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STEADY-STATE QUANTILE ESTIMATION USING STANDARDIZED TIME SERIES

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ABSTRACT

Extending developments of Calvin and Nakayama in 2013 and Alexopoulos et al. in 2019, we formulate point and confidence-interval (CI) estimators for given quantiles of a steady-state simulation output process based on the method of standardized time series (STS). Under mild, empirically verifiable conditions, including a geometric-moment contraction (GMC) condition and a functional central limit theorem for an associated indicator process, we establish basic asymptotic properties of the STS quantile-estimation process. The GMC condition has also been proved for many widely used time-series models and a few queueing processes such as M/M/1 waiting times. We derive STS estimators for the associated variance parameter that are computed from nonoverlapping batches of outputs, and we combine those estimators to build asymptotically valid CIs. Simulated experimentation shows that our STS-based CI estimators have the potential to compare favorably with their conventional counterparts computed from nonoverlapping batches.

1 INTRODUCTION

Discrete-event simulation can be used to analyze many types of stochastic processes. Simulation output analyses often report point and confidence interval (CI) estimators for steady-state performance measures such as the mean and selected quantiles of the underlying process. Since the early 1950s, research on simulation-based estimation of the steady-state mean has grown rapidly. By contrast since the mid-1970s, research on simulation-based estimation of steady-state quantiles has grown much less rapidly owing to the more-difficult challenges encountered when the output process (i) is contaminated by warm-up effects due to non-steady-state initialization of the simulation; (ii) is autocorrelated; (iii) has a heavy-tailed distribution; (iv) does not have a probability density function (p.d.f.); (v) has a p.d.f. with multiple modes; or (vi) has a p.d.f. with discontinuities, vertical asymptotes, or other departures from global smoothness. While issues (iv) and (vi) have relatively little impact on steady-state mean estimation, they complicate steady-state quantile estimation significantly. To address challenges (i)–(iii), several steady-state quantile estimation procedures have been developed; see Alexopoulos et al. (2017, p. 22:3) and Alexopoulos et al. (2019a, §1).

Of particular note are two recent sequential procedures for estimating a given steady-state p-quantile for $p \in (0,1)$ that address issues (i)–(iii). Sequest (Alexopoulos et al. 2019a) is designed for estimating nonextreme quantiles—i.e., $p \in [0.05, 0.95]$; and Sequem (Alexopoulos et al. 2017) is designed for estimating "extreme" quantiles—i.e., $p \in (0.0005, 0.05) \cup (0.95, 0.9995)$. These sequential procedures use batch quantile estimators (BQEs) computed from nonoverlapping batches to deliver CIs for a given quantile that have been shown on a large battery of test cases to exhibit ease of use, close conformance to user-specified requirements on CI coverage probability and precision, and high efficiency with respect to sampling effort.

In this paper we develop a class of quantile-estimation methods based on a standardized time series (STS) that addresses challenges (i)–(vi) and is an alternative (or potential companion) to conventional BQE-based methods. STS-based methods have been studied extensively in the context of point and CI estimation of the steady-state mean (Schruben 1983; Glynn and Iglehart 1990; Goldsman et al. 1990), where they are shown to have certain performance advantages over other methods. Here we apply the STS method to steady-state quantile estimation by extending the developments of Calvin and Nakayama (2013) for independent and identically distributed (i.i.d.) data and Alexopoulos et al. (2019b, §4) for dependent data. In Section 2 we formulate our key assumptions, which are substantially weaker than those of Calvin and Nakayama (2013, p. 603). In Section 3 we use the basic asymptotic properties derived by Alexopoulos et al. (2019b, Theorems 1–3) for the STS quantile-estimation process associated with a dependent output process in order to establish the limiting distributions of the STS "area" variance estimators (Theorem 4) and the asymptotic validity of CIs based on the nonoverlapping-batch STS method for quantile estimation (Theorem 5). Section 4 details some initial simulated experimentation revealing that the STS-based quantile estimators work as predicted by the asymptotic theory, yielding CIs that are comparable to conventional CIs based on BQEs. Finally in Section 5 we summarize our findings and discuss directions for future work.

2 PRELIMINARIES

For given $p \in (0,1)$, we formulate point and confidence-interval (CI) estimators of the steady-state p-quantile x_p of a simulation-generated response X based on the STS method of output analysis. We use the following conventional notation: $\mathbb{R} \equiv (-\infty, \infty)$ denotes the set of real numbers; $\mathbb{R}^+ \equiv [0, \infty)$ denotes the set of nonnegative real numbers; and $\mathbb{Z} \equiv \{0, \pm 1, \pm 2, \ldots\}$ denotes the set of integers. If it is clear from the context that, for example, k is a nonnegative (respectively, positive) integer-valued variable, then for simplicity we often write $k \geq 0$ (respectively, $k \geq 1$). For each $x \in \mathbb{R}$, we let $F(x) \equiv \Pr\{X \leq x\}$ denote the cumulative distribution function (c.d.f.) of the steady-state response so that we have $x_p = F^{-1}(p) \equiv \inf\{x : F(x) \geq p\}$. If $F(x)$ is absolutely continuous, then we let $f(x)$ denote the p.d.f. of $F(x)$.

