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OVERLAPPING BATCH QUANTILES

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ABSTRACT

In this paper we show that although overlapping batch quantiles (OBQ) is asymptotically very similar to overlapping batch means, its performance for finite sample sizes is not. We show that the bias, the variance and the mean-squared-error of OBQ are not smooth functions of the batch size but rather cyclic. The cyclic behavior of OBQ depends on the marginal distribution, the point estimator of quantiles and the autocorrelation function and it diminishes with the sample size.

We conclude that very large sample sizes and batch sizes are needed to obtain reliable standard error estimators when using OBQ, even for independently and identically distributed data.

1 INTRODUCTION

In some simulation applications quantiles are of interest instead of, or in addition to, the mean and the variance. Given that simulation output $\{X\}$ comes from a process with marginal cdf F_X, the q^{th} quantile, x_q, of the process satisfies $F_X(x_q) = \mathrm{P}\{X \le x_q\} = q$. Throughout this paper we assume that there is a unique x_q satisfying the above equation and that the marginal density g_X is continuous around x_q.

In this paper we analyze overlapping batch quantiles (OBQ) as the standard error estimator of the point estimators of the quantiles. More specifically we introduce two versions of OBQ and four point estimators of quantiles and analyze the asymptotic and finite sample size properties of OBQ for each point estimator.

We show that the bias and the variance of OBQ estimators go to zero with the same rate as the bias and the variance of overlapping batch means (OBM). We also show that the asymptotic relations between OBM and non-overlapping batch means (NBM) exist between OBQ and non-overlapping batch quantiles (NBQ).

Finite sample size performance of OBQ is, however, more problematic than that of OBM. The main problem arises from the fact that the expected value and the variance of OBQ are cyclic functions of the batch size, m. Therefore the performance of OBQ highly depends on the choice of batch size within a cycle. Furthermore the "best" batch size within a cycle changes with the distribution shape, the quantile value, q, and the choice of point estimator for the quantile. We show that no point estimator performs better than the others for all q and all distributions. The classical factors that affect OBM also affect OBQ, namely the sample size and the autocorrelation structure. They determine the choice of the "best" cycle. The term "best" may be used to refer to minimal bias, minimal variance or to minimal mse.

In this paper we present results of analytical studies and conjectures derived from the empirical studies. Because of space limitations, this paper includes no proofs and only a bit empirical evidence. Details of this study can be found in Wood (1995).

In Section 2 we present a literature survey of the four point estimators of quantiles as well as their standard error estimators. In Section 3 we introduce the two versions of OBQ that we analyze. Sections 4 and 5 contain our analysis and discussion of the asymptotic and finite sample size performance of OBQ, respectively. In Section 6 we present the results of our empirical comparison of OBQ and NBQ. In Section 7 we summarize our findings and discuss the difficulties with practical applications of OBQ.

2 A LITERATURE SURVEY OF QUANTILE ESTIMATORS

We survey point estimators of quantiles and their statistical properties. We then survey methods for estimating the standard error of quantile estimators.

2.1 Point Estimators of Quantiles

We study and compare four point estimators of quantiles from among the many in the literature. After introducing these four estimators together with their statistical properties we mention some of the other point estimators. For all four point estimators, implicitly or explicitly, data need to be ordered. Given the data set $\{X_1, X_2, \ldots, X_n\}$ let $X_{(1)} \le X_{(2)} \le \cdots \le X_{(n)}$ denote the ordered set. Then $X_{(r)}$ is called the r^{th} order statistic. The first two point estimators that we study consist of a single order statistic and the last two are linear combinations of two order statistics.

The first point estimator chooses the order statistic by taking the *ceiling* function of nq. That is, the point estimator is $\hat{x}_q(ce) = X_{(r)}$, where $r = \lceil nq \rceil$ is the smallest integer greater than or equal to nq. The second estimator chooses the order statistic by taking the *floor* function of nq. We denote this estimator by $\hat{x}_q(fl)$ and it is equal to $X_{(r)}$, where $r = \lfloor nq \rfloor$ is the largest integer smaller than or equal to nq.

Approximations for the expected value and the variance of $\hat{x}_q(ce)$ and $\hat{x}_q(fl)$ are (see, e.g., Gibbons 1971, p. 36).

$$\mathrm{E}\left(X_{(r)}\right) \approx F_X^{-1}\left(\frac{r}{n+1}\right)$$

and for identically and independently distributed (iid) data

$$\mathrm{V}\left(X_{(r)}\right) \approx \frac{r(n+1-r)}{(n+2)(n+1)^2}\left\{g_X\left[F_X^{-1}\left(\frac{r}{n+1}\right)\right]\right\}^{-2}.$$

The above equations hold exactly for uniform distributions and are large sample size approximations for other continuous distributions.

