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THIRTY YEARS OF "BATCH SIZE EFFECTS"

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ABSTRACT

The method of non-overlapping batch means is the standard for constructing a confidence interval for the mean of a steady-state simulation output. In "Batch Size Effects in the Analysis of Simulation Output," published in *Operations Research* in 1982, Schmeiser recast the problem of selecting a batch size by examining the marginal benefit of attaining the largest number of batches (smallest batch size) that still yields a valid confidence interval. His formulation of the problem, and the conclusions he reached, influenced nearly all later work on batching and batching algorithms for confidence-interval estimation.

1 INTRODUCTION

Assigning a measure of error to an estimate of the mean of a steady-state simulation is a research problem with a long history, and for which there have been many lasting contributions. When the measure of error is a confidence interval, the method of batch means is both widely known and routinely applied; it is even incorporated as an automated procedure in some commercial simulation products.

In brief, the method of batch means takes a single run of n output observations, partitions it into k batches of size $m = n/k$ consecutive observations, and then treats the sample means of the batches as independent and identically normally distributed. Therefore, a standard t-distribution confidence interval can be derived. If n is large enough that it is reasonable to apply the method of batch means, then the next practical question is, into how many batches k should the output be divided?

Schmeiser (1982) attacked this question in an elegant and innovative way, providing insight that has influenced virtually all later work on what is now known as the method of non-overlapping batch means. The summary insight, as stated in the paper itself, is this:

> The results of Sections 1 and 2 show that the practitioner should seldom exert much effort to increase the number of batches beyond $k = 30$, regardless of the number of observations n. (Schmeiser 1982, p. 564)

In this paper we describe the basis for this insight as well as some of its impact on work that followed. However, we first review the "batch size" problem as it was understood prior to Schmeiser (1982). Throughout the paper we use the phrase "method of batch means" as short for obtaining a confidence interval (CI) by employing sample means from non-overlapping batches of observations from a single simulation run.

2 BACKGROUND

We adopt the notation used in Schmeiser (1982). Let $X_1, X_2, \ldots, X_n$ be the output of a single replication of a steady-state simulation. There are many, sometimes equivalent, definitions, of "steady-state simulation," but a common one is that the output process $X_i \Rightarrow X$ as $i \to \infty$, where $\Rightarrow$ denotes weak convergence. Here we are interested in estimating $\mu = \mathrm{E}\{X\}$. The estimator we will employ is the sample mean $\bar{X} = \sum_{i=1}^{n} X_i/n$, and the problem for which the method of batch means is a potential solution is obtaining a CI for μ.

From the original output process, the method forms k batch means, where the ith batch mean is $\bar{X}_i = \sum_{j=(i-1)m+1}^{im} X_j/m$, and $m = n/k$ is the batch size. The hope is that if k is small enough (equivalently m large enough), then the batch means $\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_k$ will be approximately uncorrelated and normally distributed. When this is a valid approximation it justifies the $(1-\alpha)100\%$ confidence interval $\bar{X} \pm H_{\alpha,k}$, where $H_{\alpha,k} = t_{\alpha/2,k-1} S_k/\sqrt{k}$ is the half width of the CI, $t_{\alpha/2,k-1}$ is the $1-\alpha/2$ quantile of the t distribution with $k-1$ degrees of freedom, and

$$S_k^2 = \frac{1}{k-1}\left(\sum_{i=1}^{k} \bar{X}_i^2 - k\bar{X}^2\right)$$

is the sample variance of the batch means.

Later research has provided a rigorous asymptotic justification for this CI; Schmeiser (1982, p. 557) assumed the then prevalent heuristic justification that (i) initial transient effects on the output process had been removed, yielding a covariance stationary process with mean μ, variance σ^2 and lag h autocorrelations $\rho_h, h = 1, 2, \ldots$; and (ii) that there exists a number of batches $k^* \geq 2$ such that for all $k \leq k^*$ the dependence and non-normality of the batch means was negligible. Under these conditions the method of batch means made sense, provided $k \leq k^*$.

In light of assumptions (i)–(ii), and the fact that the degrees of freedom associated with $H_{\alpha,k}$ depend on the number of batch means k, it seemed obvious that selecting k as large as possible, and ideally $k = k^*$, was a sensible objective. A well-known and widely used batching algorithm by Fishman (1978) embodied this approach:

Fishman's Batching Algorithm

1. $m \leftarrow 1$
2. $k \leftarrow \lfloor n/m \rfloor$
3. If $k < 8$ then return indicating failure
4. Compute the batch means $\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_k$
5. Test the hypothesis $H_0 : \mathrm{Corr}(\bar{X}_i, \bar{X}_{i+1}) = 0$
6. If the test fails, then $m \leftarrow 2m$ and go to 2
7. Otherwise, $k' \leftarrow k$
8. Compute $S_{k'}^2$
9. Return the CI: $\bar{X} \pm H_{\alpha,k'}$

Notice that the algorithm starts with the largest possible number of batches ($k = n$) and then halves the number of batches until either the hypothesis test is passed, or the number of batches becomes too small to justify the assumptions behind the hypothesis test. Halving the number of batches was computationally convenient because the new batch means could be formed by averaging pairs of the previous ones. Schriber and Andrews (1979) modified this algorithm so that it considered every possible batch size yielding $k \geq 8$. The important observation is that this and other batching algorithms at that time attempted to find a large, or even the largest, value of k that also yielded a valid confidence interval, where validity meant correct coverage: $\Pr\{|\bar{X} - \mu| \leq H_{\alpha,k}\} \approx 1 - \alpha$.

