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JACKKNIFED VARIANCE ESTIMATORS FOR SIMULATION OUTPUT ANALYSIS

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ABSTRACT

We develop new point estimators for the variance parameter of a steady-state simulation process. The estimators are based on jackknifed versions of nonoverlapping batch means, overlapping batch means, and standardized time series variance estimators. The new estimators have reduced bias—and can be manipulated to reduce their variance and mean-squared error—compared with their predecessors, facts which we demonstrate analytically and empirically.

1 INTRODUCTION

A fundamental goal in simulation output analysis is the estimation of the unknown mean μ of a steady-state simulation-generated output process, $\{Y_j : j = 1, 2, \ldots, n\}$. The obvious point estimator for this task is the sample mean, $\overline{Y}_n \equiv n^{-1}\sum_{i=1}^{n} Y_i$. It also proves useful to get a handle on the sample mean's variability, so a long-standing area of research has involved estimating the measure $\sigma_n^2 \equiv n\,\mathrm{Var}(\overline{Y}_n)$ or (almost equivalently) the *variance parameter*, $\sigma^2 \equiv \lim_{n\to\infty}\sigma_n^2 = \sum_{j=-\infty}^{\infty} R_j$, where the covariance function $R_j \equiv \mathrm{Cov}(Y_1, Y_{1+j})$, for $j = 0, 1, \ldots$. Knowledge of σ^2 helps us to make precision and confidence statements about $\overline{Y}_n$ as an estimator for μ.

Over the years, a significant literature has developed with the problem of estimating σ^2 in mind, for example, the methods of nonoverlapping batch means (NBM) (Schmeiser 1982), overlapping batch means (OBM) (Meketon and Schmeiser 1984), and standardized time series (STS) (Schruben 1983). These methods typically divide the time series $\{Y_j : j = 1, 2, \ldots, n\}$ into possibly overlapping batches of size m, and calculate estimators for σ^2 that have been proven to be consistent as m and $b \equiv n/m$ both go to infinity—that is, the mean squared errors (MSEs) of these estimators go to zero as m and $b \to \infty$.

Broadly speaking, the batch size m governs the bias component of the estimator's MSE, while the quantity b most directly affects the variance component of MSE (Goldsman and Meketon 1986, Song and Schmeiser 1995, and Aktaran-Kalaycı et al. 2011). When the budget n is fixed, one faces the classical bias-variance trade-off when selecting m and b. The goal of this paper is to use simple jackknifing technology to facilitate large reductions in bias at the price of only modest increases in variance—the result of which will be improved MSE.

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This article is organized as follows. We present background material in Section 2 to introduce the NBM, OBM, and STS variance estimators that will be used in the sequel. The main jackknifing results for these estimators are given in Section 3. A comparison of the various estimators is undertaken in Section 4. Conclusions and ongoing work are detailed in Section 5.

2 BACKGROUND

In this section, we define the NBM, OBM, and STS estimators for σ^2.

2.1 Nonoverlapping Batch Means Estimator

Here we divide the steady-state output $\{Y_j : j = 1,2,\ldots,n\}$ into b contiguous, nonoverlapping batches of observations, each of length m, where we assume that $n = bm$. Thus, the ith nonoverlapping batch consists of observations $\{Y_{(i-1)m+k} : k = 1,2,\ldots,m\}$ for $i = 1,2,\ldots,b$. We define the nonoverlapping batch means by $\overline{Y}_{i,m} \equiv m^{-1}\sum_{k=1}^{m} Y_{(i-1)m+k}$, for $i = 1,2,\ldots,b$. It is well known that under mild moment and mixing conditions, these batch means can be regarded as approximately independent and identically distributed (i.i.d.) normal random variables as the batch size m increases. This immediately allows us to use the scaled sample variance of the batch means as the NBM estimator for σ^2 (Glynn and Whitt 1991, Steiger and Wilson 2001),

$$\mathscr{N}(b,m) \equiv \frac{m}{b-1}\sum_{i=1}^{b}(\overline{Y}_{i,m} - \overline{Y}_n)^2 \Rightarrow \frac{\sigma^2\chi^2_{b-1}}{b-1} \quad \text{as } m \to \infty,$$

where the symbol $\Rightarrow$ denotes convergence in distribution and χ^2_ν is a χ^2 random variable with ν degrees of freedom. Under mild conditions, several papers (e.g., Chien, Goldsman, and Melamed 1997, Goldsman and Meketon 1986, Song and Schmeiser 1995) find the expected value of the NBM estimator. For instance, consider the following standing assumption.

Assumption A: The process $\{Y_j\}$ is stationary with mean μ and exponentially decaying covariance function $|R_j| = O(\delta^j)$ for some $\delta \in (0,1)$, so that

$$\sum_{j=m}^{\infty} j^\ell |R_j| = O(m^\ell \delta^m) \quad \text{and} \quad \sum_{j=1}^{m} j^\ell R_j = \frac{\gamma_\ell}{2} + O(m^\ell \delta^m) \quad \text{for } \ell = 0,1,2,\ldots,$$

where the "Big-Oh" notation $g(m) = O(h(m))$ means that for some finite constants C and m_0, we have $|g(m)| \le C|h(m)|$ for all $m \ge m_0$, and where $\gamma_\ell \equiv 2\sum_{j=1}^{\infty} j^\ell R_j$, $\ell = 0,1,2,\ldots$.