We seek to estimate x_p from the stationary process $\{Y_k : k \geq 1\}$, which is a warmed-up (i.e., truncated-and-reindexed) version of the original sequence of simulation outputs $\{X_i : i \geq 1\}$ as documented in Alexopoulos et al. (2019a, §3.1). For each $x \in \mathbb{R}$ and $k \geq 1$, we define the indicator random variable (r.v.) $I_k(x) \equiv 1$ if $Y_k \leq x$, and $I_k(x) \equiv 0$ otherwise. For a sample of size $n \geq 1$, we let $\bar{I}(x_p, n) \equiv n^{-1} \sum_{k=1}^{n} I_k(x_p)$; and when $n = 0$, we let $\bar{I}(x_p, n) \equiv 0$. For each $\ell \in \mathbb{Z}$, we let $\rho_I(\ell) \equiv \mathrm{Corr}[I_k(x_p), I_{k+\ell}(x_p)]$ denote the autocorrelation at lag ℓ in the indicator process; and we assume $\sum_{\ell \in \mathbb{Z}} |\rho_I(\ell)| < \infty$ so that we can define the variance parameter of the indicator process,

$$\sigma_I^2 \equiv \lim_{n \to \infty} n \mathrm{Var}\big[\bar{I}(x_p, n)\big] = p(1-p) \sum_{\ell \in \mathbb{Z}} \rho_I(\ell) \in (0, \infty). \tag{1}$$

Let D denote the space of real-valued ($\mathbb{R}$-valued) functions on $[0,1]$ that are right-continuous with left-hand limits (Billingsley 1999, §12; Whitt 2002, §3.3). We assume that the warmed-up output process $\{Y_k : k \geq 1\}$ and the associated indicator process $\{I_k(x_p) : k \geq 1\}$ satisfy the following conditions.

Geometric-Moment Contraction (GMC) Condition The process $\{Y_k : k \geq 1\}$ is defined by a function $\xi(\cdot)$ of a sequence of i.i.d. r.v.'s $\{\varepsilon_j : j \in \mathbb{Z}\}$ such that $Y_k = \xi(\ldots, \varepsilon_{k-1}, \varepsilon_k)$ for $k \geq 1$. Moreover, there exist constants $\psi > 0$, $C > 0$, and $r \in (0,1)$ such that for two independent sequences $\{\varepsilon_j : j \in \mathbb{Z}\}$ and $\{\acute{\varepsilon}_j : j \in \mathbb{Z}\}$ each consisting of i.i.d. r.v.'s distributed like ε_0, we have

$$\mathrm{E}\Big[\big|\xi(\ldots, \varepsilon_{-1}, \varepsilon_0, \varepsilon_1, \ldots, \varepsilon_k) - \xi\big(\ldots, \acute{\varepsilon}_{-1}, \acute{\varepsilon}_0, \varepsilon_1, \ldots, \varepsilon_k\big)\big|^{\psi}\Big] \leq Cr^k \text{ for } k \geq 0. \tag{2}$$

Density-Regularity (DR) Condition The c.d.f. $F(x)$ has a p.d.f. $f(x)$ that is continuous at every $x \in \mathbb{R}$, and $\sup_{x \in \mathbb{R}} f(x) < \infty$; moreover at the quantile x_p to be estimated, we have $f(x_p) > 0$, and the derivative $f'(x_p)$ exists.

Functional Central Limit Theorem (FCLT) for the Indicator Process We define the following sequence of random functions $\{\mathscr{I}_n(\cdot; x_p) : n \geq 1\}$ in D,

$$\mathscr{I}_n(t; x_p) \equiv \frac{\lfloor nt \rfloor}{\sigma_I n^{1/2}}\big[\bar{I}(x_p, \lfloor nt \rfloor) - p\big] \text{ for } n \geq 1 \text{ and } t \in [0,1], \tag{3}$$

where $\lfloor \cdot \rfloor$ denotes the floor function. We assume that the sequence (3) satisfies the functional central limit theorem (FCLT),

$$\mathscr{I}_n(\cdot; x_p) \underset{n \to \infty}{\Longrightarrow} \mathscr{W}(\cdot), \tag{4}$$

where $\mathscr{W}(\cdot)$ denotes standard Brownian motion on $[0,1]$; and $\underset{n \to \infty}{\Longrightarrow}$ denotes weak convergence in D as $n \to \infty$ (Billingsley 1999, §§2–3, §8, §13).

Using the full sample $\{Y_1, \ldots, Y_n\}$ of size $n \geq 1$, we sort the responses in ascending order to obtain the order statistics $Y_{(1)} \leq \cdots \leq Y_{(n)}$. The full-sample point estimator of x_p is defined as $\widetilde{y}_p(n) \equiv Y_{(\lceil np \rceil)}$ when $n \geq 1$, where $\lceil \cdot \rceil$ denotes the ceiling function; and when $n = 0$, we let $\widetilde{y}_p(n) \equiv 0$.

We assume that a batch count $b \geq 2$ is given. For $j = 1, \ldots, b$, the jth nonoverlapping batch of size $m \geq 1$ consists of the response subsequence $\{Y_{(j-1)m+1}, \ldots, Y_{jm}\}$. From the jth batch of size $m \geq 1$, we compute the batch mean of the associated indicator r.v.'s, $\bar{I}_j(x_p, m) \equiv m^{-1} \sum_{\ell=1}^{m} I_{(j-1)m+\ell}(x_p)$; and when $m = 0$, we let $\bar{I}_j(x_p, m) \equiv 0$. When $m \geq 1$, we sort the responses from the jth batch in ascending order to obtain the order statistics $Y_{j,(1)} \leq \cdots \leq Y_{j,(m)}$. Then the jth batch quantile estimator (BQE) of x_p is defined as $\widehat{y}_p(j, m) \equiv Y_{j,(\lceil mp \rceil)}$ when $m \geq 1$; and we let $\widehat{y}_p(j, m) \equiv 0$ when $m = 0$.

