Derandomizing and Rerandomizing Variance Estimators

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December 22, 1997

Abstract

This technical report is meant to accompany the paper [7] and should be read in conjunction with that work. It describes several concepts which were alluded to in [7] but not elaborated on.

We give algorithms for computing the derandomized estimator, introduce the concept of rerandomization, examine heuristically the question of how the derandomized and standard variance estimators behave as the splitting constants get small, and consider the use of the derandomized estimator in sequential stopping situations.

1 Introduction

In [7] we described the concept of derandomization for Markov chain regenerative simulations. The purpose of this technical report is to discuss the issues we chose to omit from that paper. Specifically, we will address four issues: calculation of the derandomized variance estimator, rerandomization, asymptotics for the variance of the variance estimators for small splitting constants, and sequential calculation of the derandomized estimate.

In Section 2 we restate our general framework. This section includes a more extensive discussion of the splitting concept than in [7], as this idea is key to understanding rerandomization.

Then, in Section 3, we discuss two algorithms for computing the derandomized estimator. The first algorithm requires $O(n^2)$ computational effort for a simulation run of length n. The second requires $O(n)$ computational effort and is also discussed in [7]. The decrease in computational effort comes at the expense of *possible* numerical instability. In all of the examples we have considered, instability has not occurred, but we believe an unstable example could be constructed.

In order to obtain a numerically stable $O(n)$ algorithm, we introduce the concept of *rerandomization* in Section 4. Instead of computing the derandomized estimator, we compute a rerandomized estimator. A numerically stable $O(n)$ algorithm is presented for computing the rerandomized estimator. The improved computational properties of the rerandomized estimator come at the cost of some statistical efficiency, but the loss is shown through a numerical example to be relatively small.

In practice, the splitting constants used to derive regenerations may be extremely small, and so it is of interest to see how the derandomized and standard variance estimators behave in such situations. We examine this question in the context of a specific example in Section 5 to show that both estimators asymptotically have variances of the same order, although the derandomized estimator must have lower variance.

Our discussion thus far focuses on fixed run-length simulations, when the simulation run-length is determined in advance. Another approach is to run the simulation until some stopping criteria are met. Such simulations are termed "sequential" methods. We examine the problem of updating the derandomized variance estimator sequentially, i.e., updating the variance estimator when one further observation is added to the sample path. The approach we describe is potentially numerically unstable.

2 Framework

2.1 The process X

Let $X = \{ X_n : n \geq 0 \}$ be a Markov chain on a complete separable metric space S. Suppose that X is positive Harris recurrent, so that X possesses an invariant probability distribution π. Then there is an $m \geq 1$, a probability distribution φ, and a non-negative function λ such that:

1. $P^m(x,\cdot) \stackrel{\triangle}{=} P(X_m \in \cdot | X_0 = x) \geq \lambda(x)\varphi(\cdot) \ \ \forall x \in S$;
2. $\int_S \lambda(x)\pi(dx) > 0$.

Definition 1 *We say that (λ, φ) is an m-minorization of X if 1 and 2 hold.*

For the remainder of this section we will assume that $m = 1$. Let us write

$$P(x,\cdot) = \lambda(x)\varphi(\cdot) + (1 - \lambda(x))Q(x,\cdot), \tag{1}$$

where

$$Q(x,\cdot) \stackrel{\triangle}{=} \frac{P(x,\cdot) - \lambda(x)\varphi(\cdot)}{1 - \lambda(x)} \tag{2}$$

when $\lambda(x) < 1$ and (arbitrarily) a point mass at x when $\lambda(x) = 1$. This decomposition lies at the heart of the splitting variable approach to regenerative simulation.

2.2 Splitting the Markov Chain

The material in this section is adapted from [9] and [5]. The decomposition (1) suggests generating a transition of the Markov chain from $X_n = x$ in the following way. First, flip a Bernoulli rvZ_n with success probability $\lambda(x)$. If $Z_n = 1$, generate X_{n+1} from φ, otherwise generate X_{n+1} from Q. The important idea here is that if $Z_n = 1$, X_{n+1} is distributed according to φ *independently* of X_n. We can simulate X using this 2 step process, and when $Z_n = 1$, $n+1$ is a regeneration time.

A difficulty with this approach is that when $Z_n = 0$, we must generate random variables from the distribution Q, which may be a prohibitive task. It turns out, however, that we can avoid doing so. Suppose X_{n+1} is generated from $X_n = x$ by sampling from the distribution $P(x,\cdot)$. Given that $X_n = x$, and $X_{n+1} = y$, there is some probability that X_{n+1} is distributed according to φ (ie $Z_n = 1$). (1) implies that the measure $\lambda(x)\varphi(\cdot)$ is absolutely continuous with respect to $P(x,\cdot)$. Hence there is a density $w(x,y)$ such that

$$\lambda(x)\varphi(dy) = w(x,y)P(x,dy)$$

and then it is easy to see that

$$P(Z_n = 1 | X_n = x, X_{n+1} = y) = w(x,y).$$

This suggests the following approach. Simulate X in any convenient way, generating a sample path $X_0, \ldots, X_N$. Then generate Z_n for $n = 0, \ldots, N-1$ with success probability $w(X_n, X_{n+1})$. A regeneration occurs at time $n+1$ if $Z_n = 1$.

We may look at the above construction from another point of view, and this will be helpful in section 4. We will give a similar development to that in Meyn and Tweedie [9]. We say that B is an *atom* for a Markov chain if $P(x,\cdot)$ does not depend on x for every $x \in B$. If $X_n \in B$ then X_{n+1} is independent of X_n, so that $n+1$ is a regeneration time. The above construction amounts to defining a new Markov chain X' on an expanded state space $S \times \{0,1\}$ and then noting that $S \times \{1\}$ is an atom for X'.