Under Assumption A, Aktaran-Kalaycı et al. (2007) show that

$$\mathrm{E}[\mathscr{N}(b,m)] = \sigma^2 - \frac{\gamma_1(b+1)}{mb} + O(\delta^m). \tag{1}$$

In addition, the NBM estimator's variance is given by

$$\lim_{m\to\infty}(b-1)\,\mathrm{Var}[\mathscr{N}(b,m)] = 2\sigma^4 \quad \text{for fixed } b.$$

2.2 Overlapping Batch Means Estimator

Now we form $n-m+1$ *overlapping* batches, each of size m. In particular, the ith overlapping batch is composed of the observations $\{Y_{i+k} : k = 0,1,\ldots,m-1\}$, for $i = 1,2,\ldots,n-m+1$; and the ith overlapping batch mean is $\overline{Y}^{\mathrm{O}}_{i,m} \equiv m^{-1}\sum_{k=0}^{m-1} Y_{i+k}$, for $i = 1,2,\ldots,n-m+1$. Finally, the OBM estimator for σ^2 is the appropriately scaled sample variance of the overlapping batch means (Meketon and Schmeiser 1984),

$$\mathscr{O}(b,m) \equiv \frac{nm}{(n-m+1)(n-m)}\sum_{i=1}^{n-m+1}(\overline{Y}^{\mathrm{O}}_{i,m} - \overline{Y}_n)^2.$$

Under Assumption A with $b = n/m \geq 2$, Aktaran-Kalaycı et al. (2007) show that

$$\mathrm{E}[\mathscr{O}(b,m)] \;=\; \sigma^2 - \frac{\gamma_1(b^2+1)}{n(b-1)} + \frac{\gamma_1+\gamma_2}{(n-m)(n-m+1)} + O(\delta^m) \tag{2}$$

(also see Goldsman and Meketon 1986 and Song and Schmeiser 1995, among others). Further, Damerdji (1995) finds that for large batch size m and fixed sample-to-batch-size ratio b,

$$\lim_{m\to\infty} \mathrm{Var}[\mathscr{O}(b,m)] \;=\; \frac{(4b^3-11b^2+4b+6)\sigma^4}{3(b-1)^4} \;\approx\; \frac{4\sigma^4}{3b} \quad \text{for large } b.$$

So the OBM estimator has about the same bias as, but only 2/3 the variance of the NBM estimator.

2.3 Standardized Time Series Nonoverlapping Area Estimator

For purposes of this subsection, we divide the steady-state simulation output $\{Y_j : j = 1,2,\ldots,n\}$ into $b = n/m$ nonoverlapping batches, as in Section 2.1. Schruben (1983) defined the standardized time series from nonoverlapping batch i by

$$T_{i,m}(t) \;\equiv\; \frac{\lfloor mt \rfloor(\overline{Y}_{i,m} - \overline{Y}_{i,\lfloor mt \rfloor})}{\sigma\sqrt{m}} \quad \text{for } t \in [0,1] \text{ and } i = 1,2,\ldots,b,$$

where $\lfloor\cdot\rfloor$ is the floor function and $\overline{Y}_{i,j} \equiv j^{-1}\sum_{k=1}^{j} Y_{(i-1)m+k}$ is the jth cumulative sample mean from batch i, for $i = 1,2,\ldots,b$ and $j = 1,2,\ldots,m$. The STS nonoverlapping area estimator for σ^2, based on b batches and weight function $f(\cdot)$, is defined as

$$\mathscr{A}(f;b,m) \;\equiv\; \frac{1}{b}\sum_{i=1}^{b} A_i(f;m),$$

where

$$A_i(f;m) \;\equiv\; \left[\frac{1}{m}\sum_{k=1}^{m} f(k/m)\sigma T_{i,m}(k/m)\right]^2 \quad \text{for } i = 1,2,\ldots,b,$$

and where $f(\cdot)$ satisfies the conditions

$$\int_0^1\!\!\int_0^1 f(s)f(t)\big(\min(s,t)-st\big)\,ds\,dt \;=\; 1 \quad \text{and} \quad \tfrac{d^2}{dt^2}f(t) \text{ is continuous at every } t\in[0,1]. \tag{3}$$

Under a mild functional central limit theorem assumption (cf. Goldsman, Meketon, and Schruben 1990), it turns out that $\mathscr{A}(f;b,m) \Rightarrow \sigma^2\chi_b^2/b$ as $m \to \infty$. Moreover,

$$\mathrm{E}[\mathscr{A}(f;b,m)] \;=\; \sigma^2 - \frac{[(F-\overline{F})^2+\overline{F}^2]\gamma_1}{2m} + O(1/m^2), \tag{4}$$

where

$$F(s) \equiv \int_0^s f(t)\,dt \;\text{ for } s\in[0,1],\;\; F \equiv F(1),\;\; \overline{F}(u) \equiv \int_0^u F(s)\,ds \;\text{ for } u\in[0,1],\;\text{ and }\; \overline{F} \equiv \overline{F}(1).$$