A large sample size approximation for the variance of $\hat{x}_q(ce)$, and therefore $\hat{x}_q(fl)$, for autocorrelated data is, from Heidelberger and Lewis (1984),

$$\mathrm{V}\left(X_{(r)}\right) \approx n^{-1} p_0\, g_X^{-2}\left(\hat{x}_q(ce)\right),$$

where

$$p_0 = q(1-q) + 2\sum_{h=1}^{n-1}\left(1-\frac{h}{n}\right)\mathrm{Cov}\left(I_1, I_{1+h}\right)$$

and

$$I_h = \begin{cases} 1 & \text{if } X_h < x_q \\ 0 & \text{otherwise} \end{cases}. \qquad (1)$$

The third estimator, proposed by Avramidis and Wilson (1995), is the linear combination

$$\hat{x}_q(lcA) = \alpha X_{(\lceil nq+0.5\rceil-1)} + (1-\alpha)X_{(\lceil nq+0.5\rceil)},$$

where $\alpha = \lceil nq+0.5\rceil - (nq+0.5)$. The weights result from taking the empirical cdf to be a piece-wise linear function, $\hat{F}_X(x)$, equal to $(i-0.5)/n$ at $x = X_{(i)}$ and equal to zero for $x < X_{(1)}$ and equal to one for $x > X_{(n)}$.

The fourth estimator, from Schmeiser (1975), is the linear combination

$$\hat{x}_q(lcS) = \alpha X_{(\lfloor (n+1)q\rfloor+1)} + (1-\alpha)X_{(\lfloor (n+1)q\rfloor)},$$

where $\alpha = (n+1)q - \lfloor (n+1)q \rfloor$. The weights are chosen so that the estimator is unbiased for data with uniform marginals.

All four point estimators are consistent estimators of the quantile, x_q; that is, their bias and variance go to zero as the sample size increases.

All four point estimators share the same average cycle length, $\mathrm{ACL} = 1/\min\{q, (1-q)\}$. There is a single cycle length, $\mathrm{CL} = \mathrm{ACL}$, if ACL is an integer. Otherwise there are two cycle lengths: $\lfloor \mathrm{ACL} \rfloor$ and $\lceil \mathrm{ACL} \rceil$. The two cycle lengths occur in a frequency such that they average to ACL in the long run. For example when $q=0.1$ (or 0.9) the cycle length is 10. When $q=0.3$ or (0.7) there are two cycles of length 3 and 4 averaging to $1/0.3$.

Some of the other methods for estimating quantiles include the use of histograms and empirical cdf's (Schmeiser 1977, and Jain and Chlamtac 1985). Another method, developed primarily for estimating quantiles for autocorrelated data, is the maximum transformation method (Heidelberger and Lewis 1984).

2.2 Standard-Error Estimators of Quantiles

The literature on standard-error estimation for quantiles is limited. Iglehart (1976) discusses the use of regenerative cycles. Seila (1982) discusses batching regenerative cycles. A method that does not require regenerative systems is the maximum transformation method of Heidelberger and Lewis (1984).

Overlapping batch quantiles is first proposed by Schmeiser, Avramidis and Hashem (1980). Hashem and Schmeiser (1994) contains a C code for OBQ.

We analyze overlapping batch quantiles in Sections 4 and 5 and provide empirical comparison to NBQ in Section 6.

3 DEFINITIONS OF OBQ

In this section we first review the original definition of OBQ from Schmeiser, Avramidis and Hashem (1990), and then propose a second version by changing the centering term. We argue that the second version smoothes the cyclic behavior of OBQ.

Assume that one of the four point estimators of the q^{th} quantile is chosen. Let the point estimator be $\hat{x}_q(\bullet) = f(X_1, X_2, \ldots, X_n)$. Then by definition the j^{th} batch estimator is $\hat{x}_q^j(\bullet) = f(X_j, X_{j+1}, \ldots, X_{j+m-1})$. The original definition of OBQ is

$$\text{OBQ}(1) = \frac{m}{(n-m)(n-m+1)} \sum_{j=1}^{n-m+1} \left(\hat{x}_q^j(\bullet) - \hat{x}_q(\bullet)\right)^2 .$$

The choice of m affects the statistical properties of $\hat{x}_q^j(\bullet)$, especially for small values of m. The value of the centering term, $\hat{x}_q(\bullet)$, however, is independent of the batch size. It is our intuition that the independence of $\hat{x}_q(\bullet)$ from the choice of m increases the sensitivity of OBQ to cyclic effects. The alternative centering term we propose is the average of the batch quantiles $\bar{x}_q(\bullet) = (n-m+1)^{-1} \sum_{j=1}^{n-m+1} \hat{x}_q^j(\bullet)$. The second version of OBQ then is

$$\text{OBQ}(2) = \frac{m}{(n-m)(n-m+1)} \sum_{j=1}^{n-m+1} \left(\hat{x}_q^j(\bullet) - \bar{x}_q(\bullet)\right)^2 .$$

The centering term, $\bar{x}_q$, has the same cyclic properties of the batch estimators and therefore, intuitively, decreases the effects of cycles on OBQ.