Before developing the main results, we finish describing our basic notation. If the r.v.'s $\mathscr{S}$ and $\mathscr{U}$ have the same distribution, then we write $\mathscr{S} \overset{\mathrm{d}}{=} \mathscr{U}$. We let $N(0,1)$ denote the standard normal distribution so that a standard normal r.v. $Z \overset{\mathrm{d}}{=} N(0,1)$ has mean 0 and variance 1; and we let $\mathbf{Z}_b = [Z_1, \ldots, Z_b]^{\mathsf{T}}$ denote a $b \times 1$ standard normal random vector so that its entries $\{Z_i : i = 1, \ldots, b\}$ are i.i.d. $N(0,1)$. If $\{\mathscr{U}_n : n \geq 1\}$ is a sequence of r.v.'s and $\{a_n : n \geq 1\}$ is a sequence of nonnegative constants, then the expression $\mathscr{U}_n = O_{\text{a.s.}}(a_n)$ means there is a real-valued r.v. $\mathfrak{U}$ and an integer $n_0 \geq 1$ such that $|\mathscr{U}_n| \leq \mathfrak{U} a_n$ for $n \geq n_0$ almost surely (a.s.) (Wu 2005, p. 1934). Note that $\mathfrak{U}$ does not depend on n and $\mathfrak{U} \in \mathbb{R}^+$, but $\mathfrak{U}$ is not necessarily a bounded r.v. Based on this setup, Alexopoulos et al. (2019a) prove the following result.

Theorem 1 If the batch count $b \geq 2$ is given, the batch size $m \geq 1$, and the process $\{Y_k : k \geq 1\}$ satisfies the GMC and DR conditions as well as the FCLT (4), then

$$\widehat{y}_p(j, m) = x_p - \frac{\bar{I}_j(x_p, m) - p}{f(x_p)} + O_{\text{a.s.}}\left[\frac{(\log m)^{3/2}}{m^{3/4}}\right] \text{ as } m \to \infty \text{ for } j = 1, \ldots, b; \text{ and} \tag{5}$$

$$m^{1/2}\big[\widehat{y}_p(1, m) - x_p, \ldots, \widehat{y}_p(b, m) - x_p\big]^{\mathsf{T}} \underset{m \to \infty}{\Longrightarrow} \big[\sigma_I / f(x_p)\big]\mathbf{Z}_b. \tag{6}$$

Equation (5) is the Bahadur representation for the BQE $\widehat{y}_p(j,m)$. To elaborate the significance of Theorem 1 as it will be used in the following development, we state an immediate consequence of this result as it applies to the full-sample quantile estimator $\widetilde{y}_p(n)$.

Corollary 1 If the sample size $n \geq 1$, and $\{Y_k : k \geq 1\}$ satisfies the GMC and DR conditions as well as the FCLT (4), then the remainder

$$Q_n \equiv \widetilde{y}_p(n) - x_p + \frac{\bar{I}(x_p, n) - p}{f(x_p)} \text{ for } n \geq 1 \tag{7}$$

in the Bahadur representation for $\widetilde{y}_p(n)$ has an associated real-valued r.v. $\mathfrak{U}$ and an integer $n_0 \geq 1$ such that

$$|Q_n| \leq \mathfrak{U}\frac{(\log n)^{3/2}}{n^{3/4}} \text{ for } n \geq n_0 \text{ a.s.} \tag{8}$$

Thus the Bahadur representation for $\widetilde{y}_p(n)$ has the form

$$\widetilde{y}_p(n) = x_p - \frac{\bar{I}(x_p, n) - p}{f(x_p)} + O_{\text{a.s.}}\left[\frac{(\log n)^{3/2}}{n^{3/4}}\right] \text{ as } n \to \infty, \tag{9}$$

and the central limit theorem (CLT) for quantile estimation in dependent sequences has the form

$$n^{1/2}\big[\widetilde{y}_p(n) - x_p\big] \underset{n\to\infty}{\Longrightarrow} [\sigma_I / f(x_p)]Z. \tag{10}$$

Remark 1 The proof of Theorem 1 requires a minor modification in the proof for Theorem 4 of Wu (2005) as detailed in Alexopoulos et al. (2019a, Electronic Companion, Equations (EC.14)–(EC.15)). It must be noted, however, that another minor modification of Wu's proof can be used to ensure that the conclusions of Theorem 1 and Corollary 1 hold when the DR condition is replaced by the following much weaker condition.

Local Distribution-Regularity (LDR) Condition In some neighborhood of x_p, the c.d.f. $F(x)$ has a positive first derivative $F'(x)$ and a bounded second derivative $F''(x)$.

All the following results hold if the DR condition is replaced by the LDR condition. Moreover, the LDR condition holds for all the test processes evaluated in Alexopoulos et al. (2019a, §4), whereas the DR condition does not hold for the queue-waiting-time processes evaluated in Alexopoulos et al. (2019a, §§4.2–4.4) because the distribution of each associated response has an atom at $x = 0$, the lower end-point of its support, and thus does not possess a p.d.f. The LDR condition can also hold when the p.d.f. $f(x)$ exists but has a finite number of (i) discontinuities (e.g., $f(x)$ is an exponential, Pareto, or uniform p.d.f.); or (ii) vertical asymptotes (e.g., $f(x)$ is a beta, gamma, or Weibull p.d.f. with a shape parameter less than 1)—provided, of course, that x_p is not one of the points in $\mathbb{R}$ of type (i) or (ii). ◄

3 BASIC ASYMPTOTIC PROPERTIES OF STS QUANTILE ESTIMATORS

In this section we build on Theorem 1 and Corollary 1 to establish the asymptotic behavior of two STS-based quantile-estimation processes on D. We start with the centered-and-scaled quantile-estimation process,

$$\mathscr{Y}_n(t; x_p) \equiv \frac{\lfloor nt \rfloor}{n^{1/2}}\big\{x_p - \widetilde{y}_p(\lfloor nt \rfloor)\big\} = \frac{\sigma_I}{f(x_p)}\mathscr{I}_{\lfloor nt \rfloor}(t; x_p) - \frac{\lfloor nt \rfloor}{n^{1/2}}Q_{\lfloor nt \rfloor} \text{ for } n \geq 1 \text{ and } t \in [0, 1], \tag{11}$$

where the remainder terms $\{Q_u : u \geq 1\}$ associated with the Bahadur representation for $\widetilde{y}_p(u)$ are defined by Equation (7), while we let $Q_0 \equiv 0$ so that Equation (11) holds not only when $u = \lfloor nt \rfloor \geq 1$ but also when $u = \lfloor nt \rfloor = 0$. Thus we obtain the Bahadur representation for $\mathscr{Y}_n(t; x_p)$,

$$\mathscr{Y}_n(t; x_p) = \frac{\sigma_I}{f(x_p)} \mathscr{I}_n(t; x_p) + O_{\text{a.s.}}\left[\frac{(\log n)^{3/2}}{n^{1/4}}\right] \text{ as } n \to \infty \text{ and } t \in [0, 1]. \tag{12}$$

The following intermediate result is proved in Alexopoulos et al. (2019b, Theorem 2).