Further, under mild conditions and as long as the weight function $f(\cdot)$ satisfies Conditions (3), we have for fixed b,

$$\lim_{m\to\infty} b\,\mathrm{Var}[\mathscr{A}(f;b,m)] \;=\; 2\sigma^4.$$

Schruben's original area estimator uses the constant weight $f_0(t) \equiv \sqrt{12}$ for all $t \in [0,1]$, for which under Assumption A, Aktaran-Kalaycı et al. (2007) derive the fine-tuned result

$$\mathrm{E}[\mathscr{A}(f_0;b,m)] \;=\; \sigma^2 - \frac{3\gamma_1}{m} - \frac{\sigma^2}{m^2} + \frac{\gamma_1 + 2\gamma_3}{m^3} + O(\delta^m), \tag{5}$$

indicating that $\mathscr{A}(f_0;b,m)$ is somewhat biased in m. The good news is that it is easy to choose a weight such as $f_2(t) \equiv \sqrt{840}(3t^2 - 3t + 1/2)$ that yields an estimator having $F = \overline{F} = 0$ in Equation (4), i.e., which is first-order unbiased for σ^2. In fact, under Assumption A, Aktaran-Kalaycı et al. (2007) obtain the fine-tuned result

$$\mathrm{E}[\mathscr{A}(f_2;b,m)] \;=\; \sigma^2 + \frac{7(\sigma^2 - 6\gamma_2)}{2m^2} + \frac{35(\gamma_1 + 2\gamma_3)}{2m^3} + O(1/m^4). \tag{6}$$

3 MAIN RESULTS

In this section, we deliver the main results of the article. Section 3.1 describes a simple jackknife calculation that reduces estimator bias. Then Sections 3.2–3.4 show how to use the jackknife on the NBM, OBM, and STS nonoverlapping area estimators. Section 4 compares the performances of the various estimators.

3.1 A Rough and Ready Tool

One of the easiest ways to reduce estimator bias is via the use of jackknifing (Quenouille 1949, Quenouille 1956, Tukey 1958, Efron 1982). In the ensuing discussion, we will work with simple "block" jackknife versions of our original NBM, OBM, and STS estimators. In order to provide motivation, suppose that $\mathscr{V}(n)$ is a generic estimator for σ^2 based on n observations. Further suppose that $\mathrm{E}[\mathscr{V}(n)] = \sigma^2 + c/n + O(1/n^2)$ for some appropriate c. If we define a jackknife version of $\mathscr{V}(n)$ by

$$\mathscr{V}_{\mathrm{J}}(n) \;\equiv\; \frac{\mathscr{V}(n) - r\mathscr{V}(rn)}{1-r}, \quad 0 < r < 1, \tag{7}$$

then an elementary calculation reveals that $\mathrm{E}[\mathscr{V}_{\mathrm{J}}(n)] = \sigma^2 + O(1/n^2)$, thereby yielding a first-order unbiased estimator for σ^2. While this bias reduction is greatly satisfying, the party is spoiled a bit by a variance increase,

$$\begin{aligned}
\mathrm{Var}[\mathscr{V}_{\mathrm{J}}(n)] &= \frac{1}{(1-r)^2}\big(\mathrm{Var}[\mathscr{V}(n)] + r^2\mathrm{Var}[\mathscr{V}(rn)] - 2r\mathrm{Cov}[\mathscr{V}(n), \mathscr{V}(rn)]\big) \\
&\approx \frac{1}{(1-r)^2}\big((1+r^2)\mathrm{Var}[\mathscr{V}(n)] - 2r\mathrm{Cov}[\mathscr{V}(n), \mathscr{V}(rn)]\big),
\end{aligned}$$

where the approximation is due to the fact that $\mathrm{Var}[\mathscr{V}(n)]$ and $\mathrm{Var}[\mathscr{V}(rn)]$ (for fixed r) typically converge to the same constant for large n.

We will use this trick—or an easy variant—in the upcoming sections.

3.2 Jackknifing the NBM Estimator

We apply a slight variant of Equation (7) to obtain the jackknifed NBM estimator,

$$\mathscr{N}_{\mathrm{J}}(b,m,r) \;\equiv\; \beta_{\mathrm{N}}(b,r)\mathscr{N}(b,m) + [1 - \beta_{\mathrm{N}}(b,r)]\mathscr{N}(b/r, mr), \tag{8}$$

where we assume for convenience that b/r and rm are integers and we take

$$\beta_{\mathrm{N}}(b,r) \;\equiv\; \frac{b+r}{b(1-r)}.$$

Equations (1) and (8) immediately reveal that $\mathrm{E}[\mathscr{N}_{\mathrm{J}}(b,m,r)] = \sigma^2 + O(\delta^m)$, i.e., $\mathscr{N}_{\mathrm{J}}(b,m,r)$ has exponentially decaying bias. After carrying out additional algebra, the details of which are given in Dingeç et al. (2015), one can calculate the variance of the jackknifed NBM estimator,

$$\lim_{m\to\infty} \mathrm{Var}[\mathscr{N}_{\mathrm{J}}(b,m,r)] \;=\; \frac{2\sigma^4}{b-1}\left[\frac{\left(1+r-r^2\right)b^2+(r+r^2)b+r^2}{(1-r)b(b-r)}\right] \;\equiv\; \frac{2\sigma^4}{b-1}W(b,r),$$

where $W(b,r)$ represents a variance inflation factor over the original NBM estimator $\mathscr{N}(b,m)$, with

$$\lim_{b\to\infty} W(b,r) \;=\; \frac{1+r-r^2}{1-r} \;>\; 1 \quad \text{for } 0<r<1.$$

For example, for $r = 1/8$ and 1/2, the above limiting inflation factors are $71/56 \approx 1.3$ and 5/2, respectively.

