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ASYMPTOTIC AND FINITE-SAMPLE CORRELATIONS BETWEEN OBM ESTIMATORS

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ABSTRACT

Linear combinations of estimators offer a variety of good computational and statistical properties. The values of the optimal linear-combination weights depend upon the estimators' covariances. We investigate the asymptotic covariances and correlations between overlapping-batch-means estimators of the variance of the sample mean when applied to a common sample from a stationary finite-order moving-average data process. After reviewing the asymptotic formulas, we report a Monte Carlo study that suggests that the asymptotic correlation formula provides a good approximation to the true finite-sample correlation if (1) the sample size n is at least several multiples of γ_0 and (2) the both batch sizes are between γ_0 and $n/2$, where γ_0 is the sum of all autocorrelation.

1 INTRODUCTION

Engineers are faced with real-world stochastic systems that are frequently too complex to allow an analytical evaluation. Often, in such cases, a computer simulation model must be developed and Monte Carlo techniques used to study these systems. Stochastic simulation experiments create statistical point estimators to infer the value of system performance measures. Because of this inferential nature of Monte Carlo techniques, it is necessary to indicate how likely these statistics are to be wrong and by how much. Usually the uncertainty is measured in terms of estimator variance. We refer to the the process of estimating the variance of the point estimator as *output analysis*.

Classical issues in output analysis of a simulation study include (1) how to obtain good estimates of some measure of performance, (2) how to evaluate the quality of these estimates, and (3) how to determine the goodness of the quality measure. Often in simulation the measure of performance is a population mean, the point estimator is the sample mean, and the goodness of the point estimator is measured by its standard error.

Several procedures for estimating the standard error from stationary autocorrelated data have been proposed: For example, direct (DI) [Hannan, 1957, and Moran, 1975], spectral (SP) [Bratley, Fox and Schrage, 1987; Heidelberger and Welch, 1981], non-overlapping-batch-means (NBM) [Schmeiser, 1982], overlapping-batch-means (OBM) [Meketon and Schmeiser, 1984], standardized-time-series-area (STS.A) [Schruben, 1983] and orthonormally weighted (STS.W) [Foley and Goldsman, 1988]. No type of estimator dominates the others in terms of computational and statistical properties across all types of time-series data.

Our main objective is to develop robust and computationally efficient methodology to estimate the variance of the sample mean. Previous studies [Politis and Romano, 1992, Song and Schmeiser, 1988b] suggest that linear combinations of estimators of the variance of the sample mean lead to better estimators; i.e., with smaller mean squared error (mse) than the component estimators. We consider the problem of determining the minimal mse optimal linear combination weights of OBM estimators. We study OBM estimators since they are conceptually simple methods, they are easy to compute, and they can be written as quadratic forms, which leads to tractable analysis.

The key to using linear combinations, as discussed in Section 2.3, is to derive the asymptotic covariance/correlation between OBM estimators. In Section 3 we present our asymptotic results and in Section 4 we show empirically that the asymptotic correlation formula provides a good approximation to the finite-sample correlation, except when the batch size is quite small or larger than half the sample size. Here *small* is with respect to the sum of autocorrelations.

2 BACKGROUND

Bratley, Fox and Schrage [1987] and other simulation textbooks discuss output analysis. Here we summarize background information about the variance of the sample mean, batch means estimators, and optimal linear combinations.

2.1 The Variance of the Sample Mean

For stationary time series $\{X_i\}$ a natural unbiased estimator of the population mean μ_X is the sample mean

$$\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i, \qquad (1)$$

where n is the number of observations. The variance of any sample mean is

$$\text{var}(\bar{X}) = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \text{cov}(X_i, X_j). \qquad (2)$$