Theorem 2 If $\{Y_k : k \geq 1\}$ satisfies the assumptions of Theorem 1, then

$$[f(x_p)/\sigma_I]\, \mathscr{Y}_n(t; x_p) \underset{n \to \infty}{\Longrightarrow} \mathscr{W}(\cdot). \tag{13}$$

Next we obtain the FCLT required for an STS-based quantile-estimation procedure. As the STS counterpart of Equation (11), we define the STS quantile-estimation process,

$$T_n(t) \equiv \frac{\lfloor nt \rfloor}{n^{1/2}}\left[\, \widetilde{y}_p(n) - \widetilde{y}_p(\lfloor nt \rfloor)\right] \text{ for } n \geq 1 \text{ and } t \in [0, 1], \tag{14}$$

where $\widetilde{y}_p(\lfloor nt \rfloor)$ is the estimator of the p-quantile (x_p) based on the partial sample $\{Y_1, \ldots, Y_{\lfloor nt \rfloor}\}$; and we let $\mathscr{B}(t) \equiv \mathscr{W}(t) - t\mathscr{W}(1)$ for $t \in [0, 1]$ denote a standard Brownian bridge that is independent of $\mathscr{W}(1)$ (Billingsley 1999, pp. 101–102). The following intermediate result is proved in Alexopoulos et al. (2019b, Theorem 3).

Theorem 3 If $\{Y_k : k \geq 1\}$ satisfies the assumptions of Theorem 1, then

$$\left[f(x_p)/\sigma_I\right]\left\{n^{1/2}\left[x_p - \widetilde{y}_p(n)\right], T_n(\cdot)\right\} \underset{n \to \infty}{\Longrightarrow} [\mathscr{W}(1), \mathscr{B}(\cdot)]. \tag{15}$$

3.1 Weak Convergence of the Full-Sample STS Area Variance Estimator

Let $w(t)$, $t \in [0, 1]$, denote a deterministic weighting function that has a continuous second derivative on $[0, 1]$. The full-sample STS area variance estimator is $\mathscr{A}_n^2(w)$, where

$$\mathscr{A}_n(w) \equiv n^{-1} \sum_{k=1}^{n} w(k/n) T_n(k/n) \text{ for each } n \geq 1. \tag{16}$$

In Equation (16), we select $w(\cdot)$ to yield $\mathrm{E}\left\{\left[\int_0^1 w(t)\mathscr{B}(t)\,\mathrm{d}t\right]^2\right\} = 1$ so that $\int_0^1 w(t)\mathscr{B}(t)\,\mathrm{d}t \stackrel{\mathrm{d}}{=} N(0, 1)$. Since $|w(t)|$ is nontrivial and continuous on $[0, 1]$, it attains a finite nonzero upper bound $M \equiv \sup_{0 \leq t \leq 1} |w(t)| \in (0, \infty)$. To establish the asymptotic distribution of $\mathscr{A}_n^2(w)$ as $n \to \infty$, we define the following functionals for each $y \in D$:

$$\Delta_n(y) \equiv n^{-1} \sum_{k=1}^{n} w(k/n) y(k/n) \text{ for each } n \geq 1, \text{ and } \Delta(y) \equiv \int_0^1 w(t) y(t)\,\mathrm{d}t. \tag{17}$$

Since each $y \in D$ is bounded and has at most countably many discontinuities in $[0, 1]$ (Billingsley 1999, p. 122), the function $w(t)y(t)$ has the same properties and thus is Riemann integrable over $[0, 1]$.

Theorem 4 If $\{Y_k : k \geq 1\}$ satisfies the assumptions of Theorem 1, then

$$\mathscr{A}_n^2(w) \underset{n \to \infty}{\Longrightarrow} \frac{\sigma_I^2}{f^2(x_p)} \chi_1^2, \tag{18}$$

where χ_ν^2 denotes a chi-squared random variable with ν degrees of freedom for $\nu \geq 1$.

Proof Pick $y \in D$ arbitrarily. Let $\{y_n : n \geq 1\}$ denote an arbitrary sequence in D such that $y_n \longrightarrow y$, which implies that $\lim_{n\to\infty} \|y_n - y\| = 0$. By the triangle inequality, we have

$$|\Delta_n(y_n) - \Delta(y)| \leq |\Delta_n(y_n) - \Delta_n(y)| + |\Delta_n(y) - \Delta(y)| \text{ for each } n \geq 1. \tag{19}$$

Since $w(t)y(t)$ is Riemann integrable over $[0,1]$, we have $\lim_{n\to\infty} \Delta_n(y) = \Delta(y)$. We also observe that

$$|\Delta_n(y_n) - \Delta_n(y)| \leq \Delta_n(|y_n - y|) \leq \Delta_n(\|y_n - y\|) \leq M\|y_n - y\|. \tag{20}$$