3.3 Jackknifing the OBM Estimator

We can remove the OBM estimator's first-order bias term displayed in Equation (2) by jackknifing,

$$\mathscr{O}_{\mathrm{J}}(b,m,r) \;\equiv\; \beta_{\mathrm{O}}(b,r)\mathscr{O}(b,m) + (1-\beta_{\mathrm{O}}(b,r))\mathscr{O}(b/r,mr),$$

where we again assume for convenience that b/r and rm are integers and we take

$$\beta_{\mathrm{O}}(b,r) \;\equiv\; \frac{(b-1)\left(b^2+r^2\right)}{(1-r)b\left[b^2-b(r+1)-r\right]}.$$

After some algebra, we find that the expected value of the jackknifed OBM estimator is

$$\mathrm{E}[\mathscr{O}_{\mathrm{J}}(b,m,r)] \;=\; \sigma^2 + \frac{\left[(b^3-br+r^2-r)m+b^2-r\right](\gamma_1+\gamma_2)}{bm\left[(b-1)m+1\right]\left[(b-r)m+1\right]\left[b^2-(1+r)b-r\right]} + O(\delta^m). \tag{9}$$

Thus, $\mathscr{O}_{\mathrm{J}}(b,m,r)$ is first-order unbiased for σ^2, which is an improvement over the analogous expected value result for $\mathscr{O}(b,m)$ from Equation (2). Moreover, Dingeç et al. (2015) find that $\lim_{b\to\infty}\mathrm{E}[\mathscr{O}_{\mathrm{J}}(b,m,r)] = \sigma^2 + O(\delta^m)$, suggesting that the bias will exhibit exponential decay for large b. Dingeç et al. (2015) also obtain the variance of the jackknifed OBM estimator,

$$\mathrm{Var}[\mathscr{O}_{\mathrm{J}}(b,m,r)] \;\approx\; \frac{4\sigma^4}{3b}(1+2r) + O(1/b^2) \quad \text{for large } b.$$

For $r = 1/2$ and large b, the jackknifed OBM estimator has approximately 2 times the variance of the regular OBM estimator; this penalty goes up to a factor of at most 3 for $r \approx 1$.

3.4 Jackknifing the STS Nonoverlapping Area Estimator

For notational convenience, we temporarily work with area estimators consisting of $b = 1$ batch of m observations; modifications for $b > 1$ batches of m observations will be discussed starting in Section 3.4.3. Therefore, consider Section 2.3's area estimator from the first batch of m observations, $A(f;m) \equiv A_1(f;m)$. We will examine the effects of jackknifing on this area estimator with weights $f_0(t)$ and $f_2(t)$.

3.4.1 Area Estimator with Weight $f_0(t)$

Recall that the expected value of the area estimator with constant weight $f_0(t) = \sqrt{12}$ is given by Equation (5), where it is revealed that $A(f_0;m)$ is first-order biased as an estimator of σ^2. The good news is that Equation (7) gives us a recipe to eliminate this first-order bias via the jackknifed estimator

$$A_{\mathrm{J}_1}(f_0;m,r) \;\equiv\; \frac{A(f_0;m)-rA(f_0;rm)}{1-r}.$$

After some algebra, our hopes are realized, since

$$\mathrm{E}[A_{\mathrm{J}_1}(f_0;m,r)] \;=\; \sigma^2 + \frac{\sigma^2}{rm^2} - \frac{(1+r)(\gamma_1+2\gamma_3)}{r^2m^3} + O(\delta^m).$$

However, Dingeç et al. (2015) show that there is a steep price to be paid in terms of variance for this first-order unbiasedness. Namely,

$$\frac{\mathrm{Var}[A_{\mathrm{J}_1}(f_0;m,r)]}{\mathrm{Var}[A(f_0;m)]} \;\to\; \frac{1+r^2-2r^4}{(1-r)^2}; \tag{10}$$

for instance, if $r=1/2$, the variance inflates by a factor of 4.5, so that $\mathrm{Var}[A_{\mathrm{J}_1}(f_0;m,r)] \to 9\sigma^4$.

Without becoming discouraged by this variance inflation, let us apply our jackknifing technology again to remove other bias terms. In fact, if we are interested in eliminating a generic area estimator's $O(1/m^\ell)$ bias term for some positive integer ℓ, Dingeç et al. (2015) show that the estimator

$$A_{\mathrm{J}_\ell}(f;m,r) \;\equiv\; \frac{A(f;m)-r^\ell A(f;rm)}{1-r^\ell}, \quad r\in(0,1), \tag{11}$$

does the trick. Similarly, if we want to simultaneously eliminate two bias terms, say of orders $O(1/m^{\ell_1})$ and $O(1/m^{\ell_2})$ for positive integers ℓ_1 and ℓ_2 with $\ell_2 > \ell_1$, then it is easy to show that the following estimator is right for the job,

$$A_{\mathrm{J}_{\ell_1,\ell_2}}(f;m,r) \;\equiv\; \frac{A(f;m)-(r^{\ell_1}+r^{\ell_2})A(f;rm)+r^{\ell_1+\ell_2}A(f;r^2m)}{(1-r^{\ell_1})(1-r^{\ell_2})}, \quad r\in(0,1).$$

.