The centering term affects the performance of OBQ when the point estimator is either the ceiling function, $\hat{x}_q(ce)$, or the floor function, $\hat{x}_q(fl)$. The point estimators that use a linear combination of two order statistics, $\hat{x}_q(lcA)$ and $\hat{x}_q(lcS)$, seem to be affected insignificantly by the centering term. This behavior was observed for all marginal distributions and quantile values studied.

The decrease in the cyclic behavior from OBQ(1) to OBQ(2) makes the choice of the "best" batch size within a cycle less important and the penalty for choosing a wrong m less significant.

4 ASYMPTOTIC PERFORMANCE OF OBQ

In this section we show that the asymptotic properties of OBQ resemble those of OBM (and overlapping batch variances (OBV), in all aspects except the cyclic behavior. In all limits we assume that the batch size, m, is an increasing function of the sample size, n.

We show that as the sample size, n, and the batch size, m, go to infinity

(i) nm bias(OBQ) is finite and attains CL different values (or $\lceil \text{ACL} \rceil + \lfloor \text{ACL} \rfloor$ values if ACL is not an integer) depending on the position of the batch size within a cycle,

(ii) the batch size that minimizes nm bias(OBQ) depends on the distribution shape, quantile value, q, the point estimator, and the autocorrelation function,

(iii) (n^3/m) V(OBQ) goes to a finite constant independent of the distribution shape and point estimator.

In the next two subsections we discuss the asymptotic properties of OBQ, first for iid data and then for autocorrelated data.

4.1 IID Data

Results 1 and 2 concern nm bias(OBQ(1)) for iid uniform data.

Result 1: For iid uniform data with density function g_X, point estimator $\hat{x}_q(ce)$, and for batch sizes that satisfy $\lceil mq \rceil/(m+1) = q$,

$$\lim_{n\to\infty} nm\, \text{bias}(\text{OBQ}(1)) = -2q(1-q)g_X^{-2} .$$

The importance of Result 1 is that, unlike OBM for iid data, the limit is not zero even when the batch size is chosen so that the batch estimator is unbiased. Changing the coefficients of OBQ from $m[(n-m)(n-m+1)]^{-1}$ to $(m+2)[(n-m)(n-m+1)]^{-1}$ makes nm bias(OBQ(1)) go to zero instead of to $-2q(1-q)g_X^{-2}$. However this would be a distribution-specific change.

Result 2: While estimating the median, $q=0.5$, for iid uniform data with density g_X and point estimator $\hat{x}_q(ce)$,

$$\lim_{n\to\infty} nm\,\text{bias}(\text{OBQ}(1)) = \begin{cases} -q(1-q)g_X^{-2} & \text{if } m \text{ is even} \\ -2q(1-q)g_X^{-2} & \text{if } m \text{ is odd} \end{cases}.$$

If the point estimator is $\hat{x}_q(fl)$

$$\lim_{n\to\infty} nm\,\text{bias}(\text{OBQ}(1)) = \begin{cases} -q(1-q)g_X^{-2} & \text{if } m \text{ is even} \\ +2q(1-q)g_X^{-2} & \text{if } m \text{ is odd} \end{cases},$$

and if the point estimator is either $\hat{x}_q(lcA)$ or $\hat{x}_q(lcS)$

$$\lim_{n\to\infty} nm\,\text{bias}(\text{OBQ}(1)) = \begin{Bmatrix} -3q(1-q)g_X^{-2} & \text{if } m \text{ is even} \\ -2q(1-q)g_X^{-2} & \text{if } m \text{ is odd} \end{Bmatrix}.$$

No point estimator and no batch size makes nm bias(OBQ(1)) go to zero in this special case. Empirical evidence shows that the same is true for OBQ(2) when estimating the median for iid uniform data.

Empirical evidence also shows that nm bias(OBQ) attains CL (or $\lceil \text{ACL} \rceil + \lfloor \text{ACL} \rfloor$) finite values for other marginal distributions and quantiles and that (n^3/m) V(OBQ) attains a single finite value.