Equations (19)–(20) ensure that

$$\lim_{n\to\infty} \Delta_n^2(y_n) = \Delta^2(y). \tag{21}$$

Using Theorem 3 and Equation (21), we can apply the generalized continuous-mapping theorem (Whitt 2002, Theorem 3.4.4) to conclude that

$$\mathscr{A}_n^2(w) = \Delta_n^2(T_n) \underset{n\to\infty}{\Longrightarrow} \Delta^2\left[\frac{\sigma_I}{f(x_p)}\mathscr{B}\right] = \frac{\sigma_I^2}{f^2(x_p)}\left[\int_0^1 w(t)\mathscr{B}(t)\,\mathrm{d}t\right]^2 \overset{\mathrm{d}}{=} \frac{\sigma_I^2}{f^2(x_p)}\chi_1^2. \quad \blacksquare \tag{22}$$

3.2 Asymptotically Valid CIs for the Nonoverlapping-Batch STS Method

From the jth batch ($j = 1, \ldots, b$), we compute the statistic $\widehat{y}_p(j,m)$, the r.v. $\bar{I}_j(x_p, m)$, and the random process $\left\{\bar{I}_j(x_p, \lfloor mt \rfloor) : t \in [0,1]\right\}$ to obtain the associated STS quantile-estimation process,

$$T_{j,m}(t) \equiv \frac{\lfloor mt \rfloor}{m^{1/2}}\left[\widehat{y}_p(j,m) - \widehat{y}_p(j, \lfloor mt \rfloor)\right] \text{ for } m \geq 1 \text{ and } t \in [0,1]. \tag{23}$$

Then for $j = 1, \ldots, b$, from Theorem 3 adapted to a batch of size m rather than the full sample of size $n = bm$, we have

$$\left[f(x_p)/\sigma_I\right]\left\{m^{1/2}\left[x_p - \widehat{y}_p(j,m)\right], T_{j,m}(\cdot)\right\} \underset{m\to\infty}{\Longrightarrow} [\mathscr{W}_j(1), \mathscr{B}_j(\cdot)], \tag{24}$$

where $\mathscr{W}_j(1)$ and $\mathscr{B}_j(\cdot)$ are independent. If we prove that the random vectors $\left\{\left[\mathscr{W}_j(1), \Delta^2(\mathscr{B}_j)\right]^\mathsf{T} : j = 1, \ldots, b\right\}$ are i.i.d., then we can also show that as $m \to \infty$, an asymptotically valid $100(1-\alpha)\%$ CI for x_p is given by

$$\overline{\overline{y}}_p(b,m) \pm t_{1-\alpha/2,b}\left[\mathscr{A}_{b,m}^2/n\right]^{1/2}, \tag{25}$$

where:

$$\overline{\overline{y}}_p(b,m) \equiv b^{-1}\sum_{j=1}^{b}\widehat{y}_p(j,m) \quad \text{and} \quad \mathscr{A}_{b,m}^2 \equiv b^{-1}\sum_{j=1}^{b}\Delta_m^2(T_{j,m}) \tag{26}$$

respectively denote the average of the BQEs and the average of the STS area variance estimators computed from each of the nonoverlapping batches; and $t_{\beta,\nu}$ denotes the β-quantile for Student's t-distribution with ν degrees of freedom when $\beta \in (0,1)$ and $\nu \geq 1$.

Theorem 5 If $\{Y_k : k \geq 1\}$ satisfies the assumptions of Theorem 1, then in Equation (24) we have

$$\left\{\left[\mathscr{W}_j(1), \Delta^2(\mathscr{B}_j)\right]^\mathsf{T} : j = 1, \ldots, b\right\} \text{ are i.i.d.} \tag{27}$$

so that Equation (25) is an asymptotically valid $100(1-\alpha)\%$ CI estimator of x_p as $m \to \infty$.

Proof For each $\omega \in D$ and $j \in \{1, \dots, b\}$, define the functional $\mathfrak{B}_j : D \mapsto D$ by

$$\mathfrak{B}_j \circ \omega(t) \equiv b^{1/2}\Big[\omega\Big(\frac{t+j-1}{b}\Big) - \omega\Big(\frac{j-1}{b}\Big)\Big] - tb^{1/2}\Big[\omega\Big(\frac{j}{b}\Big) - \omega\Big(\frac{j-1}{b}\Big)\Big] \text{ for } t \in [0,1]. \tag{28}$$

For the batch size $m \geq 1$, define the corresponding Riemann-sum functional Δ_m as in Equation (17). Pick $\omega \in D$ arbitrarily. Let $\{\omega_m : m \geq 1\}$ denote an arbitrary sequence in D such that $\omega_n \to \omega$ so that $\lim_{m\to\infty} \|\omega_m - \omega\| = 0$. We can show that

$$\big|\mathfrak{B}_j \circ \omega_m(t) - \mathfrak{B}_j \circ \omega(t)\big| \leq 4b^{1/2}\|\omega_m - \omega\|. \tag{29}$$

By the triangle inequality, we have

$$|\Delta_m(\mathfrak{B}_j \circ \omega_m) - \Delta(\mathfrak{B}_j \circ \omega)| \leq |\Delta_m(\mathfrak{B}_j \circ \omega_m) - \Delta_m(\mathfrak{B}_j \circ \omega)| + |\Delta_m(\mathfrak{B}_j \circ \omega) - \Delta(\mathfrak{B}_j \circ \omega)| \tag{30}$$

for $m \geq 1$. Because $w(t)\mathfrak{B}_j \circ \omega(t)$ is Riemann integrable over $[0,1]$, we have $\lim_{m\to\infty} \Delta_m(\mathfrak{B}_j \circ \omega) = \Delta(\mathfrak{B}_j \circ \omega)$. We can also show that

$$|\Delta_m(\mathfrak{B}_j \circ \omega_m) - \Delta_m(\mathfrak{B}_j \circ \omega)| \leq 4b^{1/2}M\|\omega_m - \omega\|. \tag{31}$$