To be precise, let $S' = S \times \{0,1\}$ and let $X' = \{ X'_n : n \geq 0 \}$ be a Markov chain on S' with initial distribution μ' and transition kernel $P'(x,\cdot)$. We will define these measures shortly, but first some more notation. For a given measure ν on S define ν^* on S' by

$$\nu^*(dy, ds) \stackrel{\triangle}{=} \begin{cases} (1 - \lambda(y))\nu(dy) & \text{if } s = 0; \\ \lambda(y)\nu(dy) & \text{if } s = 1. \end{cases} \tag{3}$$

Now, if μ is the distribution of X_0 then define

$$\mu'(A \times \{0\}) = \mu(A) \text{ and } \mu'(A \times \{1\}) = 0.$$

Next define P' as

$$\begin{aligned} P'((x,0),\cdot) &= \frac{P^*(x,\cdot) - \lambda(x)\varphi^*(\cdot)}{1 - \lambda(x)} \text{ and} \\ P'((x,1),\cdot) &= \varphi^*(\cdot). \end{aligned}$$

X' lives on the two-layered space S'. At each transition it moves to $S \times \{1\}$ with some probability, otherwise it goes to $S \times \{0\}$. If $X'_n \in S \times \{1\}$ we see that X'_{n+1} will be distributed according to φ^* independently of X'_n, so that $S \times \{1\}$ is an atom for X'. The final observation to make here is that we can "peel off" X from the "first co-ordinate" of X'. ie. X is a marginal chain of X'.

To conclude this section we describe some of the notation we will use throughout the remainder of this report.

2.3 Notation

Let $f : S \to \mathbb{R}$ be a real-valued function on S. Define the long-run average cost by

$$\alpha \stackrel{\triangle}{=} \pi f \stackrel{\triangle}{=} \int_S f(x)\pi(dx).$$

Let $T_0 = 0$, let $T_1, T_2, \ldots$ be regeneration times for X and let $\tau_k = T_k - T_{k-1}$ for $(k = 1, 2, \ldots)$ be the associated cycle lengths. Let $g : S \to \mathbb{R}$ and define $Y_k(g)$ as

$$Y_k(g) \stackrel{\triangle}{=} \sum_{j=T_{k-1}}^{T_k - 1} g(X_j).$$

At the regeneration times T_k, $X_{T_k} \sim \varphi$ where φ is the splitting distribution on S and $\sim$ should be read "is distributed according to ". Define $\ell(n) = \sup\{k \geq 0 : T_k \leq n\}$, the number of regenerations to occur by time n.

Define $E_\varphi(\cdot)$ as $\int_S E(\cdot|X_0 = x)\varphi(dx)$ and $P_\varphi(A) = E_\varphi I_A$, the expected value of the indicator function of A. Standard arguments (see, for example, Chung 1967) establish that if $E_\varphi((Y_1(|f|))^2 + \tau_1^2) < \infty$ then

$$\alpha_n \stackrel{\triangle}{=} \frac{1}{n}\sum_{k=0}^{n-1} f(X_k) \to \alpha \text{ a.s. as } n \to \infty,$$

and

$$\sqrt{n}(\alpha_n - \alpha) \Rightarrow \sigma N(0, 1)$$

where $\Rightarrow$ denotes convergence in distribution. Let $f_c(x) \stackrel{\triangle}{=} f(x) - \alpha$ and $f_n(x) \stackrel{\triangle}{=} f(x) - \alpha_n$. The constant σ^2 may be written as

$$\sigma^2 = \frac{E_\varphi(Y_1(f_c))^2}{E_\varphi \tau_1}. \tag{4}$$

Finally let $\bar{w}(x, y) = 1 - w(x, y)$, where $w(x, y)$ is a density of $\lambda(x)\varphi(\cdot)$ with respect to $P(x, \cdot)$.

3 Algorithms

The first term in the derandomized estimator (see Equation (9) of [7]) presents no difficulty, so we concentrate on the second term, B_n, where

$$B_n = \frac{2}{n}\sum_{j=0}^{n-1} f_n(X_j) \sum_{k=j+1}^{n} f_n(X_k) \prod_{i=j}^{k-1} \overline{w}(X_i, X_{i+1}). \tag{5}$$

A simple algorithm for calculating this quantity is given by Algorithm 1.

Algorithm 1: Calculation of B_n

$B = 0$
for $j = 0, \ldots, n-1$
  $Z = f_n(X_j)$
  $k = j$
  repeat

$k = k + 1$
$Z = Z\overline{w}(X_{k-1}, X_k)$
$B = B + f_n(X_k)Z$
until $(k = n)$ or $(Z = 0)$
end for
$B_n = 2B/n$
End: Calculation of B_n

If $\overline{w}(X_{k-1}, X_k) > 0$ for all k and we work with exact arithmetic, then this algorithm will take $O(n^2)$ time to compute B_n. In that case, for large n the effort required to compute V_n ultimately dominates the computational effort devoted to simulating X. We need to adopt a more efficient approach. We now outline an algorithm that runs in $O(n)$ time. It is possible that this new algorithm could exhibit numerical instability, although that has not been our experience with the approach. In Section 4 an approach will be discussed that overcomes such potential difficulties.