For stationary time series, $\text{cov}(X_i, X_{i+h}) = R(h)$ is a constant, yielding

$$\text{var}(\bar{X}) = \frac{R(0)}{n} \sum_{h=-n}^{n} \left(1 - \frac{|h|}{n}\right) \rho(h), \qquad (3)$$

where $R(0) = \text{var}(X)$ and $\rho(h) = \text{corr}(X_i, X_{i+h})$. Define

$$\gamma_0 = \sum_{h=-\infty}^{\infty} \rho(h). \qquad (4)$$

If $\gamma_0 < \infty$ then

$$\lim_{n \to \infty} n \, \text{var}(\bar{X}) = \gamma_0 \, R(0), \qquad (5)$$

as shown in, for example, Anderson [1971, p. 460]. For independent and identically distributed (iid) data, $\gamma_0 = 1$. More generally, Equation 5 implies that γ_0 can be thought of as the number of contiguous observations that carry the same information as one independent observation. The rate of convergence in Equation 5 depends on

$$\gamma_1 = \sum_{h=-\infty}^{\infty} |h| \, \rho(h) = 2 \sum_{h=1}^{\infty} h \, \rho(h), \qquad (6)$$

the weighted sum of the correlations. In particular, Schmeiser and Song [1989] show that if $\gamma_1 < \infty$ then

$$n \, \text{var}(\bar{X}) = \gamma_0 \, R(0) - \frac{\gamma_1 R(0)}{n} + o\left(\frac{1}{n}\right). \qquad (7)$$

2.2 The Batch-Means Methodology and the OBM Estimator of var($\bar{X}$)

The batch-means methodology is based on dividing the n observations X_1, X_2, ..., X_n into b batches of size m. Thus batch 1 consists of observations X_1, ..., X_m and batch i consists of observations $X_{l(i-1)+1}$, ..., $X_{l(i-1)+m}$ where l is the "lag" between the first observations of two consecutive batches. For $l = 1$ there is full overlap and the estimator is called overlapping-batch-means (OBM) [Meketon and Schmeiser, 1984] and for $l = m$ there is no overlap and the estimator is the non-overlapping-batch-means (NBM) [Schmeiser, 1982]. The main concept underlying the NBM methodology is to transform correlated data into fewer batch means that are normally distributed and uncorrelated. OBM also batches observations but the batches contain common observations and are therefore correlated. The OBM estimator of var($\bar{X}$) is asymptotically equivalent to the Bartlett spectral estimator, and therefore it has only 2/3 the asymptotic variance of NBM's [Meketon and Schmeiser, 1984].

The overlapping-batch-means (OBM) estimator of var($\bar{X}$) is defined as

$$\hat{V} = \frac{1}{d} \sum_{i=1}^{b} (\bar{X}_i - \bar{X})^2 , \qquad (8)$$

where $b = n - m + 1$, $d = (n - m + 1)(n - m)/m$, $1 \le m \le n - 1$, and

$$\bar{X}_i = \frac{1}{m} \sum_{j=i}^{i-1+m} X_j .$$

This estimator is unbiased for iid data for any sample size n and any batch size m, but it is biased in general.

For normal iid data and fixed batch size m the following equation holds:

$$\lim_{n \to \infty} n^3 \text{var}(\hat{V}) = \frac{2R(0)^2}{3} \left(2m + \frac{1}{m}\right), \qquad (9)$$

[Song and Schmeiser, 1988a]. This limit can be compared to the analogous expression $2mR(0)^2$ for the NBM estimator, to conclude that the asymptotic ratio is two-thirds.

The OBM is a quadratic-form estimator since it can be written as

$$\hat{V} = \sum_i \sum_j q_{ij} X_i X_j \qquad (10)$$

for constant coefficients q_{ij}, or equivalently

$$\hat{V} = \underline{X}^t Q \underline{X}, \qquad (11)$$

where $\underline{Q}$ is a constant symmetric matrix, $\underline{Q} = [q_{ij}]_{i,j=1}^{n}$, and $\underline{X}$ is the vector of observations. An extensive study of the quadratic-form class is presented in Song and Schmeiser [1993].

The quadratic-form coefficients of the OBM estimator of $\text{var}(\bar{X})$ are

$$q_{ij} = \frac{1}{d}\left[\frac{a_{ij}}{m^2} - \frac{a_{ii}+a_{jj}}{m\ n} + \frac{n-m+1}{n^2}\right], \quad (12)$$

where a_{ij}, the number of batches that includes both X_i and X_j, is defined by

$$\begin{aligned} a_{ij} &= \min[n-m+1, \max(0, m-|j-i|), \\ &\quad \min(i,j), n-\max(i,j)+1]. \quad (13) \end{aligned}$$

the first term, $n-m+1$, is the number of batches; the second reflects the batch size m and lag of cross product; the third and fourth terms are end effects [Song and Schmeiser, 1993].