Equations (29)–(31) ensure that

$$\lim_{m\to\infty} \Delta_m^2(\mathfrak{B}_j \circ \omega_m) = \Delta^2(\mathfrak{B}_j \circ \omega) \text{ for } j = 1, \dots, b. \tag{32}$$

In terms of the random function $\mathscr{I}_n(\cdot; x_p) = \mathscr{I}_{bm}(\cdot; x_p)$ in D defined by Equation (3), we can apply Equation (32), the FCLT (4), and the generalized continuous mapping theorem to conclude that

$$\big[\Delta_m^2(\mathfrak{B}_1 \circ \mathscr{I}_{bm}), \dots, \Delta_m^2(\mathfrak{B}_b \circ \mathscr{I}_{bm})\big]^{\mathsf{T}} \underset{m\to\infty}{\Longrightarrow} \big[\Delta^2(\mathfrak{B}_1 \circ \mathscr{W}), \dots, \Delta^2(\mathfrak{B}_b \circ \mathscr{W})\big]^{\mathsf{T}} \tag{33}$$

$$\stackrel{\mathrm{d}}{=} \big[\chi_1^2(1), \dots, \chi_1^2(b)\big]^{\mathsf{T}}, \tag{34}$$

where the $\{\chi_1^2(j) : j = 1, \dots, b\}$ are i.i.d. chi-squared random variables, each with 1 degree of freedom. Note that Equation (34) follows from the observation that if we let

$$\mathscr{W}_j(t) \equiv b^{1/2}\Big[\mathscr{W}\Big(\frac{t+j-1}{b}\Big) - \mathscr{W}\Big(\frac{j-1}{b}\Big)\Big] \text{ for } t \in [0,1] \text{ and } j = 1, \dots, b, \tag{35}$$

then we have

$$\mathfrak{B}_j \circ \mathscr{W}(t) = \mathscr{W}_j(t) - t\mathscr{W}_j(1) \equiv \mathscr{B}_j(t) \stackrel{\mathrm{d}}{=} \mathscr{W}(t) - t\mathscr{W}(1) \text{ for } t \in [0,1] \text{ and } j = 1, \dots, b \tag{36}$$

because Brownian motion is self-similar with Hurst index $1/2$ (Whitt 2002, §4.2.2). Moreover, the conclusion (27) follows from (i) the property that $\mathscr{W}(1)$ and $\mathscr{B}(\cdot)$ are independent; and (ii) the independent increments property of $\mathscr{W}$ because the random functions $\{\mathscr{B}_j(\cdot) : j = 1, \dots, b\}$ are respectively defined in terms of increments of $\mathscr{W}(\cdot)$ on the nonoverlapping subintervals $\big\{\big((j-1)/b, j/b\big] : j = 1, \dots b\big\}$ of $[0,1]$ (Whitt 2002, §1.2.3).

From the foregoing discussion, we see that the $\{\widehat{y}_p(j,m) : j = 1, \dots, b\}$ and the $\{\Delta_m^2(T_{j,m}) : j = 1, \dots, \}$ are all asymptotically mutually independent as $m \to \infty$. From the observation that

$$\Pr\Big\{b^{-1}\sum_{j=1}^{b}\chi_1^2(j) \stackrel{\mathrm{d}}{=} \chi_b^2/b > 0\Big\} = 1, \tag{37}$$

together with Equation (6), Theorem 4, Equation (26), and the generalized continuous mapping theorem, we see that

$$\frac{\overline{\overline{y}}_p(b,m)-x_p}{\left(\mathscr{A}^2_{b,m}/n\right)^{1/2}}=\frac{n^{1/2}\left[\overline{\overline{y}}_p(b,m)-x_p\right]}{\mathscr{A}_{b,m}}\underset{m\to\infty}{\Longrightarrow}\frac{Z}{\left(\chi^2_b/b\right)^{1/2}}\stackrel{\mathrm{d}}{=}t_b, \tag{38}$$

where Z is independent of χ^2_b/b, and t_b denotes a Student's t random variable with b degrees of freedom. This establishes the asymptotic validity of the CI (25). ∎

Remark 2 The quantities $\Delta_m(T_{j,m})$ in Equation (26) can be computed in $O\big(m\log_2 m\big)$ time by sorting the sample corresponding to each batch, using pointers, and computing the expressions $\Delta_m(T_{j,m})$ backwards. Then the overall computational complexity for the STS area estimator amounts to $O\big(n\log_2 m\big)$. So, aside from some additive overhead related to updating the pointers, the STS area estimator has the same complexity as the estimator based on the sample variance of the BQEs in Equation (39) below. ◀

4 EXPERIMENTAL RESULTS

In this section we conduct an empirical evaluation of the performance of the batched area variance estimator $\mathscr{A}^2_{b,m}$ in Equation (26) against the "classical" variance estimator based on the BQEs $\big\{\widehat{y}_p(j,m)\big\}$, namely $mS^2_{b,m}$, where

$$S^2_{b,m}\equiv(b-1)^{-1}\sum_{j=1}^{b}\left[\widehat{y}_p(j,m)-\overline{\overline{y}}_p(b,m)\right]^2, \tag{39}$$

and the average $\overline{\overline{y}}_p(b,m)$ is defined in Equation (26); see Alexopoulos et al. (2019a). The respective approximate $100(1-\alpha)\%$ CI for x_p based on Equation (39) is

$$\widetilde{y}_p(n)\pm t_{1-\alpha/2,b-1}S_{b,m}/b^{1/2}. \tag{40}$$

We compared the latter interval against the following analogue of (25) based on the constant weight function $w(t)=\sqrt{12}$, $t\in[0,1]$ (Schruben 1983) and centered at $\widetilde{y}_p(n)$:

$$\widetilde{y}_p(n)\pm t_{1-\alpha/2,b}\left[\mathscr{A}^2_{b,m}/n\right]^{1/2}. \tag{41}$$

The sole purpose of this evaluation is to validate the convergence of the batched area variance estimator $\mathscr{A}^2_{b,m}$ and the asymptotic validity of the CI in Equation (41). The evaluation of estimators $\mathscr{A}^2_{b,m}$ based on alternative weight functions (cf. Goldsman et al. 1990) as well as linear combinations of $\mathscr{A}^2_{b,m}$ and $S^2_{b,m}$ (cf. Schruben 1983) is the subject on ongoing work.