4.2 Autocorrelated Data

The arguments in this section are based on the reciprocal relationship between the quantiles and the probabilities: $P\{X_i \le x_q\} = q$. When we are interested in estimating the q^{th} quantile of a process, q is known and the unknown quantity is x_q. When we are interested in estimating the probability that any observation is less then x_q, the unknown quantity is q. Furthermore the variances of the quantile estimator and the probability estimator are related by $\text{V}(\hat{x}_q(ce)) = \text{V}(\hat{q})\, g_X^{-2}(x_q)$ for large sample sizes. We use this relation between the variances of the estimators and the asymptotic properties of overlapping batch probabilities (OBP) to obtain Conjecture 1 below.

The usual estimator of probability is $\hat{q} = n^{-1}\sum_{i=1}^{n} I_i$, where I_i is the indicator function defined by (1). Since the probability estimator is the sample mean of the indicator function, the asymptotic properties of OBM apply to OBP. That is, from Song and Schmeiser (1995),

$$\lim_{n\to\infty} nm\,\text{bias}(\text{OBP}) = -\gamma_1^P$$

and

$$\lim_{n\to\infty} \frac{n^3}{m}\text{V}(\text{OBP}) = \frac{4}{3}\left(\gamma_0^P\right)^2,$$

where

$$\gamma_1^P = 2\sum_{h=1}^{\infty} h\,\text{Cov}\left(I_1, I_{1+h}\right),$$

and

$$\gamma_0^P = 1 + 2\sum_{h=1}^{\infty}\text{Cov}\left(I_1, I_{1+h}\right).$$

Conjecture 1 : For covariance stationary data

$$\lim_{n\to\infty} nm\,\text{bias}(\text{OBQ}) = -\gamma_1^P g_X^{-2}(x_q) + C_b(\varphi)$$

and

$$\lim_{n\to\infty} \frac{n^3}{m}\text{V}(\text{OBQ}) = \frac{4}{3}\left(\gamma_0^P g_X^{-2}(x_q)\right)^2,$$

where $C_b(\varphi)$ attains CL (or $\lceil \text{ACL} \rceil + \lfloor \text{ACL} \rfloor$) finite values as a function of the position of the subsequence of batch sizes within a cycle.

Conjecture 1 implies that nOBQ is an mse consistent estimator of $n\,\text{V}(\hat{x}_q)$, since it shows that the bias of OBQ is proportional to $1/(nm)$, and the variance is proportional to m/n^3. It also shows that similar to OBM (and OBV) mse optimal batch size should be proportional to $n^{1/3}$. In addition, given that m is proportional to $n^{1/3}$, the ratio of mse(OBQ) to $\left[\text{V}(\hat{x}_q)\right]^2$ goes to zero with $n^{2/3}$.

5 FINITE-SAMPLE SIZE PERFORMANCE OF OBQ

In Sections 5 and 6 we consider only OBQ(2), and write OBQ, for the reason discussed in Section 3: smoother behavior.

In this section we show that the cyclic behavior of OBQ, and the changes in the cyclic behavior depending on the distribution shape and the quantile value, make it very difficult to choose the "best" batch size and the "best" point estimator.

In our finite sample size discussions we use the criterion that an acceptable mse is one that satisfies

$$\sqrt{\text{mse(OBQ)}} \le \text{V}(\hat{x}_q(\bullet))/10. \qquad (2)$$

For all of our figures we indicate the mse value that satisfies the above criterion with a solid line.

In the next subsection we present examples with iid data that show that the performance of OBQ depends on the point estimator, marginal distribution, quantile value, and the sample size.

5.1 IID Data

5.1.1 Effects of the Marginal Distribution

For $q=0.1$ and $n=10000$, Figures 1 and 2 show the bias, variance, and mse of the OBQ estimator plotted as a function of batch size. The four curves in each subfigure correspond to the four point estimators, as indicated in the legend. In the first figure data are Uniform$(-1/0.6\ ,\ 1/0.6)$ and in the second they are Exponential $(1/0.3)$. To simplify comparison the distribution coefficients are chosen such that $q(1-q)\, g_X^{-2}(x_q) = 1$. Therefore, the value of our maximum-mse criterion is 10^{-10} for both distributions.