2.3 Linear-Combination Estimators of $\text{var}(\bar{X})$

There are several examples in the literature of using linear combinations of estimators to obtain a better estimator in terms of statistical properties: small variance, bias or mean squared error. The OBM estimator can be viewed as a linear combination of NBM estimators [Meketon and Schmeiser, 1984]. Schruben [1983] considered a linear combination of the STS.A and the NBM estimators, which are asymptotically independent. Politis and Romano [1992] propose a linear combination of two Bartlett estimators of the spectral density with different bandwidths for the reduction of the bias.

The linear combination of OBM's is

$$\widehat{V}^{LC} = \sum_{i=1}^{p} \alpha_i \widehat{V}_i, \quad (14)$$

where p is the number of components, the α_i's are the L.C. coefficients and the $\widehat{V}_i$'s are the OBM component estimators applied to the same data but each with a different batch size m_i. By definition, the bias of $\widehat{V}^{LC}$ is

$$\begin{aligned} \text{bias}\left(\widehat{V}^{LC}\right) &= E\left(\widehat{V}^{LC}\right) - \text{var}(\bar{X}) \\ &= \sum_{i=1}^{p} \alpha_i \,\text{bias}\left(\widehat{V}_i\right) \\ &\quad + \left(-1 + \sum_{i=1}^{p} \alpha_i\right) \text{var}(\bar{X}), \quad (15) \end{aligned}$$

and the variance is

$$\text{var}\left(\widehat{V}^{LC}\right) = \sum_{i=1}^{p}\sum_{j=1}^{p} \alpha_i\, \alpha_j \,\text{cov}\left(\widehat{V}_i, \widehat{V}_j\right). \quad (16)$$

Since the linear-combination variance depends upon the various estimator covariances, any method to select optimal linear-combination parameters must consider the estimator covariances. In Section 3 we state the asymptotic covariances, which in Section 4 we see empirically provide a good approximation to the finite-sample covariances. In the rest of this section, we review how these covariances can be used to select the optimal linear-combination weights.

Song and Schmeiser [1988b] address the problem of selecting the component estimators and determining the optimal linear combination coefficients given the covariances between component estimators and their individual biases. They consider two problems: ($P1$) the weights sum to one, and ($P2$) no constraint on the weights. Let

1. $\underline{\widehat{V}}$ be the vector of estimators;
2. $\underline{\Lambda}$ be the $p \times p$ matrix whose $(i,j)^{th}$ element is
$$\Lambda_{ij} = \text{bias}(\widehat{V}_i) \times \text{bias}(\widehat{V}_j);$$
3. $\underline{\Sigma}$ be the $p \times p$ dispersion matrix,
$$\Sigma_{ij} = \text{cov}(\widehat{V}_i, \widehat{V}_j);$$
4. $\underline{\Delta}$ be the "risk" matrix, i.e.,
$$\underline{\Delta} = \beta_1 \underline{\Lambda} + \beta_2 \underline{\Sigma},$$
where β_1 and β_2 are positive constants that reflect the relative weight that we want to give to the bias and the variance;
5. $\underline{\alpha}$ be the vector of the coefficients of the linear combinations and $\underline{\alpha}^*$ the vector of optimal weights.