Remark 3 Recently we proved that under the assumptions of Theorem 1 as $m\to\infty$, (i) the CI (40) is asymptotically exact; and (ii) $\mathrm{Bias}\big[\mathscr{A}^2_{b,m}\big]\equiv\mathrm{E}\big[\mathscr{A}^2_{b,m}\big]-\sigma^2_I/f^2(x_p)=O(m^{-1/4})$. Moreover, we showed that in steady-state operation, the M/M/1 queue waiting times satisfy the GMC condition. Proofs of these results will appear in follow-up work. These results provide the basis for the following example. ◀

Example: M/M/1 Queue Waiting Times Our test process $\{X_k : k\geq 1\}$ was generated by a stationary M/M/1 queueing system with first-in-first-out (FIFO) service discipline, arrival rate $\lambda=0.8$, and service rate $\omega=1$. Specifically, X_k is the time spent in the queue by the kth arriving customer prior to service.

In this system the steady-state server utilization is $\rho=\lambda/\omega=0.8$, and the steady-state c.d.f. of X_k is

$$F(x)=\begin{cases}0 & \text{if } x<0,\\ 1-\rho & \text{if } x=0,\\ 1-\rho e^{-\omega(1-\rho)x} & \text{if } x>0;\end{cases} \tag{42}$$

hence the steady-state distribution of X_k has mean $\mu_X = \rho/(\omega-\lambda) = 4$, and the quantiles of this distribution are easily evaluated by inverting Equation (42). This steady-state distribution is markedly nonnormal, having an atom at zero, an exponential tail, and a skewness of $2(3-3\rho+\rho^2)/[\rho^{1/2}(2-\rho)^{3/2}] \approx 2.1093$. The latter properties can induce a significant skewness in the corresponding BQEs $\{\widehat{y}_p(j,m)\}$ that can degrade the performance of the CI given in Equation (40), resulting in a coverage probability that can be substantially below the nominal level (Alexopoulos et al. 2019a). Because of the atom at zero in the c.d.f. (42), we only considered values of $p > 1-\rho = 0.20$.

The variance parameter σ_I^2 of the indicator process was computed from Equation (22) of Blomqvist (1967). After some algebra, we obtained the following analytical expression for the asymptotic variance $\sigma^2 \equiv \sigma_I^2/[f(x_p)]^2$:

$$\sigma^2 = \frac{1}{\omega^2(1-\rho)^4}\left\{\frac{[-2+p(3-\rho)+2\rho](1+\rho)}{1-p} - 4\rho\ln\left(\frac{\rho}{1-p}\right)\right\}. \tag{43}$$

We generated the stationary version $\{Y_k : k \geq 1\}$ of this waiting-time process by sampling Y_1 using Equation (42), and then using Lindley's recursion. Table 1 below studies the performance of the aforementioned variance estimators and the approximate 95% CIs computed based on Equations (40) and (41) for a fixed batch count $b = 32$ and increasing batch sizes $m = 2^\ell$, $\ell = 10, 11, \ldots, 20$. We note that batch sizes with $\ell \leq 15$ are inadequate for variance estimation in this problem (Alexopoulos et al. 2019a). All entries are based on 2,500 independent replications using the random-number package of L'Ecuyer et al. (2002). We selected two values of p, the upper quartile ($p = 0.75$) and the extreme value $p = 0.99$. Column 1 contains the values p, x_p, and σ^2 (in **bold red type**); and column 2 lists $\ell = \log_2(m)$. Columns 3 and 8 display the averages of the variance estimates $\mathscr{A}_{b,m}^2$ (labeled as "STS Area Variance Estimator") and $mS_{b,m}^2$ based on Equation (39) (labeled as "NBQ Variance Estimator"), while columns 4 and 9 display the averages of the bias of the respective replicate variance estimates. Columns 5 and 10 list the standard deviations of the STS area and NBQ variance estimators, while columns 6 and 11 contain the respective standard errors (CI half-lengths divided by the associated t-quantile). Finally, columns 7 and 12 display the estimated coverage probabilities of the 95% CIs in Equations (39) and (41), respectively.

A careful examination of Table 1 revealed the presence of substantial bias in the variance estimates; this bias apparently became more prominent for extreme quantiles. For example, when $p = 0.75$ the average relative bias (bias divided by the true variance) of the STS area estimator decreased slowly from a whopping 47.1% above the asymptotic variance for $m = 2^{10}$ to about 0.2% for $m = 2^{20}$. When $p = 0.99$, the variance estimates approached their limit even more slowly, with a relative bias that started at nearly 85% below the asymptotic variance for $m = 2^{10}$, became positive near $m = 2^{15}$, and then dropped slowly as m increased. Notice that for $m = 2^{20}$ (total sample size $n = 2^{25} \approx 33$ million), the average relative bias of the STS area estimator was 1.17% while the average relative bias of the NBQ variance estimator was a bit lower (0.94%). These nonmonotone convergence patterns became more transparent from Figures 1 and 2. The behavior of the bias of both estimators is an open problem and a subject of ongoing research. At this juncture, we would like to caution the reader that for this extreme value of p, the automated sequential procedure of Alexopoulos et al. (2019a), that is based on the BQEs in Equations (39)–(40), often delivered CIs that exhibited significant undercoverage while requiring excessive sample sizes. This motivated the development of the Sequem procedure (Alexopoulos et al. 2017) for the more-difficult problem of estimating extreme quantiles.