Schmeiser (1982) noted that maximizing the number of batches k is not without risk. The magic number of batches k^* is unknown, and in fact it is hard to define a "negligible" departure from independence and normality. The premise behind batch means implies that the assumptions of nearly independent and approximately normally distributed batch means—assumptions that are critical to the coverage of the confidence interval—are most likely to be approximately correct when k is small. In fact, if coverage close to $1-\alpha$ were the only criterion, then $k=2$ would usually be optimal. Of course, the degrees of freedom penalty for $k=2$ is substantial. This lead Schmeiser to formulate the batch-size question in a new way: How important is it to get close to k^*?

3 ANALYSIS

Although maximizing the degrees of freedom seemed like a sensible objective, Schmeiser (1982) observed that the effect of increasing the degrees of freedom by rebatching a fixed quantity of data is less dramatic than the effect of obtaining additional data. This matters, because in reality there will be a trade off between coverage, for which $k=2$ is best, and degrees of freedom, for which $k=n$ dominates. The research challenge was finding a way to examine this effect that provided general guidance and was not dependent on the run length n or the myriad of correlation structures that an output process might have.

The central insight that made a meaningful and general analysis possible was this: *The biggest penalty for using $k<k^*$ (smaller than necessary) occurs when the batch means $\bar{X}_1,\bar{X}_2,\ldots,\bar{X}_k$ are precisely i.i.d. normal for all $k \le k^*$.* This is because the number of batches k could be increased right up to k^* without any degradation in coverage. By taking coverage off the table, the full effect of degrees of freedom could be assessed. Further, there was no need to consider different simulation output processes, nor was it necessary to specify n, as long as the analysis was limited to $k \le k^*$ (see further discussion below).

Because $\Pr\{|\bar{X}-\mu| \le H_{\alpha,k}\} = 1-\alpha$ for all $k \le k^*$ under this assumption, Schmeiser (1982) focused on other measures of CI performance:

Width: $\mathrm{E}\{H_{\alpha,k}\}$ is perhaps the most important performance measure after coverage, since a wide CI implies that μ is not well estimated.

Stability: Both $\sqrt{\mathrm{Var}\{H_{\alpha,k}\}}$ and $\mathrm{CV}\{H_{\alpha,k}\}$ quantify the likelihood that a practitioner actually achieves a CI with width close to $\mathrm{E}\{H_{\alpha,k}\}$. This is important because decisions are based on $H_{\alpha,k}$ not on $\mathrm{E}\{H_{\alpha,k}\}$.

Specificity: $\beta_{\alpha,k}(\mu_1) = \Pr\{|\bar{X}-\mu_1| \le H_{\alpha,k}\}$ for $\mu_1 \ne \mu$ is the probability that the CI covers values that are not the desired value μ. This is important because one interpretation of a CI is that the true value of μ could be any value in $[\bar{X}-H_{\alpha,k}, \bar{X}+H_{\alpha,k}]$.

Schmeiser also pointed out that under assumptions (i)–(ii) we have

$$\mathrm{E}\{S_k^2/k\} = \mathrm{Var}\{\bar{X}\} = c\sigma^2/n$$

for any $k \le k^*$, where $c = 1+2\sum_{h=1}^{n}(1-h/n)\rho_h$. Therefore, quantities like $\mathrm{E}\{H_{\alpha,k}\}$ and $\sqrt{\mathrm{Var}\{H_{\alpha,k}\}}$ could be expressed in units of $\sqrt{c\sigma^2/n}$, freeing them from dependence on the correlation structure ρ_h or n. Similarly, deviations $|\mu_1-\mu|$ could be given in the same units when evaluating $\beta_{\alpha,k}(\mu_1)$.

To illustrate the analysis, Table 1 shows a portion of Table I from Schmeiser (1982). Consider first the expected half width of a 95% CI, $\mathrm{E}\{H_{0.05,k}\}$, and suppose that the number of batches we intend to use is $k=10$. Then if $k^*=61$ we would only decrease the expected half width by 9% in moving from $k=10$ to $k=61$ (remembering that the total sample size n is fixed). Even moving from $k=10$ to the (conceptual value of) $k^*=\infty$ only reduces the expected half width 11%.

The standard deviation and coefficient of variation of the half width, on the other hand, are more sensitive at small values of k. Schmeiser concludes from these results that there is little benefit (and of course, some risk) in going beyond $k=30$; the coverage results $\beta_{\alpha,k}(\mu_1)$ reinforce these conclusions. These results have immediate implications for batching algorithms, as they remove the pressure to try to maximize the number of batches.