For example, suppose that we would like to simultaneously eliminate the first- and third-order bias terms for the area estimator with weight f_0. Then we find after a bit of algebra that the expected value of the estimator $A_{\mathrm{J}_{1,3}}(f_0;m,r)$ is

$$\mathrm{E}[A_{\mathrm{J}_{1,3}}(f_0;m,r)] \;=\; \sigma^2\left(1+\frac{1-r}{r(1-r^3)m^2}\right)+O(\delta^m),$$

where the first- and third-order bias terms have indeed been eliminated, while the second-order term still remains. Fortuitously, we can avoid a third jackknife and eliminate the $O(1/m^2)$ bias term by applying a simple manipulation. Let

$$\zeta(m,r) \;\equiv\; \frac{r(1-r^3)m^2}{1-r+r(1-r^3)m^2},$$

so that the estimator

$$A^\star_{\mathrm{J}_{1,3}}(f_0;m,r) \;\equiv\; \zeta(m,r)A_{\mathrm{J}_{1,3}}(f_0;m,r) \tag{12}$$

has exponential convergence of its expected value to σ^2,

$$\mathrm{E}\big[A^\star_{\mathrm{J}_{1,3}}(f_0;m,r)\big] \;=\; \sigma^2+O(\delta^m).$$

As with Equation (10), Dingeç et al. (2015) find that as $m\to\infty$, the asymptotic variance inflation caused by the "double jackknife" is

$$\frac{\mathrm{Var}[A^\star_{\mathrm{J}_{1,3}}(f_0;m,r)]}{\mathrm{Var}[A(f_0;m)]} \to \frac{1+r^2+r^3+r^5}{(1-r)^3\,(1+r+r^2)}, \quad r\in(0,1);$$

and for $r=0.5$, this ratio is $45/7\approx 6.4$, so that $\mathrm{Var}[A^\star_{\mathrm{J}_{1,3}}(f_0;m,r)] \to 12.857\sigma^4$.

3.4.2 Area Estimator with Weight $f_2(t)$

We apply the technology of Equation (11) with $\ell = 2$ to Equation (6) with $b = 1$ to remove the quadratic bias term, resulting in

$$\mathrm{E}[A_{\mathrm{J}_2}(f_2;m,r)] \;=\; \frac{\mathrm{E}[A(f_2;m)] - r^2\mathrm{E}[A(f_2;rm)]}{1-r^2} \;=\; \sigma^2 - \frac{35(\gamma_1+2\gamma_3)}{2r(1+r)m^3} + O(1/m^4), \quad r\in(0,1),$$

which is second-order unbiased, as promised. Similar to Equation (10), we calculate the asymptotic variance inflation caused by the jackknife as $m\to\infty$,

$$\frac{\mathrm{Var}[A_{\mathrm{J}_2}(f_2;m,r)]}{\mathrm{Var}[A(f_2;m)]} \;\to\; \frac{1+r^4-\frac{1}{2}r^5\left[7+3r(-7+4r)\right]^2}{(1-r^2)^2}, \quad r\in(0,1),$$

so that for $r = 0.5$, the inflation factor is about 1.88194, i.e., $\mathrm{Var}[A_{\mathrm{J}_2}(f_2;m,r)] \to 3.764\sigma^4$. Notice that this inflation factor is significantly smaller than the inflation factors for $A_{\mathrm{J}_1}(f_0;m,r)$ and $A^{\star}_{\mathrm{J}_{1,3}}(f_0;m,r)$.

We can repeat the jackknifing exercise to remove higher-order bias terms, but instead refer the reader to Dingeç et al. (2015) for the detailed results.

3.4.3 Batching of Jackknifed Area Estimators

The single-batch variance estimators $A_{\mathrm{J}_\ell}(f;m,r)$ and $A^{\star}_{\mathrm{J}_{1,3}}(f_0;m,r)$ defined by Equations (11) and (12) are easily generalized for $b>1$ batches. Simply let

$$\mathscr{A}_{\mathrm{J}_\ell}(f;b,m,r) \;\equiv\; \frac{1}{b}\sum_{i=1}^{b} A_{\mathrm{J}_\ell,i}(f;m,r) \quad \text{and} \quad \mathscr{A}^{\star}_{\mathrm{J}_{1,3}}(f_0;b,m,r) \;\equiv\; \frac{1}{b}\sum_{i=1}^{b} A^{\star}_{\mathrm{J}_{1,3},i}(f_0;m,r),$$

where the i subscript indicates that the component estimator is from the ith nonoverlapping batch, $i = 1,2,\ldots,b$. Assuming that the $A_{\mathrm{J}_\ell,i}(f;m,r)$ estimators from different nonoverlapping batches are i.i.d., we see that $\mathrm{E}[\mathscr{A}_{\mathrm{J}_\ell}(f;b,m,r)] = \mathrm{E}[A_{\mathrm{J}_\ell}(f;m,r)]$ and $\mathrm{Var}\big[\mathscr{A}_{\mathrm{J}_\ell}(f;b,m,r)\big] = \mathrm{Var}\big[A_{\mathrm{J}_\ell}(f;m,r)\big]/b$; and similarly for $\mathscr{A}^{\star}_{\mathrm{J}_{1,3}}(f_0;b,m,r)$.

4 COMPARISON OF ESTIMATORS

In this section, we compare the performances of different jackknifed estimators presented in Section 3 based on their biases, variances, and MSEs.

4.1 Bias, Variance, and Mean Squared Error

Table 1 summarizes the main results from Section 3 for $r = 1/2$, along with asymptotically optimal MSE results. The MSE of an estimator for the variance parameter σ^2 balances bias and variance. To this end, consider the generic variance estimator $\mathscr{V}(n)$ for σ^2. Suppose that the bias of $\mathscr{V}(n)$ is of the form $\mathrm{Bias}[\mathscr{V}(n)] = c/m^k$ for some constant c, batch size m, and $k>0$, where we ignore smaller-order terms. Further suppose that the variance of $\mathscr{V}(n)$ is of the form $\mathrm{Var}[\mathscr{V}(n)] = v/b$ for some constant v and sample-to-batch-size ratio $b = n/m$.