Let $\underline{\alpha}^t\ \underline{\Delta}\ \underline{\alpha} = \beta_1\ \text{bias}^2(\underline{\alpha}^t\underline{\widehat{V}}) + \beta_2\ \text{var}(\underline{\alpha}^t\underline{\widehat{V}})$. The optimal $\underline{\alpha}$ for

$$(P1) \quad \text{Minimize } \underline{\alpha}^t\ \underline{\Delta}\ \underline{\alpha} \quad \text{s.t. } \underline{\alpha}^t\underline{1} = 1,$$

is

$$\underline{\alpha}^* = \frac{\underline{\Delta}^{-1}\ \underline{1}}{\underline{1}^t\ \underline{\Delta}^{-1}\ \underline{1}}, \quad (17)$$

and for

$$(P2) \quad \text{Minimize } \underline{\alpha}^t\ \underline{\Delta}\ \underline{\alpha}$$

is

$$\underline{\alpha}^* = \beta_1 \text{var}(\bar{X}) \left[\beta_1 E(\underline{\widehat{V}})E(\underline{\widehat{V}})^t + \beta_2 \underline{\Sigma}\right]^{-1} E(\underline{\widehat{V}}). \quad (18)$$

Their work also includes a numerical study, based on AR(1) data, of effect on the mse of combining two estimators of the same or different types. The results suggest that the use of linear combinations can lead to substantial improvements.

The $\underline{\alpha}^*$ formulas (Equations 17 and 18) show, again, that the optimal linear-combination estimator depends on the covariance/correlation coefficients between the component estimators of the variance of the sample mean.

3 ASYMPTOTIC COVARIANCE/CORRELATION FORMULAS

In this section we present the asymptotic covariance and correlation between two OBM estimators of the variance of the sample mean with batch sizes m_1 and m_2 from n observations. The derivation and additional details are in Pedrosa and Schmeiser [1993b].

Suppose that the observations $\{X_i\}$ are from a stationary time series and these data can be expressed using a moving-average model of order q, i.e.,

$$X_i = b_0\varepsilon_i + b_1\varepsilon_{i-1} + \cdots + b_q\varepsilon_{i-q}, \quad (19)$$

where $b_0, ..., b_q$ are constants and $\{\varepsilon_i\}$ is a sequence of iid random variables with finite variance $\sigma_\varepsilon{}^2$, fourth cumulant $K_{\varepsilon,4}$ and mean μ_ε.

The asymptotic results are derived using the OBM quadratic forms. The end-effects cannot be ignored unless we assume conditions $C1$: as $n \to \infty$, $m_1 \to \infty$ and $m_2 \to \infty$ while simultaneously $m_1/n \to 0$ and $m_1/m_2 \to c$, where c is a non-negative constant. Notice that the limits of Equations 21 and 22 exist only if $m_1/m_2 \to c$.

Assume, without loss of generality, that $m_2 \geq m_1$. Then

$$\lim_{C1}\left\{\frac{n^3}{m_1}\operatorname{var}(\widehat{V_1})\right\} = \lim_{C1}\left\{\frac{n^3}{m_2}\operatorname{var}(\widehat{V_2})\right\} = \frac{4}{3}\gamma_0{}^2 R(0)^2, \quad (20)$$

$$\lim_{C1}\left\{\frac{n^3}{m_1}\operatorname{cov}\left(\widehat{V_1},\widehat{V_2}\right)\right\} = \lim_{C1}\left\{\frac{4}{3}\gamma_0{}^2 R(0)^2\left[1+\frac{1}{2}\left(\frac{m_2-m_1}{m_2}\right)\right]\right\}, \quad (21)$$

and

$$\lim_{C1}\left\{\operatorname{corr}\left(\widehat{V_1},\widehat{V_2}\right)\right\} = \lim_{C1}\left\{\left(\frac{m_1}{m_2}\right)^{\frac{1}{2}}\left[1+\frac{1}{2}\left(\frac{m_2-m_1}{m_2}\right)\right]\right\}, \quad (22)$$

where $\widehat{V_1}$ and $\widehat{V_2}$ are two OBM estimators of $\operatorname{var}(\bar{X})$ with batch sizes m_1 and m_2, γ_0 is the sum of correlations, and $R(0)$ is the data variance. A similar result for the variance (Equation 9) was obtained by Song and Schmeiser [1988a].

The asymptotic variance of the OBM estimator is proportional to the square of the sum of the correlations γ_0, and the population variance $R(0)$. It is also directly proportional to the the batch size and inversely proportional to n^3. Using Equation 5, Equation 20 can be rewritten as

$$\lim_{C1}\left\{\frac{n}{m_1}\frac{\operatorname{var}(\widehat{V_1})}{\left[\operatorname{var}(\bar{X})\right]^2}\right\} = \frac{4}{3}. \quad (23)$$

This result shows that, for a large fixed value of n, the variance of the OBM estimator is directly proportional to m_1 and the square of the variance of the sample mean.