Suppose (for now) that $\overline{w}(X_i, X_{i+1}) > 0 \; \forall i$. Define

$$\Lambda_j = \prod_{i=0}^{j-1} \overline{w}(X_i, X_{i+1})$$

for $j \geq 1$ and $\Lambda_0 = 1$. Then

$$\begin{aligned} \frac{n}{2}B_n &= \sum_{j=0}^{n-1} f_n(X_j) \sum_{k=j+1}^{n} f_n(X_k)\Lambda_k/\Lambda_j \\ &= \sum_{j=0}^{n-1} f_n(X_j)/\Lambda_j \sum_{k=j+1}^{n} f_n(X_k)\Lambda_k \\ &= \sum_{j=0}^{n-1} f_n(X_j)b_j/\Lambda_j \text{ say.} \end{aligned}$$

Now consider the more general case where we do not exclude the possibility that $\overline{w}(X_i, X_{i+1}) = 0$ (i.e., $i+1$ is a regeneration time with probability 1). In this case, many of the terms that comprise B_n are 0. Let $U(1), ..., U(r^* - 1)$ be the indices such that $\overline{w}(X_{U(i)-1}, X_{U(i)}) = 0$, and define $U(0) = 0, U(r^*) = n+1$. Then we can write

$$\begin{aligned} \frac{n}{2}B_n &= \sum_{r=1}^{r^*} \sum_{j=U(r-1)}^{U(r)-2} \sum_{k=j+1}^{U(r)-1} f_n(X_j)f_n(X_k) \prod_{i=j}^{k-1} \overline{w}(X_i, X_{i+1}) \\ &= \sum_{r=1}^{r^*} \sum_{j=U(r-1)}^{U(r)-2} f_n(X_j)b_j/\Lambda_j. \end{aligned}$$

where

$$\begin{aligned} \Lambda_{U(r)} &= 1, \text{ for } r = 0, 1, 2, ..., r^* - 1, \\ \Lambda_k &= \prod_{i=U(r-1)}^{k-1} \overline{w}(X_i, X_{i+1}) \text{ if } U(r-1) < k < U(r), \text{ and} \\ b_j &= \sum_{k=j+1}^{U(r)-1} f_n(X_k)\Lambda_k \text{ if } U(r-1) \leq j < U(r) - 1. \end{aligned}$$

We therefore obtain the following algorithm for computing B_n.

Algorithm 2: Calculation of B_n

$B = 0$
for $r = 1, ..., r^*$
start $= U(r-1)$, stop $= U(r) - 1$
if stop $>$ start then (the sum is not vacuous)
$\Lambda_{\text{start}} = 1$
for $j =$ (start $+ 1$), ..., stop
$\Lambda_j = \Lambda_{j-1}\overline{w}(X_{j-1}, X_j)$
end for
$b = 0$
for $j =$ stop down to (start $+ 1$)
$b = b + f_n(X_j)\Lambda_j$
$B = B + bf_n(X_{j-1})/\Lambda_{j-1}$
end for
end if
end for
$B_n = 2B/n$
End: Calculation of B_n

This new algorithm runs in $O(n)$ time. Notice however, that in Algorithm 2 we divide certain quantities by $\Lambda_j \in (0, 1)$, where the Λ's are products of $\overline{w}$'s. If $0 < \overline{w}(X_i, X_{i+1}) < 1$ for all i, then Λ_j will be small for large j. Consider, for example, the situation where $\overline{w}$ is constant and equal to 10^{-1}. On a machine that can represent real numbers between 10^{-99} and 10^{99}, Λ_j is calculated to be 0 for $j > 99$, even though its true value is 10^{-j}. This means that the above algorithm can exhibit instability. One solution to this problem is to use Algorithm 1 instead of Algorithm 2. This solution is unattractive due to the $O(n^2)$ running time of Algorithm 1. A second solution is to somehow force $\overline{w}(X_i, X_{i+1}) = 0$ for several i, thereby truncating the products that comprise the Λ's. (Recall that

$$\Lambda_k = \prod_{i=U(r-1)}^{k-1} \overline{w}(X_i, X_{i+1}) \text{ if } U(r-1) < k < U(r),$$

so that Λ_k is a product of $k - U(r-1)$ terms. By increasing the frequency of the epochs when $\overline{w}(X_i, X_{i+1}) = 0$, we decrease the number of products required to calculate Λ_k. By doing so, we immediately see that Algorithm 1 will run in $O(n)$ time owing to the fact that the number of products in the inner loop becomes stochastically bounded. Furthermore, the number of products required to produce the Λ_j's in Algorithm 2 also becomes stochastically bounded, thereby improving its numerical properties. We will show how to force $\overline{w}(X_i, X_{i+1}) = 0$ infinitely often (i.o.) in the next section, using a device we call rerandomization.

4 Rerandomization

The goal of this section is to derive the rerandomized estimator, and present a stable and efficient algorithm for computing it. Let us assume (for now) that the minorization constant $m = 1$. We will relax this assumption later in the section. In [7] we showed that the completely derandomized variance estimator is given by

$$V_n \stackrel{\triangle}{=} \frac{1}{n}\sum_{k=0}^{n-1} f_n(X_k)^2 + \frac{2}{n}\sum_{j=0}^{n-1} f_n(X_j) \sum_{k=j+1}^{n} f_n(X_k) \prod_{i=j}^{k-1} \overline{w}(X_i, X_{i+1}). \tag{6}$$

This estimator is based on the standard estimator

$$\tilde{V}_n = \frac{1}{n}\sum_{j=0}^{n-1} f_n(X_j)^2 + \frac{2}{n}\sum_{j=0}^{n-1} f_n(X_j) \sum_{k=j+1}^{(T_{\ell(j)+1}-1)\wedge n} f_n(X_k) \tag{7}$$

In [7] we wanted a CLT for V_n, but it was not readily apparent that such a CLT existed, because in the process of derandomizing, we removed the regenerative structure of the variance estimator. The

rerandomized estimator fits between the standard estimator and the completely derandomized estimator in that it does take some advantage of derandomization while still retaining regenerative structure. Perhaps the major quality of the rerandomized estimator is that $\overline{w}(X_i, X_{i+1}) = 0$ i.o and the times at which this occurs give rise to regeneration times. Let us proceed to an intuitive discussion of rerandomization, followed by the theoretical development.

