)} = f(U)$ , and  $X^{(2)} = f(1 - U)$ , assuming that  $X = f(U)$  where  $U \sim U(0, 1)$ . A very simple case is when  $X = f(U) = aU + b$  where  $U \sim U(0, 1)$  (so  $f$  is an affine function). Then, AV gives  $X_a = a/2 + b$ , a constant, so we have zero variance. This also works for a linear function of several variables. If  $f$  is monotone, AV always reduces the variance, but not to zero unless  $f$  is linear.

Zero variance (or faster convergence than  $O(n^{-1/2})$ ) can also be obtained for certain spaces of nonlinear functions by more refined GAV schemes which are better known under the name of randomized quasi-Monte Carlo (RQMC). The usual RQMC framework is as follows. Suppose  $X$  can be written as  $X = f(\mathbf{U})$  where  $\mathbf{U}$  is a vector of  $s$  independent  $U(0, 1)$  random variables. Any expectation that admits an unbiased estimator by simulation can be written in this form, sometimes with  $d = \infty$  (to cover the case where the required number of uniforms is random). An RQMC estimator has the form

$$\hat{\mu}_{n,\text{rqmc}} = \frac{1}{n} \sum_{i=0}^{n-1} f(\mathbf{U}_i), \tag{16}$$

where  $\{\mathbf{U}_0, \dots, \mathbf{U}_{n-1}\}$  is a set of  $n$  random points that cover the unit hypercube  $[0, 1]^s$  very evenly (or uniformly, as a set) and such that each individual point is a random vector with the uniform distribution over  $(0, 1)^s$ .

Two examples of such an RQMC point sets are a lattice rule with a random shift modulo 1 and a digital net with a random digital shift; see Niederreiter (1992), Sloan and Joe (1994), Owen (2003), L'Ecuyer and Lemieux (2002), L'Ecuyer (2008) for their definitions. The uniformity of these point sets is often measured by a figure of merit that provides a bound on the worst-case variance over a given Hilbert space of functions. For example, for the Sobolev space of functions  $f : [0, 1]^s \rightarrow \mathbb{R}$  with square integrable mixed partial derivatives up to order  $\alpha$ , for any  $\delta > 0$ , it is known that there exist RQMC rules giving  $O(n^{-2\alpha-1+\delta})$  worst-case variance (Hickernell 2003) and it is not difficult to find (by computer search) RQMC rules that achieve  $O(n^{-2\alpha+\delta})$  worst-case variance (Dick et al. 2004, Dick et al. 2006).

In the case of a randomly-shifted lattice rule, the variance can be written exactly as

$$\text{Var}[\hat{\mu}_{n,\text{rqmc}}] = \sum_{\mathbf{0} \neq \mathbf{h} \in L_s^*} |\hat{f}(\mathbf{h})|^2, \quad (17)$$

where the  $\hat{f}(\mathbf{h})$  are the coefficients of the Fourier expansion of the function  $f$  and  $L_s^*$  is the dual lattice, defined as the set of vectors  $\mathbf{h} \in \mathbb{Z}_s^*$  whose scalar product modulo 1 with any point of the integration lattice is zero. If we can construct a lattice rule whose dual lattice contains none of the vectors  $\mathbf{h}$  for which  $\hat{f}(\mathbf{h}) \neq 0$ , this gives a zero variance RQMC estimator. In particular, this is always possible (with a large enough  $n$ ) if  $f$  has a Fourier expansion with a finite number of nonzero Fourier coefficients. For an arbitrary  $f$ , (17) indicates that we should try to select the lattice in order to minimize this expression. This can be achieved (in principle) by making sure that the dual of the selected lattice does not contain the vectors  $\mathbf{h}$  associated with the largest square Fourier coefficients. This idea is discussed in L'Ecuyer and Lemieux (2000) and L'Ecuyer (2008), for example. However, much research work is still needed for its practical implementation, which should involve adaptive algorithms.

Similar properties hold for digital nets with a random digital shift, with the coefficients of the Fourier expansion replaced by those of the Walsh coefficients (Dick 2008).

## 7 CONCLUSION

In theory, both IS and CV can achieve zero-variance for the simulation of a Markov chain. In practice, zero-variance sampling can only be approximated, usually by approximating the value function  $\mu$ , and good approximations can be difficult to find in general. Least-squares approximation by a linear combination of a small (fixed) set of basis functions seems to be the natural solution in the case of continuous or very large state spaces. The main difficulty then is the choice of those basis functions. In the case

of IS, another hurdle is that the approximation must be selected in a way that random variate generation from the modified distribution is not too hard. This problem does not appear with CV. Despite these difficulties, there are situations where approximate zero-variance sampling can provide very significant gains in efficiency, as exemplified by the numerical experiments reported in recent articles listed in our bibliography. More applications could benefit from this technology. This offers a fertile and exciting area for further research.

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