In such cases, the MSE of $\mathscr{V}(n)$ as an estimator of σ^2 is

$$\mathrm{MSE}[\mathscr{V}(n)] \;=\; \mathrm{Bias}^2[\mathscr{V}(n)] + \mathrm{Var}[\mathscr{V}(n)] \;\approx\; \frac{c^2}{m^{2k}} + \frac{v}{b},$$

where the approximation is the direct result of ignoring small-order terms. As described in Goldsman and Meketon (1986), Song and Schmeiser (1995), and Aktaran-Kalaycı et al. (2011), the minimum value of

Table 1: Approximate bias, variance, and optimal MSE formulas for large b and m and $r = 1/2$. (Bias results for $\mathscr{O}_{\mathrm{J}}(b,m,1/2)$ are for the special case in which $b \to \infty$.)

Estimator	Bias	$b \cdot \text{Variance}/\sigma^4$	MSE*
$\mathscr{N}(b,m)$	$-\dfrac{\gamma_1}{m}$	2	$3\left(\dfrac{\gamma_1\sigma^4}{n}\right)^{2/3}$
$\mathscr{N}_{\mathrm{J}}(b,m,1/2)$	$O(\delta^m)$	5	$O(\ell\mathrm{n}(n)/n)$
$\mathscr{O}(b,m)$	$-\dfrac{\gamma_1}{m}$	$4/3$	$2.289\left(\dfrac{\gamma_1\sigma^4}{n}\right)^{2/3}$
$\mathscr{O}_{\mathrm{J}}(b,m,1/2)$	$O(\delta^m)$	$8/3$	$O(\ell\mathrm{n}(n)/n)$
$\mathscr{A}(f_0;b,m)$	$-\dfrac{3\gamma_1}{m}$	2	$6.240\left(\dfrac{\gamma_1\sigma^4}{n}\right)^{2/3}$
$\mathscr{A}_{\mathrm{J}_1}(f_0;b,m,1/2)$	$\dfrac{2\sigma^2}{m^2}$	9	$12.622\left(\dfrac{\sigma^5}{n}\right)^{4/5}$
$\mathscr{A}^\star_{\mathrm{J}_{1,3}}(f_0;b,m,1/2)$	$O(\delta^m)$	$90/7$	$O(\ell\mathrm{n}(n)/n)$
$\mathscr{A}(f_2;b,m)$	$\dfrac{7(\sigma^2-6\gamma_2)}{2m^2}$	2	$4.740\left[\dfrac{(\sigma^2-6\gamma_2)\sigma^8}{n^2}\right]^{2/5}$
$\mathscr{A}_{\mathrm{J}_2}(f_2;b,m,1/2)$	$\dfrac{-70(\gamma_1+2\gamma_3)}{3m^3}$	3.764	$11.545\left[\dfrac{(\gamma_1+2\gamma_3)\sigma^{12}}{n^3}\right]^{2/7}$

this quantity (at least asymptotically for large values of the run length n and hence for large m and b) is

$$\mathrm{MSE}^\star[\mathscr{V}(n)] \;=\; (1+2k)\left[c\left(\frac{v}{2nk}\right)^k\right]^{\frac{2}{1+2k}}.$$

For the variance estimators $\mathscr{N}_{\mathrm{J}}(b,m,r)$, $\mathscr{O}_{\mathrm{J}}(b,m,r)$, and $\mathscr{A}^\star_{\mathrm{J}_{1,3}}(f_0;b,m,r)$ for which the bias is of the form $O(\delta^m)$, a more-delicate analysis is required to show that the minimum MSE is of order $O(\ell\mathrm{n}(n)/n)$; see Dingeç et al. (2015).

4.2 Exact Bias Example

We present exact closed-form bias results for a particular stochastic process—a stationary autoregressive process of order 1 [AR(1)]. The AR(1) is defined by $Y_i = \phi Y_{i-1} + \varepsilon_i$ for $i = 1,2,\ldots$, where $-1 < \phi < 1$, $Y_0 \sim N(0,1)$, and the ε_i's are i.i.d. $N(0,1-\phi^2)$ random variables, independent of Y_0. The covariance function of the process is $R_j = \phi^{|j|}$, for $j = 0,\pm1,\pm2,\ldots$. As shown by Aktaran-Kalaycı et al. (2007), we have $\sigma^2 = (1+\phi)/(1-\phi)$, $\gamma_1 = 2\phi/(1-\phi)^2$, $\gamma_2 = 2\phi(1+\phi)/(1-\phi)^3$, and $\gamma_3 = 2\phi(1+4\phi+\phi^2)/(1-\phi)^4$.

Aktaran-Kalaycı et al. (2007) give closed-form formulas for the expected values of $\mathscr{N}(b,m)$, $\mathscr{O}(b,m)$, and $\mathscr{A}(f_0;b,m)$ for the AR(1) process. The expected value of the vanilla NBM estimator is

$$\mathrm{E}[\mathscr{N}(b,m)] \;=\; \sigma^2 - \frac{\gamma_1}{bm}\left(b+1-\frac{b^2\phi^m-\phi^{bm}}{b-1}\right); \tag{13}$$

and, for large b, we have

$$\lim_{b\to\infty} \mathrm{E}[\mathscr{N}(b,m)] \;=\; \sigma^2 - \frac{\gamma_1\,(1-\phi^m)}{m}.$$