To derandomize the variance estimator we "smoothed over" the transitions of the Markov chain. Imagine now that we still smooth over a subset of the transitions, but on the others we toss a coin to determine whether a regeneration occurs, just as we did without any derandomization. We will therefore perform somewhere "in between" the standard and derandomized estimators. We will do the coin toss *with probability* p at each transition. It will turn out that the only way that the estimator is affected is that the regeneration density w is altered.

Let us describe the estimator and then prove that it is valid. Let p be a value between 0 and 1 which indicates the degree of rerandomization we require. Every $p > 0$ leads to an estimator satisfying a CLT. When $p = 0$ we get the derandomized estimator (6), and $p = 1$ yields the standard estimator (7). The estimator is computed as follows.

Simulate a sample path X_n for $n = 0, \ldots, N$ as before. Then define the sequence of indicator variables Z_n (for $n = 0, \ldots, N-1$) by

$$Z_n \sim \text{Bernoulli}(pw(X_n, X_{n+1})).$$

The rerandomized estimator is then given by

$$V_n(p) = \frac{1}{n}\sum_{k=0}^{n-1} f_n(X_k)^2 + \frac{2}{n}\sum_{j=0}^{n-1} f_n(X_j) \sum_{k=j+1}^{n} f_n(X_k) \prod_{i=j}^{k-1} \overline{w}'((X_i, Z_i), (X_{i+1}, Z_{i+1})) \tag{8}$$

where $\bar{w}'$ is defined as

$$\overline{w}'((x,z),(y,v)) = \begin{cases} 0 & \text{if } z = 1 \\ \frac{\overline{w}(x,y)}{1-pw(x,y)} & \text{if } z = 0 \end{cases}$$

We now prove that this representation is correct.

Let X be the Markov chain described in section 2. Then

$$P(x, \cdot) \geq \lambda(x)\varphi(\cdot) \quad \forall x.$$

But since $0 \leq p \leq 1$ it is also true that

$$P(x, \cdot) \geq p\lambda(x)\varphi(\cdot) \quad \forall x. \tag{9}$$

So let us define the split chain X' using (9) as in section 2.2. The set $S \times \{1\}$ is then an atom for X'. But now we find that X' also satisfies a minorization condition.

Lemma 1

$$P'((x,z),\cdot) \geq \delta(x,z)\varphi^*(\cdot) \quad \forall (x,z) \tag{10}$$

where

$$\delta(x,z) = \begin{cases} 1 & \text{if } z = 1 \\ \frac{(1-p)\lambda(x)}{1-p\lambda(x)} & \text{if } z = 0 \end{cases}$$

Proof:

$$P'((x,0),A') = \frac{P^*(x,A') - p\lambda(x)\varphi^*(A')}{1-p\lambda(x)}$$

and

$$\begin{aligned} P^*(x,A') &\geq \lambda(x)\varphi^*(A') \\ &= p\lambda(x)\varphi^*(A') + (1-p)\lambda(x)\varphi^*(A'). \end{aligned}$$

Moving the first term on the right hand side across to the left, and dividing by $1 - p\lambda(x)$ we obtain (10) for $x' \in S \times \{0\}$. $\delta(x,1)$ is easy to compute. Note that in this case $P'((x,1),\cdot) = \varphi^*(\cdot)$.

□

So now, what is $w'(x',\cdot)$, the density of $\delta(x')\varphi^*(\cdot)$ with respect to $P'(x',\cdot)$? We answer this question in the following lemma.

Lemma 2 *If $x' \in S \times \{1\}$ then $w'(x',y') = 1$. Otherwise $x' = (x,0)$ and then*

$$w'((x,0),(y,z)) = \frac{(1-p)w(x,y)}{1-pw(x,y)}. \tag{11}$$

Proof: If $x' \in S \times \{1\}$ then $w'(x',y')$ is a density of $\varphi^*(\cdot)$ with respect to itself and therefore 1. To complete the proof, we show that

$$w'((x,0),(y,z))P'((x,0),(dy,dz)) = \delta(x,0)\varphi^*(dy,dz)$$

where w' is defined as in (11). Suppose $z = 1$. Then

$$\begin{aligned}
& w'((x,0),(y,z))P'((x,0),(dy,dz)) \\
= & \frac{(1-p)w(x,y)}{1-pw(x,y)} \frac{\lambda(y)P(x,dy) - p\lambda(x)\lambda(y)\varphi(dy)}{1-p\lambda(x)} \\
= & \frac{(1-p)w(x,y)}{1-pw(x,y)} \frac{\lambda(y)\{P(x,dy) - p\lambda(x)\varphi(dy)\}}{1-p\lambda(x)} \\
= & \frac{(1-p)w(x,y)}{1-pw(x,y)} \frac{\lambda(y)\{P(x,dy) - pw(x,y)P(x,dy)\}}{1-p\lambda(x)} \\
= & \frac{(1-p)w(x,y)}{1-p\lambda(x)} \lambda(y)P(x,dy) \\
= & \frac{(1-p)w(x,y)\lambda(x)}{1-p\lambda(x)} \lambda(y)\varphi(dy) \\
= & \delta(x,0)\varphi^*(dy,dz).
\end{aligned}$$

The case $z = 0$ is similar.