The covariance and correlation results depend upon

$$\mathcal{G}(m_1,m_2) = 1 + \frac{1}{2}\left(\frac{m_2-m_1}{m_2}\right),$$

a simple function of the relative distance between the batch sizes.

The asymptotic covariance between two OBM estimators of $\operatorname{var}(\bar{X})$ can be viewed as the product of the asymptotic variance of the OBM estimator with smaller batch size, $\operatorname{var}(\widehat{V_1})$, by the correction factor $\mathcal{G}(m_1,m_2)$. Equation 21 can also be rewritten as

$$\lim_{C1}\left\{\frac{n}{m_1}\frac{\operatorname{cov}\left(\widehat{V_1},\widehat{V_2}\right)}{\left[\operatorname{var}(\bar{X})\right]^2}\right\} = \frac{4}{3}\left[1+\frac{1}{2}\left(\frac{m_2-m_1}{m_2}\right)\right]. \quad (24)$$

This indicates that given the data type the asymptotic covariance only depends on the relative batch sizes m_1 and m_2.

The asymptotic correlation between OBM estimators does not depend upon the data type. Rather it depends only upon the two relative batch sizes through $(m_1/m_2)^{1/2}$ and $\mathcal{G}(m_1,m_2)$.

4 FINITE-SAMPLE RESULTS

We now describe Monte Carlo experiments that estimate the correlation between two OBM estimators of $\operatorname{var}(\bar{X})$ and compare these finite-sample results to the asymptotic results of the previous section. The purpose is to study the applicability of the asymptotic formulas for finite samples and different data types. Equations 22 and 24 indicate that the quality of the covariance approximation is similar to that provided by the correlation approximation. Therefore, we consider only correlation here.

4.1 The Monte Carlo Experiment

The Monte Carlo experiment estimates corr $\left(\widehat{V}_i, \widehat{V}_j\right)$ for six cases: two sample sizes and three steady-state data processes. The sample sizes are $n = 100$ and $n = 1000$; the three data processes are iid normal ($\gamma_0 = 1$, $\gamma_1 = 0$), AR(1) normal with $\gamma_0 = 10$ and $\gamma_1 = 49.5$, and 5-state DPSS with $\gamma_0 = 10$ and $\gamma_1 = -35.2$ (and uniform marginal distribution). For each sample $\{X_1, X_2, ..., X_n\}$ from the data process, OBM estimates $\widehat{V}_m$ are computed for $m = 1, 2, ..., 99$ if $n = 100$ and for $m = 1, 10, 20, ..., 990$ if $n = 1000$. From 10,000 such samples the correlations corr $\left(\widehat{V}_i, \widehat{V}_j\right)$ are estimated to negligible sampling error.

We now briefly review the three data processes. They have different correlation structures and different marginal distributions, but all are Markov processes: the distribution of the next value depends (at most) on the current value.

The iid-normal process has "no memory" since its value at time t is independent of all past values. Therefore $\rho(h) = 0$ for all nonzero values of h, $\gamma_0 = 1$ and $\gamma_1 = 0$.

The AR(1) normal time series is $X_t = \phi X_{t-1} + \varepsilon_t$, where $|\phi| < 1$ and $\{\varepsilon_t\}$ is a sequence of iid normal random variables with zero mean and variance $\sigma_\varepsilon{}^2$. The autocovariance and autocorrelation functions are $R(h) = \sigma_\varepsilon{}^2\phi^{|h|}/(1-\phi^2)$, and $\rho(h) = \phi^{|h|}$. This geometrically decreasing correlation structure implies that the sum of correlations is $\gamma_0 = (1+\phi)/(1-\phi)$ and the weighted sum of autocorrelations is $\gamma_1 = 2\phi/(1-\phi)^2 = (\gamma_0 - 1)(\gamma_0 + 1)/2$.