Equations (8) and (13) give the expected value of the jackknifed NBM estimator,

$$\mathrm{E}[\mathscr{N}_{\mathrm{J}}(b,m,r)] \;=\; \sigma^2 - \frac{\gamma_1\left[\left(b^2-1\right)\phi^{mr} + (r^2-b^2)\phi^m + (1-r^2)\phi^{bm}\right]}{m(b-1)(1-r)(b-r)}.$$

For large b, we obtain

$$\lim_{b\to\infty} \mathrm{E}[\mathscr{N}_{\mathrm{J}}(b,m,r)] \;=\; \sigma^2 - \frac{\gamma_1\,(\phi^{mr}-\phi^m)}{m(1-r)}. \tag{14}$$

The expected value of the regular OBM estimator is

$$\mathrm{E}[\mathscr{O}(b,m)] \;=\; \sigma^2 - \frac{\left(b^2+1\right)\gamma_1}{b(b-1)m} + \frac{\gamma_1+\gamma_2}{(n-m)(n-m+1)} + \frac{\gamma_1\phi^m}{n-m}\left[b + \frac{\phi^{n-m}}{b} - \frac{2\left(1+\phi^{n-2m+1}-\phi^{n-m+1}\right)}{(1-\phi)(n-m+1)}\right].$$

We will not give the tedious expression here for $\mathrm{E}[\mathscr{O}_{\mathrm{J}}(b,m,r)]$, but as per Equation (9), the jackknifed estimator $\mathscr{O}_{\mathrm{J}}(b,m,r)$ is first-order unbiased for σ^2.

What is much more interesting is that for the special case in which we let $b\to\infty$, some algebra reveals that the expected value of the jackknifed OBM estimator is the same as the right-hand side of Equation (14). So, asymptotically, the jackknifed OBM estimator has the same bias as the jackknifed NBM estimator. But we also know that the jackknifed OBM estimator has an asymptotic variance that is smaller than that of the jackknifed NBM estimator. Thus, perhaps it will be the case that, asymptotically, $\mathscr{O}_{\mathrm{J}}(b,m,r)$ will have a smaller MSE than $\mathscr{N}_{\mathrm{J}}(b,m,r)$—though this is not quite borne out by the respective MSE* entries of Table 1, which only indicate that the MSEs are of the same order $O(\ell\mathrm{n}(n)/n)$.

Continuing, the expected value of the original area estimator $\mathscr{A}(f_0;b,m)$ is

$$\mathrm{E}[\mathscr{A}(f_0;b,m)] \;=\; \sigma^2 - \frac{3\gamma_1}{m} - \frac{\sigma^2}{m^2} + \frac{\gamma_1+2\gamma_3}{m^3} - \frac{3\gamma_1}{m}\left(1+\frac{\sigma^2}{m}\right)^2\phi^m,$$

while that of the jackknifed version turns out to be

$$\mathrm{E}\left[\mathscr{A}^\star_{\mathrm{J}_{1,3}}(f_0;b,m,r)\right] \;=\; \sigma^2 - \frac{3r^2\gamma_1\phi^{mr^2}}{m(1-r)^2\,(1+r+r^2)} + o(\phi^{mr^2}/m),$$

where the "little-oh" notation $g(m)=o(h(m))$ means that $g(m)/h(m)\to 0$ as $m\to\infty$. For this AR(1) example, note that the bias of the jackknifed area estimator is $O(\phi^{mr^2}/m)$, whereas the biases of the jackknifed NBM and OBM estimators are of the smaller order $O(\phi^{mr}/m)$.

Table 2 presents exact bias results for the regular $\mathscr{N}(b,m)$, $\mathscr{O}(b,m)$, and $\mathscr{A}(f_0;b,m)$ estimators and the jackknifed $\mathscr{N}_{\mathrm{J}}(b,m,r)$, $\mathscr{O}_{\mathrm{J}}(b,m,r)$, and $\mathscr{A}^\star_{\mathrm{J}_{1,3}}(f_0;b,m,r)$ estimators with various batches sizes m, batch count $b=n/m=10$, and $r=1/2$ for an AR(1) process with $\phi=0.9$ (in which case $\sigma^2=19$). We see that jackknifing dramatically reduces estimator bias, as anticipated by the underlying theory. Note that the $\mathscr{N}_{\mathrm{J}}(b,m,r)$ and $\mathscr{A}^\star_{\mathrm{J}_{1,3}}(f_0;b,m,r)$ estimators have exponentially decaying bias as the batch size m increases, while $\mathscr{O}_{\mathrm{J}}(b,m,r)$ seems to decay a bit more slowly (since $b=10$ is "small").

4.3 Asymptotically Optimal Mean Squared Error Example

With these exact expected bias results as well asymptotic variance results from Dingeç et al. (2015) for the general jackknife parameter r in hand, we optimize the MSEs with respect to the batch count b, the batch

Table 2: Exact biases of the $\mathscr{N}(b,m)$, $\mathscr{O}(b,m)$, and $\mathscr{A}(f_0;b,m)$ estimators and the jackknifed $\mathscr{N}_{\mathrm{J}}(b,m,r)$, $\mathscr{O}_{\mathrm{J}}(b,m,r)$, and $\mathscr{A}^{\star}_{\mathrm{J}_{1,3}}(f_0;b,m,r)$ with $b=10$ and $r=1/2$ for an AR(1) process with $\phi=0.9$ ($\sigma^2=19$).