□

In order to apply the results from Section 3 of [7] to X' we need to show that the moment conditions given for X also hold for X'. But this is immediate because τ_1' for X' is equal in distribution to τ_1 as we now show. Given X, we regenerate at time n in the X chain with probability $w(X_{n-1},X_n)$. Now let us find the probability of regeneration $q((X_{n-1},Z_{n-1}),(X_n,Z_n))$ in the X' chain (given X). We will find that it is the same.

$$\begin{aligned}
& q((X_{n-1},Z_{n-1}),(X_n,Z_n)) \\
= & (1P(Z_{n-1}=1|X) + w'((X_{n-1},0),X_n')P(Z_{n-1}=0|X)) \\
= & (pw(X_{n-1},X_n) + \frac{(1-p)w(X_{n-1},X_n)}{1-pw(X_{n-1},X_n)}(1-pw(X_{n-1},X_n)) \\
= & w(X_{n-1},X_n).
\end{aligned}$$

We can now apply the results from Section 3 of [7] to X'. We then see that (8) enjoys the properties that we showed for (6); i.e., weak consistency, and lower variance than the traditional estimator.

We now present an efficient and numerically stable algorithm for computing $V_n(p)$.

Algorithm 3: Calculation of $V_n(p)$

$\alpha = 0, V_n(p) = 0$
for $j = 0,\ldots,n-1$
    $\alpha = \alpha + f(X_j)/n$

end for
for $j = 0, \ldots, n-1$
$V_n(p) = V_n(p) + (f(X_j) - \alpha)^2$
end for
for $j = 1, \ldots, n$
Set $Z'_{j-1} = 1$ with probability $pw(X_{j-1}, X_j)$
end for
$B = 0$
for $j = 0, \ldots, n-1$
$Z = f_n(X_j)$
$k = j$
repeat
$k = k + 1$
if $Z'_{k-1} = 1$
$Z = 0$
else
$Z = Z\overline{w}(X_{k-1}, X_k)/(1 - pw(X_{k-1}, X_k))$
$B = B + f_n(X_k)Z$
until $(k = n)$ or $(Z = 0)$
end for
$V_n(p) = V_n(p) + 2B/n$
End: Calculation of $V_n(p)$

When $p > 0$, notice that the estimator $V_n(p)$ is a regenerative quantity, with regenerative cycles defined by the p-regenerations. This observation immediately yields the conclusion that (under appropriate moment conditions) $V_n(p)$ converges *almost surely* to σ^2, strengthening our earlier convergence in probability result. This result could prove useful as it is one of the requirements of sequential stopping rules as described in Glynn and Whitt (1992). In fact, for some problems $w_p(X_{k-1}, X_k) = 1$ i.o. for all p. This occurs when $\lambda(X_k) = 1$ i.o., which is the case in the setting of Andradóttir, Calvin and Glynn (1994), and so $V_n(p)$ converges a.s. to σ^2 in that case.

Using rerandomization with $p > 0$, we have achieved our goal of forcing $\overline{w}_p(X_{i-1}, X_i) = 0$ i.o. Therefore, the amount of computation in Algorithm 3 becomes $O(n)$ and Algorithm 2 is more likely to be stable. However, in Algorithm 2, it is still possible that some of the Λ_j's may be too small to accurately represent numerically. If this occurs, then the results from the algorithm could be corrupted, and so we advocate the use of Algorithm 3 in computing the rerandomized variance estimator $V_n(p)$.

We now present additional results from the second numerical example presented in [7]. These computational results show that the rerandomized estimators can be computed quickly, and little loss in statistical efficiency results. The results presented in [7] were for the fully derandomized estimator. Table 1 gives results for the rerandomized estimators, where p ranges from 0 (the derandomized estimator) to 1 (the standard estimator). The time needed to perform the computations (in seconds) is given in brackets together with the estimates of the variance of the variance estimators. By way of comparison, the simulation itself took 76 seconds.

Table 1
Variances of Variance Estimators

Derand. Est.	Rerand. $p = 0.2$	Rerand. $p = 0.4$	Rerand. $p = 0.6$	Rerand $p = 0.8$	Std. Est.
1.7(175)	1.7 (55)	1.9 (34)	2.0 (26)	2.0 (22)	2.9 (8)

In this example, we begin to see that derandomization can be useful. Using the standard estimator will result in a variance of 2.9 after 76 + 8 = 84 seconds. Using the rerandomized estimator with $p = 0.6$ results in a variance of 2.0 after 102 seconds. It would appear that in this case it is worthwhile to employ derandomization. In more complicated simulations in which it is even more expensive to perform the simulation, derandomization is definitely worth considering.