The DPSS(d, p, s, S) process models a d-state (s, S) inventory system with Bernoulli demands [Pedrosa and Schmeiser, 1993a]. At each time t the random demand is zero with probability p and is $\Delta = (S-s)/(d-1)$ units with probability $1-p$; non-zero demand at inventory s causes immediate reordering and a return to state S. The Markov chain is doubly stochastic, so the unique steady-state marginal distribution is uniform over the d states $\{S, S-\Delta, \ldots, s\}$; the steady-state mean and variance are then $\mu = (S+s)/2$ and $\text{var}(X) = (d^2-1)\Delta^2/12$. In addition to having a non-normal marginal distribution, the DPSS process differs from the AR(1) process by having a more-complex autocorrelation structure. The lag-1 autocorrelation is $\rho(1) = (d-5+6p)/(d+1)$, the sum of autocorrelations is $\gamma_0 = p/(1-p)$, and the weighted sum of autocorrelations is $\gamma_1 = \{[(19-d^2)(\gamma_0+1)]/30 - 1\}(\gamma_0+1)$.

4.2 Discussion of Experimental Results

The experimental results indicate that the quality of the approximation provided by the asymptotic correlation in Equation 22 is good if both batch sizes are between γ_0 and $n/2$. The quality is relatively insensitive to the marginal distribution and to the weighted sum of correlations γ_1.

To aid the discussion, we introduce two figures. Figure 1, for normal data, and Figure 2, for DPSS data, illustrate the results for $n = 100$, the smallest sample size considered. Each figure contains six charts, each corresponding to a batch size $m_i = 5, 10, 30, 50, 60, 90$. The horizontal axis is the other batch size m_j, ranging from 1 to $n-1$. For each chart, two curves are shown: the asymptotic correlation from Equation 22 and the true finite-sample correlation; the true correlation goes to zero for large values of m_j. The closer are the two curves the better is the approximation. The approximation is exact at $m_i = m_j$, since both the approximation and the true correlation are then one.

A relatively good approximation is shown in Figure 1. The independent normal data have $\gamma_0 = 1$, so $n = 100$ is a relatively large sample size. Whenever both batch sizes are less than $n/2$, the approximation quality is good. The quality typically degenerates as either batch size increases beyond $n/2$. The $n = 1000$ graphs (not shown) are similar to Figure 1 for all three process. In both the AR(1) and DPSS cases, $\gamma_0 = 10$, so the equivalent number of independent observations $n/\gamma_0 = 100$.

A less good approximation is shown in Figure 2. The DPSS dependent data have $\gamma_0 = 10$, so the equivalent number of independent observations is quite small, $n/\gamma_0 = 10$. Here the approximation quality degenerates when either m_j is too large or too small. Roughly, the quality is good whenever both batch sizes are between γ_0 and $n/2$. Similar graphs result for the AR(1) process with $\gamma_0 = 10$ and $n = 100$.

For sample sizes n at least a few multiples of γ_0, these experimental results suggest these four conclusions:

1. The graphs in Figure 1 are representative of the asymptotic correlations, regardless of marginal distribution and autocorrelation structure.
2. The quality of the approximation is insensitive to the marginal distribution and to γ_1.
3. The equivalent sample size n/γ_0 is sufficient information to characterize the quality of the approximation.
4. The approximation is good if both batch sizes are between γ_0 and $n/2$.