m	$\mathscr{N}(b,m)$	$\mathscr{N}_{\mathrm{J}}(b,m,r)$	$\mathscr{O}(b,m)$	$\mathscr{O}_{\mathrm{J}}(b,m,r)$	$\mathscr{A}(f_0;b,m)$	$\mathscr{A}^{\star}_{\mathrm{J}_{1,3}}(f_0;b,m,r)$
64	−3.09	−0.22	−3.14	−0.21	−7.72	−2.21
128	−1.55	−0.004	−1.58	−0.001	−4.13	−0.19
256	−0.77	−2E−06	−0.79	0.0008	−2.10	−0.002
512	−0.39	−2E−12	−0.39	0.0002	−1.05	−1E−06
1024	−0.19	−2E−24	−0.20	5E−05	−0.53	−7E−13
2048	−0.10	−3E−48	−0.10	1E−05	−0.26	−6E−25

size m, and r, for an AR(1) process with $\phi=0.9$. The optimal values are found by numerical minimization of the asymptotic MSE, which is given by the sum of the exact squared bias and the asymptotic variance. These results are displayed in Table 3 for a selection of n-values. We see that the jackknifed estimators quickly outperform their non-jackknifed counterparts in terms of optimal MSE as n increases. Specifically, $\mathscr{N}_{\mathrm{J}}(b,m,r)$ performs quite well, though for large-enough n (and hence large-enough b and m), the jackknifed OBM estimator $\mathscr{O}_{\mathrm{J}}(b,m,r)$ eventually overtakes it.

5 CONCLUSIONS AND ONGOING WORK

We have shown that the use of jackknifing is an effective way to dramatically reduce the bias and mean squared error of estimators of a steady-state simulation's variance parameter σ^2. This is particularly noteworthy in light of the fact that jackknifing typically increases estimator variance.

We presented results for nonoverlapping batch means, overlapping batch means, and certain standardized time series area estimators. In Dingeç et al. (2015), we generalize our work in the following ways:

- We consider other STS area estimator weighting functions, specifically, the general class given in Foley and Goldsman (1999).
- We consider other classes of STS estimators, for example, estimators based on Cramér von–Mises (Goldsman et al. 1999), Durbin–Watson (Batur et al. 2009), folded (Alexopoulos et al. 2010), and reflected (Meterelliyoz et al. 2015) functionals of Brownian bridges, as well as overlapping versions thereof (see, e.g., Alexopoulos et al. 2007).
- We derive approximate distributions of the various variance estimators—not just the first two central moments.
- We work with jackknife estimators that take advantage of batching in a more-efficient way.
- When carrying out simultaneous jackknifing to eliminate multiple orders of bias, we work with multiple r-values—not just a single value as in the current paper.

We are certainly encouraged by the fact that jackknifing almost always decreases bias significantly for this bulleted list of estimators—both in theory and on practical experimental stochastic processes.

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Table 3: Asymptotically optimal b, m, r, and MSE for the $\mathscr{N}(b,m)$, $\mathscr{O}(b,m)$, and $\mathscr{A}(f_0;b,m)$ estimators and the jackknifed $\mathscr{N}_{\mathrm{J}}(b,m,r)$, $\mathscr{O}_{\mathrm{J}}(b,m,r)$, and $\mathscr{A}^{\star}_{\mathrm{J}_{1,3}}(f_0;b,m,r)$ estimators for an AR(1) process with $\phi = 0.9$ ($\sigma^2 = 19$). (The optimal b and m are rounded to the nearest integer.)

	$\mathscr{N}(b,m)$			$\mathscr{N}_{\mathrm{J}}(b,m,r)$			
n	$b^\star$	$m^\star$	MSE*	$b^\star$	$m^\star$	$r^\star$	MSE*
256	9	28	120.267	12	22	0.07	130.620
512	14	36	75.764	19	27	0.13	78.367
1024	23	45	47.728	31	33	0.18	46.034
2048	36	57	30.067	53	38	0.21	26.665
4096	57	72	18.941	93	44	0.24	15.266
8192	91	90	11.932	166	49	0.26	8.647
16384	144	114	7.517	299	55	0.28	4.850
32768	229	143	4.735	545	60	0.30	2.697
65536	363	181	2.983	999	66	0.31	1.488
	$\mathscr{O}(b,m)$			$\mathscr{O}_{\mathrm{J}}(b,m,r)$			
n	$b^\star$	$m^\star$	MSE*	$b^\star$	$m^\star$	$r^\star$	MSE*
256	8	33	91.781	11	22	0.17	103.248
512	12	41	57.819	19	26	0.27	58.784
1024	20	52	36.423	34	30	0.34	33.110
2048	31	65	22.945	61	34	0.41	18.526
4096	50	82	14.455	110	37	0.46	10.300
8192	79	103	9.106	202	41	0.50	5.689
16384	126	130	5.736	373	44	0.54	3.121
32768	200	164	3.614	693	47	0.57	1.701
65536	317	207	2.276	1295	51	0.60	0.922
	$\mathscr{A}(f_0;b,m)$			$\mathscr{A}^{\star}_{\mathrm{J}_{1,3}}(f_0;b,m,r)$			
n	$b^\star$	$m^\star$	MSE*	$b^\star$	$m^\star$	$r^\star$	MSE*
256	4	59	250.166	5	47	0.03	233.765
512	7	75	157.595	8	65	0.03	151.602
1024	11	94	99.279	13	81	0.06	95.683
2048	17	118	62.542	21	96	0.10	58.631
4096	27	149	39.399	37	111	0.13	35.026
8192	44	188	24.820	64	127	0.15	20.516
16384	69	237	15.635	114	143	0.17	11.832
32768	110	298	9.850	205	160	0.18	6.739
65536	175	375	6.205	370	177	0.19	3.799

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