We believe that rerandomization is an elegant concept, and this is demonstrated by the way it can be extended to the case when the minorization constant $m > 1$. In this case the variance constant is

$$\beta^2 = \frac{E_\varphi(Y_1(f_c))^2}{E_\varphi \tau_1} + 2\frac{E_\varphi(Y_1(f_c)Y_2(f_c))}{E_\varphi \tau_1}, \tag{12}$$

the standard estimator is

$$\begin{aligned} \tilde{W}_n &= \frac{1}{n}\sum_{j=0}^{n-1} f_n^2(X_j) + \frac{2}{n}\sum_{j=0}^{n-1}\sum_{k=j+1}^{(T_{\ell(j)+1}-1)\wedge n} f_n(X_j)f_n(X_k) \\ &+ \frac{2}{n}\sum_{j=0}^{n-1}\sum_{k=j+1}^{n} f_n(X_j)f_n(X_k) I(T_{\ell(j)+1} - m < j < T_{\ell(j)+1} \le k < T_{\ell(j)+2}), \end{aligned} \tag{13}$$

(see [7]) and the rerandomized estimator is

$$\begin{aligned} W_n &= \frac{1}{n}\sum_{k=0}^{n-1} f_n(X_k)^2 + \frac{2}{n}\sum_{j=0}^{n-1} f_n(X_j)\sum_{k=j+1}^{n} f_n(X_k)\prod_{i:j<\Gamma_i\le k}\overline{w}'(X'_{\Gamma_i-m}, X'_{\Gamma_i}) + \\ &\frac{2}{n}\sum_i \sum_{j=\Gamma_i-m+1}^{\Gamma_i-1} f_n(X_j) w'(X'_{\Gamma_i-m}, X'_{\Gamma_i}) \\ &\left(\sum_{k=\Gamma_i}^{n} f_n(X_k)\prod_{h:\Gamma_i<\Gamma_h\le k}\overline{w}'(X'_{\Gamma_h-m}, X'_{\Gamma_h})\right). \end{aligned} \tag{14}$$

The proof is virtually identical to that given for the case $m = 1$, and so we omit it. The following result is proved exactly as in [7].

Theorem 1 *If $E_\varphi(T_1^2 + Y_1(|f|)^2 T_1^2) < \infty$ then W_n as defined in (14) enjoys the following properties.*

- *W_n converges in P_φ probability to β^2.*
- *Under P_φ, the L_1 error of W_n is less than that of $\tilde{W}_n$ (as given in (13), i.e.,*

$$E_\varphi|W_n - \beta^2| \le E_\varphi|\tilde{W}_n - \beta^2|.$$

- *$var_\varphi W_n \le var_\varphi \tilde{W}_n$, and the inequality fails to be strict only when $\lambda(X_{\Gamma_n - h}) \in \{0, 1\}$ $\forall n$, φ a.s.*

The following result is a central limit theorem for W_n as defined in (14).

Theorem 2 *Suppose that $E_\varphi(Y_1(|f_c|)^4 + \tau_1^4) < \infty$ and $p > 0$. Define*

$$\begin{aligned} \tilde{W}_n &= \frac{1}{n}\sum_{j=0}^{n-1} f_n^2(X_j) + \frac{2}{n}\sum_{j=0}^{n-1}\sum_{k=j+1}^{(T_{\ell(j)+1}-1)\wedge n} f_n(X_j)f_n(X_k) \\ &+ \frac{2}{n}\sum_{j=0}^{n-1}\sum_{k=j+1}^{n} f_n(X_j)f_n(X_k) I(T_{\ell(j)+1} - m < j < T_{\ell(j)+1} \le k < T_{\ell(j)+2}) \end{aligned}$$

and $W_n = E(\tilde{W}_n|X')$. Then

$$\sqrt{n}(W_n - \sigma^2) \Rightarrow \eta_2 N(0, 1).$$

Proof: Let T_i be given as in section 2. Let $T_0^* = 0$ and set $T_j^* = \inf\{n > T_{j-1}^* : \overline{w}'(X'_{\Gamma_n - m}, X'_{\Gamma_n}) = 0\}$ for $j \geq 1$. Let $\ell^*(n) = \sup\{k \geq 0 : T_k^* \leq n\}$. The times $\{T_j^* : j \geq 0\}$ break the sample path of X' into 1-dependent cycles. Each one of these cycles corresponds to a geometric sum of cycles in the X chain. To see this, recall that the Bernoulli rv's that we constructed to determine regeneration times in the X' chain have probability pw of success, whereas those in the X chain have probability w. Thus we see that (if $X_0 \sim \varphi$)

$$T_j^* - T_{j-1}^* \stackrel{\mathcal{D}}{=} T_1^* = \sum_{i=1}^{N} (T_i - T_{i-1})$$

where N is a geometric(p) rv that is *independent* of the X chain. We can write

$$\begin{aligned} W_n &= \frac{1}{n} \sum_{r=1}^{\ell^*(n)} \Big[\sum_{j=T_{r-1}^*}^{T_r^*-1} f_c(X_j)^2 + 2 \sum_{j=T_{r-1}^*}^{T_r^*-1} f_c(X_j) \sum_{k=j+1}^{T_r^*} f_c(X_k) \prod_{i: j < \Gamma_i \leq k} \overline{w}'(X'_{\Gamma_i - m}, X'_{\Gamma_i}) \\ &+ 2 \sum_{j=T_{r-1}^*}^{T_r^*-1} f_c(X_j) \sum_{k=j+1}^{T_{r+1}^*-1} f_c(X_k) \theta_{j,k} \Big] + R_n^* \end{aligned} \tag{15}$$

where R_n^* is a remainder term and $\theta_{j,k}$ is 0 if $\nexists i : j < \Gamma_i < j + m$ and

$$\theta_{j,k} = w(X_{\Gamma_i - m}, X_{\Gamma_i}) I(k \geq \Gamma_i) \prod_{h: \Gamma_i < \Gamma_h \leq k} \overline{w}(X_{\Gamma_h - m}, X_{\Gamma_h}) \leq 1$$

if $j < \Gamma_i < j + m$.