Schmeiser's analysis has occasionally been misinterpreted as implying that one should *always* use 30 batches. However, if the run length n is too short it may be that there is no number of batches, including $k=2$, that provides a valid confidence interval. And even when $m=n/30$ is a good batch size, these results say nothing about whether n is large enough to provide acceptable precision (e.g., $H_{0.05,k} \le \varepsilon$) to

Table 1: For fixed sample size n, the effect of number of batches k on properties of the half width. The $\mathrm{E}\{H_{0.05,k}\}$ and $\sqrt{\mathrm{Var}\{H_{0.05,k}\}}$ are in units of $\sqrt{c\sigma^2/n}$.

k	$\mathrm{E}\{H_{0.05,k}\}$	$\sqrt{\mathrm{Var}\{H_{0.05,k}\}}$	$\mathrm{CV}\{H_{0.05,k}\}$
2	10.1	7.66	0.76
3	3.81	1.99	0.52
4	2.93	1.24	0.42
5	2.61	0.95	0.36
6	2.45	0.79	0.32
10	2.20	0.52	0.24
30	2.03	0.27	0.13
61	1.99	0.18	0.09
121	1.98	0.13	0.06
∞	1.96	0.00	0.00

support the decision at hand. The power of Schmeiser (1982) is that it greatly reduces the range within which one should search for an acceptable number of batches, and in showing that k need not be too large, diminishes the risk of forming an invalid CI.

4 IMPACT

As of May 2011, Google Scholar listed 273 papers that cited Schmeiser (1982). These papers are not just about using batch means for confidence-interval estimation, they also span other topics that interact with batch means such a ranking & selection and variance reduction. When statistical inference will be based on using batch means, then a "batch size effects" analysis like Schmeiser (1982) in often included. A small sample of topics and representative papers follows.

While Schmeiser (1982) addressed estimating a univariate steady-state mean, a number of papers extend batching to multivariate output processes. These include Charnes (1991), Charnes and Kelton (1993), Charnes (1995) and Yang and Nelson (1992).

Ranking & selection addresses another form of multivariate estimation problem: selecting the best of several simulated systems. Multiple-comparison procedures provide simultaneous comparisons of a number of alternative systems. In a steady-state simulation context batch means may substitute for independent replications in these procedures. Papers citing Schmeiser (1982) in this vein include Batur (2006), Chen et al. (1997), Chen et al. (1998), Chen et al. (2010), Damerdji and Nakayama (1999), Goldsman and Nelson (1990), Goldsman et al. (1991), Goldsman et al. (2005), Kim and Nelson (2007), Matejcik and Nelson (1995), Nakayama (1997), Nakayama (1994) and Sullivan and Wilson (1989).

The interaction of variance-reduction techniques, particularly the method of control variates, with batching has received some attention; see for instance Añonuevo and Nelson (1986), Añonuevo and Nelson (1988), Clark (1990), Nelson (1987a), Nelson (1987b), Nelson (1990a), Sharon and Nelson (1988) and Yang and Nelson (1992).

The impact of batching on initial-condition bias has been discussed in Gallagher (1992), Kelton (1989), Nelson (1990b) and Philip and Peter (1991).

Schmeiser (1982) is cited by a number of papers on Markov chain Monte Carlo, including Chen and Schmeiser (1993), Chen et al. (2000), Geyer (1992), Jones and Hobert (2001), Lewis and Raftery (1997), Mignani and Rosa (2001) and Sung et al. (2007).

The method of batch means can be used to form a confidence interval, or simply as an estimator of the variance of the sample mean. Many other methods have been proposed, notably methods based on standardized time series. These methods are often combined with batching to increase the degrees of freedom. Papers that focus on other variance estimators, but exploit concepts in Schmeiser (1982) include Aktaran-Kalayci and Goldsman (2005), Aktaran-Kalaycı et al. (2007), Alexopoulos et al. (2004), Alexopoulos et al. (2007), Alexopoulos et al. (2007), Alexopoulos et al. (2010), Batur et al. (2009), Bischak et al. (1993), Foley and Goldsman (1999), Fox et al. (1991), Glynn and Whitt (1991), Goldsman and Schruben (1984), Goldsman et al. (1990), Goldsman and Schruben (1990), Goldsman et al. (2007), Meketon and Schmeiser (1984), Muñoz and Glynn (2001), Pedrosa and Schmeiser (1993), Schmeiser et al. (1990), Schruben (1983), Sherman (1996), Song and Schmeiser (1988), Song and Schmeiser (1993), Song and Schmeiser (1995), Song et al. (1997) and Song and Chih (2008).

5 CONCLUSIONS

Schmeiser (1982) demonstrated that asking the right question can be as powerful as a deep mathematical analysis, leading to very general and useful insights, in this case with respect to the method of batch means. His formulation of the "batch size effects" question has been repeatedly and effectively used in many contexts.

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