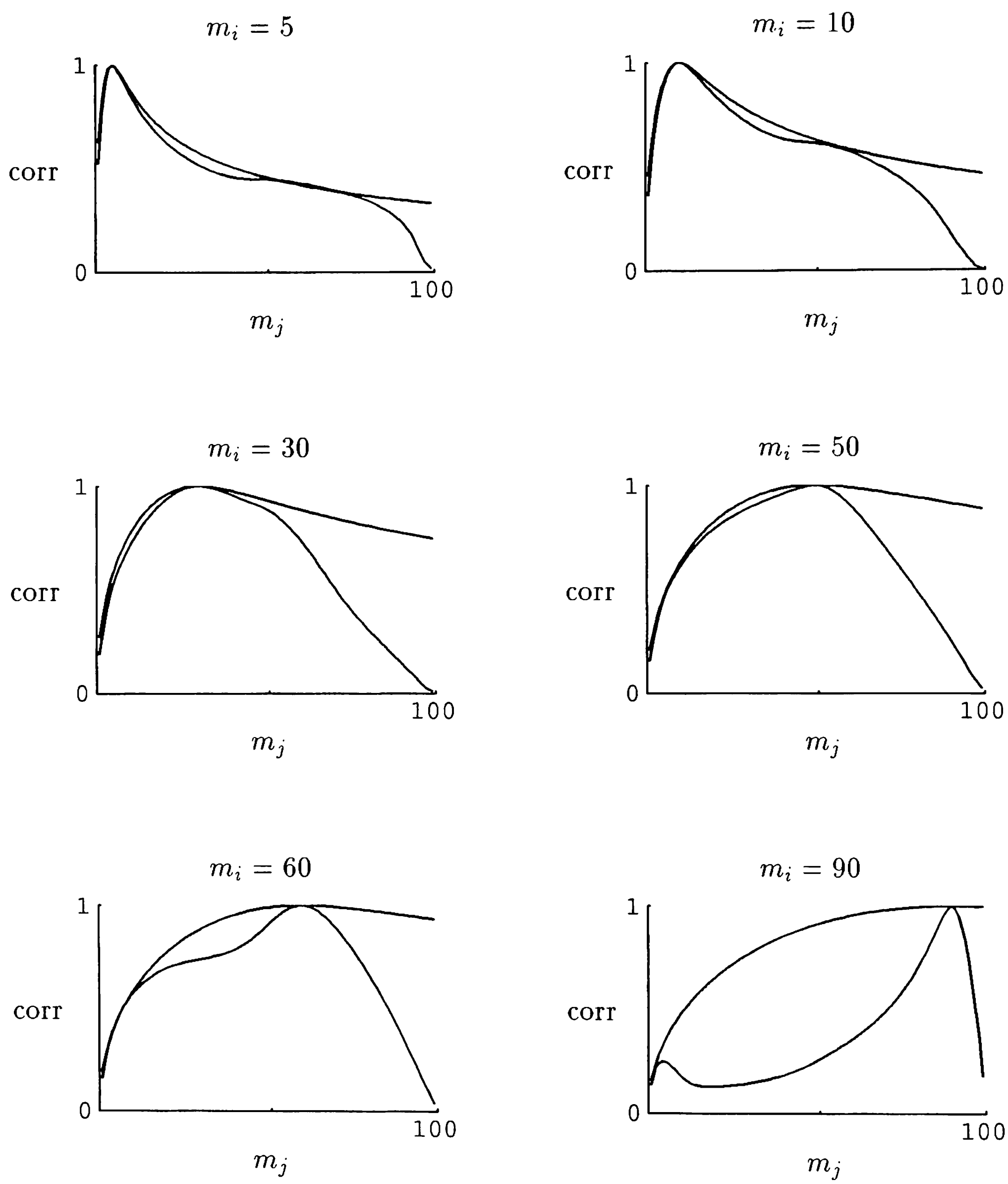

Figure 1: Correlations corr $\left(\widehat{V}_i, \widehat{V}_j\right)$ as a function of m_j for an $iid - normal$ and a sample size $n = 100$.