Notice the regenerative structure of (15). The first two terms within the brackets are defined within one cycle, whereas the last term spans two consecutive cycles. This estimator has structure that is very similar to that of $\tilde{W}_n$ (see the appendices of [7]), except that the cycles are longer! The term in square brackets is smaller in absolute value than

$$\begin{aligned} & 2 \sum_{j=T_{r-1}^*}^{T_r^*-1} |f_c(X_j)|^2 + 2 \sum_{j=T_{r-1}^*}^{T_r^*-1} |f_c(X_j)| \sum_{k=j+1}^{T_r^*} |f_c(X_k)| \\ + \quad & 2 \sum_{j=T_{r-1}^*}^{T_r^*-1} |f_c(X_j)| \left(\sum_{k=j+1}^{T_r^*-1} |f_c(X_k)| + \sum_{k=T_r^*}^{T_{r+1}^*-1} |f_c(X_k)| \right) \\ = \quad & 2 \left(\sum_{j=T_{r-1}^*}^{T_r^*-1} |f_c(X_j)| \right)^2 + 2 \sum_{j=T_{r-1}^*}^{T_r^*-1} \sum_{k=T_r^*}^{T_{r+1}^*-1} |f_c(X_k)| \\ \stackrel{\mathcal{D}}{=} \quad & 2 \left(\sum_{j=1}^{N_1} Y_j(|f_c|) \right)^2 + 2 \sum_{j=1}^{N_1} Y_j(|f_c|) \sum_{j=N_1+1}^{N_1+N_2} Y_j(|f_c|) \end{aligned}$$

where N_1 and N_2 are independent geometric(p) rv's which are independent of X. But since geometric rv's have moments of all orders, and by our moment hypotheses, this quantity has a finite second moment. It is straight-forward to show that R_n^* converges to 0. So the result follows by an application of a CLT for 2-dependent sequences, an application of Theorem 20.3 in [2], and the converging together lemma [3].

□

5 Asymptotics for Small Splitting Constants

Consider the minorization condition

$$P^m(x, \cdot) \stackrel{\triangle}{=} P(X_m \in \cdot | X_0 = x) \geq \lambda(x) \varphi(\cdot) \quad \forall x \in S.$$

In practical examples it is often the case that the best implementable value for $\lambda(x)$ is far from the theoretical maximum because $\lambda(x)$ is obtained from a series of applications of theoretical bounds, each of which could be somewhat loose [10]. This has the effect of reducing the regeneration rate and is the context in which we believe our derandomization technique is most useful. So it is of interest to see how the estimators behave for small splitting constants. We will consider a specific discrete-time Markov chain and compare the estimators via an intuitive argument.

We will find that the variances of the two estimators (standard and derandomized) are of the same order of magnitude in our special case (although of course the derandomized estimator must have a lower variance). It is our belief that this is also true of the general case, although we have no proof of this claim.

Consider a discrete-time Markov chain $X = (X_n : n \geq 0)$, consisting of iid random variables. Then

$$P(x, \cdot) \geq \lambda(x)\varphi(\cdot)$$

where $\lambda(x) \equiv 1$ and $\varphi(\cdot) = P(X_i \in \cdot)$. Let us scale $\lambda(x)$ by ϵ so that

$$P(x, \cdot) \geq \epsilon\varphi(\cdot),$$

and consider the asymptotics of our estimators as $\epsilon \searrow 0$. We will use the true centered cost f_c in our calculations for simplicity. It turns out that using the estimated function f_n does change the results slightly, but does not alter the *order* of the estimator variances, so we omit the details. As $\epsilon \searrow 0$ the cycles grow in length so we must consider our estimators evaluated over a longer period of time. Hence we consider the estimators at time t/ϵ.

First consider the standard estimator $\tilde{V}(n)$. Let $T_j(\epsilon)$ be regeneration times when the (ϵ, φ) 1-minorization is used, so that $T_j(\epsilon)$ has a geometric(ϵ) distribution. We have

$$\begin{aligned}
\tilde{V}(t/\epsilon) &\approx \frac{\epsilon}{t} \sum_{j=1}^{\ell(t/\epsilon)} \left(\sum_{k=T_{j-1}(\epsilon)}^{T_j(\epsilon)-1} f_c(X_k) \right)^2 \\
&= \frac{1}{t} \sum_{j=1}^{\ell(t/\epsilon)} \left(\epsilon^{1/2} \sum_{k=T_{j-1}(\epsilon)}^{T_j(\epsilon)-1} f_c(X_k) \right)^2 \\
&\Rightarrow \frac{1}{t} \sum_{j=1}^{N(t)} \left(\int_{T_{j-1}}^{T_j} \sigma dB(s) \right)^2
\end{aligned}$$

where $\sigma^2 = Ef_c^2(X_0)$, $B(s)$ is standard Brownian motion, $N(t)$ is a Poisson process (rate 1), T_j is the time of the j^{th} event in the Poisson process, and N is independent of the Brownian motion B. So if we assume uniform integrability, we obtain

$$\text{var } \tilde{V}(t/\epsilon) \to \text{ var } \left(\frac{\sigma^2}{t} \sum_{j=1}^{N(t)} (B(T_j) - B(T_{j-1}))^2 \right).$$

Turning now to our derandomized estimator, we note that

$$V(t/\epsilon) = \frac{\epsilon}{t} \sum_{j=0}^{t/\epsilon} f_c^2(X_j) + 2\frac{\epsilon}{t} \sum_{j=0}^{t/\epsilon} \sum_{k=j+1}^{t/\epsilon} f_c(X_j) f_c(X_k)(1-\epsilon)^{k-j}. \tag{16}$$