Figure 1 shows that the bias of OBQ has big variation within a cycle when the point estimator is either $\hat{x}_q(ce)$ or $\hat{x}_q(fl)$. OBQ has the minimal bias when the point estimator is $\hat{x}_q(lcA)$. Therefore mse of OBQ is below 10^{-10} for many batch sizes with $\hat{x}_q(lcA)$. The high variation of OBQ with other estimators makes the penalty of choosing a wrong batch size higher. Figure 2 shows, however, that the above observations are specific to the uniform distribution. For the exponential distribution the absolute bias of OBQ seems to be the same with $\hat{x}_q(lcS)$ and $\hat{x}_q(lcA)$. Since, in this case, OBQ has less variance with $\hat{x}_q(lcS)$, it has the minimal mse with $\hat{x}_q(lcS)$. Even with $\hat{x}_q(lcS)$, however, only a few batch sizes result in mse below 10^{-10}.

5.1.2 Effects of q

Estimating extreme quantiles is more difficult than estimating the median. As $|\,0.5-q\,|$ increases, estimating x_q gets more difficult, in the sense that more data are needed for the same amount of accuracy. We observe the same effect of q on the performance of OBQ. With the same sample size when $q=0.5$ more point estimators for more batch sizes satisfy our criterion given by (2) than when either $q=0.1$ or $q=0.9$. The performance of OBQ is, however, not symmetric for $q=0.1$ and $q=0.9$ even for symmetric distributions. Figure 3 shows OBQ with $q=0.75$ for 10000 independently and exponentially distributed data. Again, to simplify comparison we set the coefficient of the exponential distribution such that $q(1-q)\, g_X^{-2}(x_q) = 1$.

When $q=0.75$ mse of OBQ is below 10^{-10} for all the estimators (except $\hat{x}_q(fl)$) for batch sizes between 25 and 60. The penalty for choosing a wrong batch size is less than that observed for $q=0.1$.

5.1.3 Effects of the Sample Size, n

As our results on asymptotic behavior of OBQ imply, increasing the sample size improves the performance of OBQ. This improvement is observed in bias and variance, and consequently in mse of OBQ. Empirical evidence shows that $\sqrt{\text{mse(OBQ)}}\,/\,\text{V}(\hat{x}_q(\bullet))$, for the optimal mse, decreases with $n^{1/3}$. We observed this effect for all distributions and for all q values we studied.

Empirical evidence shows that bias(OBQ) decreases with n and that V(OBQ) decreases with n^3, consistent with the asymptotic results of Section 4. When the sample size is 1000 no batch size results in an acceptable mse level. Increasing the sample size increases the number of batches that result in an acceptable mse value.

5.1.4 Effects of Point Estimator

Our empirical study shows that the choice of point estimator effects the bias, variance and mse of OBQ for finite sample sizes. We never observed $\hat{x}_q(fl)$ resulting in the optimal or the smoothest mse curves. On the other hand, one of the linear combination point estimators, $\hat{x}_q(lcA)$ or $\hat{x}_q(lcS)$, usually produces the smoothest mse curves. No point estimator performs better than the others for all distributions and quantiles.

5.2 Autocorrelated Data

In addition to the factors discussed in the previous subsection, autocorrelation structure plays an important role in selecting the right batch size. As the data become more correlated, more specifically as γ_1^P / γ_0^P increases, the mse-optimal batch size increases. Since the cyclic behavior of OBQ diminishes with increasing batch size, the problem shifts from choosing the right cycle to choosing the right neighborhood for the right batch size.

6 COMPARISON OF NBQ AND OBQ

Our empirical study is consistent with

$$\frac{\lim_{n\to\infty} nm\ \text{bias(OBQ)}}{\lim_{n\to\infty} nm\ \text{bias(NBQ)}} = 1$$

and

$$\frac{\lim_{n\to\infty} (n^3/m)\ \text{V(OBQ)}}{\lim_{n\to\infty} (n^3/m)\ \text{V(NBQ)}} = \frac{2}{3},$$

results analogous to OBM and NBM.

7 DISCUSSION

In this paper we show that OBQ has asymptotic properties similar to OBM and that it is an mse-consistent estimator of $n\mathrm{V}\left(\hat{x}_q\right)$. However, unlike OBM, the expected value and variance of OBQ show a cyclic behavior with changing batch sizes. Therefore bias, variance and mse of OBQ may change significantly by changing the batch size by one. Since the optimal batch size depends on q and the marginal distribution, it is not easy to determine the optimal batch size in practical applications. Because of this cyclic behavior it not also sufficient to determine the neighborhood of the optimal batch size, which may include very bad batch sizes as well as the best.

The cyclic behavior of OBQ diminishes with increasing sample and batch sizes. Therefore to minimize the possibility of choosing a very bad batch size from an early cycle we advise picking from later cycles, even for iid data. This strategy of course requires a large sample size and computational time.

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