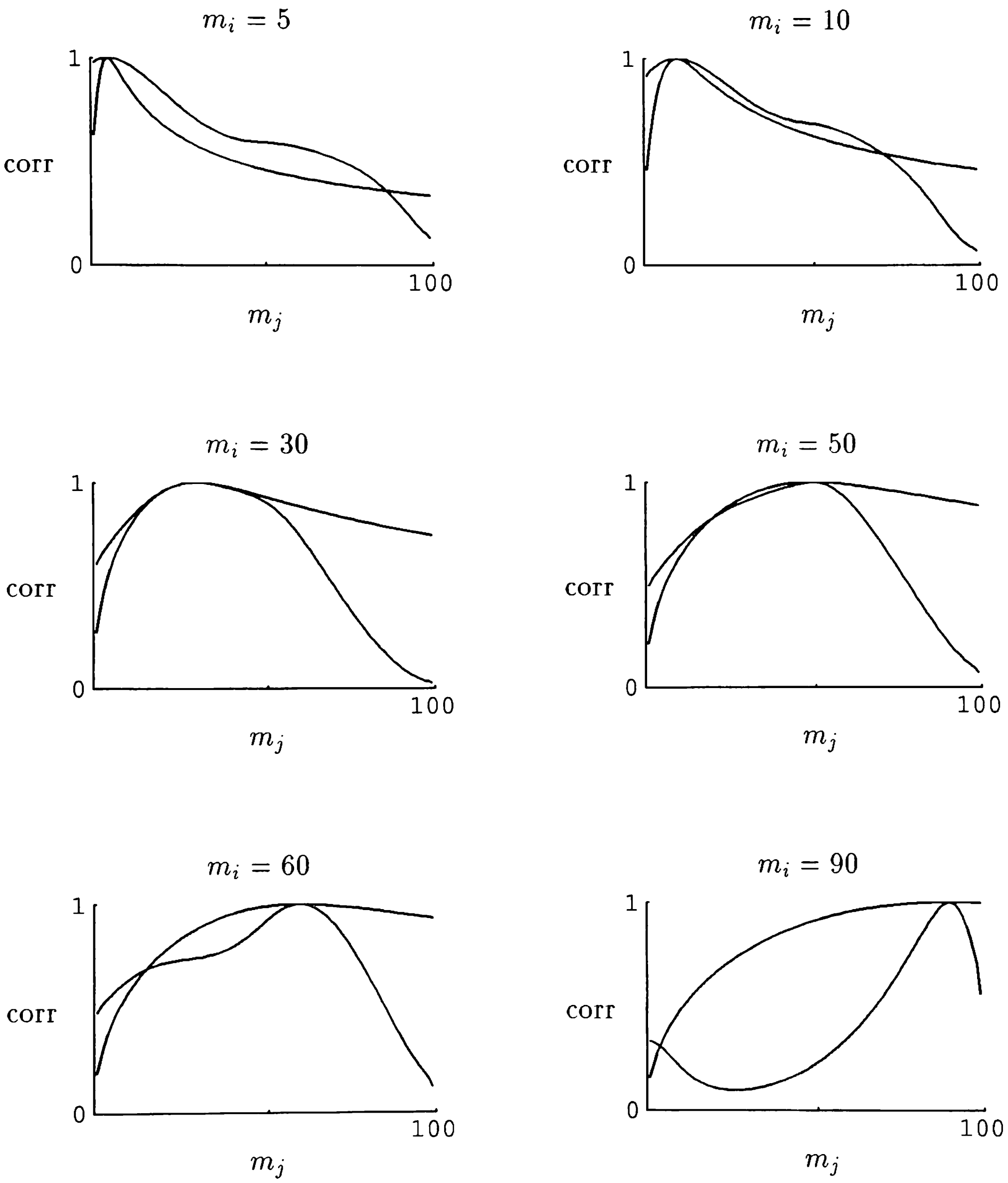

Figure 2: Correlations corr $\left(\widehat{V}_i, \widehat{V}_j\right)$ as a function of m_j for a MCBT($s = -2, S = 2, d = 5, p = 0.91$) and a sample size $n = 100$.

This robustness to batch size is encouraging since various guidelines for choosing batch size fall within this range:

1. NBM (non-overlapping batch means) batch sizes chosen for good confidence-interval performance are between $n/30$ and $n/10$ [Schmeiser, 1982];
2. The OBM estimator for the same batch size provides 50% more degrees of freedom (d.f.); then for the same d.f. good OBM batch sizes are, roughly, between $n/20$ and $n/7$;
3. The asymptotic mse-optimal batch size [Schmeiser and Song, 1989],

$$m^* = 1 + \left[\frac{3\,n}{2}\left(\frac{\gamma_1}{\gamma_0}\right)^2\right]^{\frac{1}{3}},$$

is 1 for the iid normal process, is 17 and 34 for the AR(1), and is 13 and 28 for the 5-state DPSS for $n = 100$ and $n = 1000$, respectively.

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