The first term in (16) converges to $Ef_c^2(X_0)$ as $\epsilon \searrow 0$. It will be easier to analyze the second term if we consider the Markov chain X in continuous time and use integrals instead of summations. This primarily amounts to a notational change, so that the asymptotics will not be affected. Denote the second term in (16) by $V_1(t/\epsilon)$ so that

$$V_1(t/\epsilon) \approx \frac{2\epsilon}{t} \int_0^{t/\epsilon} f_c(X_s) \int_s^{t/\epsilon} f_c(X(u)) e^{-\epsilon(u-s)} du\, ds$$

$$
\begin{aligned}
&= \frac{2\epsilon}{t}\int_0^{t/\epsilon} f_c(X_s)\int_0^{t/\epsilon-s} f_c(X(u+s))e^{-\epsilon u}du\,ds \\
&= \frac{2\epsilon}{t}\int_0^{t/\epsilon} f_c(X_s)\int_0^{t/\epsilon-s} f_c(X(u+s))\int_{\epsilon u}^{\infty} e^{-r}dr\,du\,ds \\
&= \frac{2}{t}\int_0^{t/\epsilon}\epsilon^{1/2}f_c(X_s)\int_0^{\infty} e^{-r}\int_0^{(r\wedge(t-\epsilon s))/\epsilon}\epsilon^{1/2}f_c(X(s+u))du\,dr\,ds \\
\Rightarrow\quad & \frac{2\sigma^2}{t}\int_0^t\int_0^{\infty} e^{-r}(B(s+r\wedge t)-B(s))dr\,dB(s)
\end{aligned}
$$

where the final line seems like the appropriate limit, but we have not attempted to prove it. Again assuming uniform integrability, we get

$$
\text{var } V(t/\epsilon) \to \text{ var } \left(\frac{2\sigma^2}{t}\int_0^t\int_0^{\infty} e^{-r}(B(s+r\wedge t)-B(s))dr\,dB(s)\right).
$$

So, it appears that in this case both estimators have variance of the same order of magnitude (relative to ϵ).

6 Recursive Updating of the Estimator

We will discuss this in the case where $m = 1$. Recall that while discussing the rerandomized estimator, we showed that the rerandomized estimator converges a.s. to β^2. This implies that the rerandomized estimator might be applied in conjunction with sequential stopping rules. For ease of exposition, we will further restrict ourselves to the case where $\overline{w} > 0$ a.s. Define $\Lambda_k = \prod_{i=0}^{k-1}\overline{w}(X_i, X_{i+1})$ where an empty product is taken to be 1. From (6),

$$
\begin{aligned}
V_n &= \frac{1}{n}\left(\sum_{j=0}^{n-1} f(X_j)^2 + 2\sum_{j=0}^{n-1}\sum_{k=j+1}^{n} f(X_j)f(X_k)\Lambda_k/\Lambda_j\right) \\
&- \frac{2\alpha_n}{n}\left(\sum_{j=0}^{n-1} f(X_j) + \sum_{j=0}^{n-1}\sum_{k=j+1}^{n}(f(X_j)+f(X_k))\Lambda_k/\Lambda_j\right) \\
&+ \frac{\alpha_n^2}{n}\left(n + 2\sum_{j=0}^{n-1}\sum_{k=j+1}^{n}\Lambda_k/\Lambda_j\right) \\
&= \frac{A_n}{n} - \frac{\alpha_n B_n}{n} + \frac{\alpha_n^2 C_n}{n} \text{ say.}
\end{aligned}
$$

Now,

$$
\begin{aligned}
(n+m)V_{n+m} &= A_{n+m} - \alpha_{n+m}B_{n+m} + \alpha_{n+m}^2 C_{n+m} \\
&= nV_n + (A_{n+m} - A_n) - (\alpha_{n+m}B_{n+m} - \alpha_n B_n) \\
&+ (\alpha_{n+m}^2 C_{n+m} - \alpha_n^2 C_n) \\
&= nV_n + (A_{n+m} - A_n) - (\alpha_{n+m} - \alpha_n)B_n + \alpha_{n+m}(B_n - \\
&\quad B_{n+m}) + (\alpha_{n+m}^2 - \alpha_n^2)C_n + \alpha_{n+m}^2(C_{n+m} - C_n)
\end{aligned}
$$

So to obtain a recursive update formula, we need to be able to maintain the quantities B_n, C_n, and calculate the differences $A_{n+m} - A_n$ etc quickly (it is easy to update α_n to α_{n+m}). Since $A_{n+m} - A_n$ through $C_{n+m} - C_n$ are all similar in structure, we show how to update $A_{n+m} - A_n$ alone.

$$
A_{n+m} - A_n = \sum_{j=n}^{n+m-1} f(X_j)^2 + 2\sum_{j=0}^{n-1} f(X_j)/\Lambda_j \sum_{k=n+1}^{n+m} f(X_k)\Lambda_k
$$

$$+ \quad 2 \sum_{j=n}^{n+m-1} f(X_j)/\Lambda_j \sum_{k=j+1}^{n+m} f(X_k)\Lambda_k.$$

The first and third of these terms present no problems. The second term can be handled in $O(m)$ time if we also keep track of $D_n \stackrel{\triangle}{=} \sum_{j=0}^{n-1} f(X_j)/\Lambda_j$. An examination of the quantities $B_{n+m} - B_n$ and $C_{n+m} - C_n$ reveals that we can update these values if we also keep track of $E_n \stackrel{\triangle}{=} \sum_{j=0}^{n-1} 1/\Lambda_j$.

Hence, it is possible to produce a recursive update which can be calculated in $O(m)$ time. However, the nature of the updating calculations suggests that such an approach could exhibit numerical instability. Although numerical instability has not been observed in the examples we have considered, we believe that numerically unstable examples can be constructed, and so the one-pass method suggested by the above analysis should be used with caution.

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