We now turn to the remaining statistics in Table 1. The standard deviation of the STS area estimator also converged to the theoretical limit $\left[2\sigma^4/b\right]^{1/2} = 2^{1/2}\left[\sigma_I^2/f^2(x_p)\right]/b^{1/2}$ based on Equation (22). For instance, when $p = 0.99$ and $m = 2^{20}$, the average standard deviation 48921.9 was only 4.11% larger than the theoretical limit $\sigma^2/4 = 47815.2$. When $p = 0.75$, the estimated coverage probability of the approximate 95% CIs was near the nominal rate for all batch sizes. Unfortunately, this was not the case for $p = 0.99$, when the approximate 95% CIs exhibited substantial undercoverage for moderate sample sizes; indeed, the estimated coverage probabilities started approaching 0.95 as $m \geq 2^{16}$. Overall, both methodologies appeared to be equally competitive when $p = 0.75$, while the conventional NBQ method appeared to dominate when $p = 0.99$.

Table 1: Experimental results for a stationary waiting-time process in an M/M/1 queueing system with traffic intensity $\rho = 0.8$. All estimates are based on 2500 independent replications with $b = 32$ batches and batch sizes $m = 2^\ell$, $\ell = 10, 11, \ldots, 20$.

		STS Area Variance Estimator					NBQ Variance Estimator				
p (x_p) **Variance**	ℓ	Var. Est.	Bias	St. Dev.	St. Error	95% CI Cover.	Var. Est.	Bias	St. Dev.	St. Error	95% CI Cover.
0.75	10	4853.0	1554.3	3419.9	0.3683	95.92	4798.4	1499.7	3211.7	0.3675	96.12
(5.8158)	11	4992.9	1694.2	3657.9	0.2652	96.56	4113.1	814.4	2162.2	0.2442	95.80
3298.7	12	4242.5	943.8	2046.1	0.1759	96.16	3703.1	404.4	1329.6	0.1657	95.96
	13	3819.2	520.5	1402.5	0.1189	96.32	3466.6	167.9	1036.7	0.1138	95.68
	14	3547.5	248.8	1045.6	0.0814	95.36	3366.1	67.4	905.0	0.0794	95.16
	15	3412.5	113.8	936.5	0.0565	94.64	3345.8	47.1	878.2	0.0560	94.72
	16	3356.4	57.7	873.3	0.0397	94.60	3337.2	38.5	861.3	0.0396	94.80
	17	3332.1	33.4	859.7	0.0280	94.48	3327.3	28.6	839.2	0.0279	94.68
	18	3316.1	17.4	814.8	0.0197	94.60	3312.8	14.1	829.5	0.0197	94.76
	19	3310.2	11.5	838.5	0.0139	94.36	3306.4	7.7	856.2	0.0139	94.68
	20	3292.4	−6.3	813.3	0.0098	94.64	3316.4	17.7	853.0	0.0099	95.04
0.99	10	27618.0	−163642.9	17700.9	0.8782	54.88	53584.8	−137676.1	30487.4	1.2358	71.00
(21.9101)	11	54706.7	−136554.2	37687.2	0.8694	67.96	80128.0	−111132.9	37863.4	1.0790	80.12
191260.9	12	92768.8	−98492.1	66686.8	0.7992	79.08	123087.5	−68173.4	56786.8	0.9468	89.04
	13	135781.4	−55479.5	93622.5	0.6872	87.72	179439.6	−11821.3	87474.8	0.8065	93.52
	14	179612.2	−11648.7	128351.8	0.5616	91.20	218074.5	26813.6	117142.2	0.6271	94.56
	15	204721.9	13461.0	110567.3	0.4300	94.40	213376.8	22115.9	109485.9	0.4414	94.88
	16	209708.5	18447.6	106715.1	0.3094	95.44	202610.7	11349.8	77118.1	0.3065	95.84
	17	203575.5	12314.6	70787.1	0.2174	95.32	195545.3	4284.4	55570.2	0.2138	95.00
	18	199606.7	8345.8	57125.7	0.1527	95.24	193632.8	2371.9	53765.4	0.1505	94.84
	19	196112.6	4851.7	52084.9	0.1072	95.52	192647.7	1386.8	51991.8	0.1062	95.20
	20	193492.2	2231.3	49780.2	0.0753	95.52	193054.5	1793.6	48724.2	0.0753	95.16

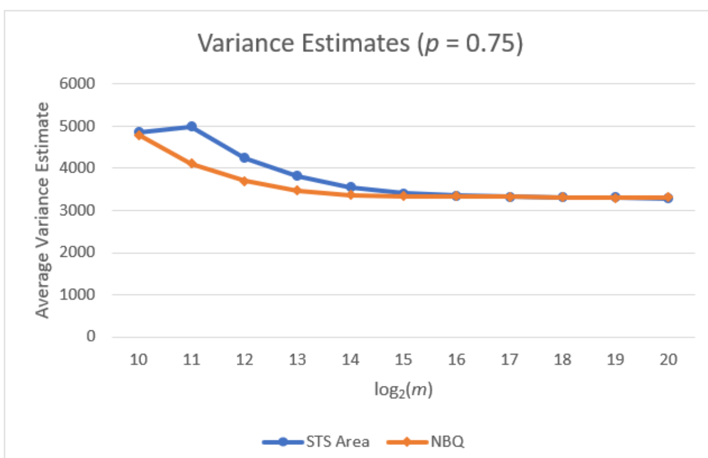

Figure 1: Average variance estimates for the marginal 0.75-quantile of a stationary waiting-time process in an M/M/1 queueing system with traffic intensity $\rho = 0.8$. All estimates are based on 2500 independent replications with $b = 32$ batches and batch sizes $m = 2^\ell$, $\ell = 10, 11, \ldots, 20$.

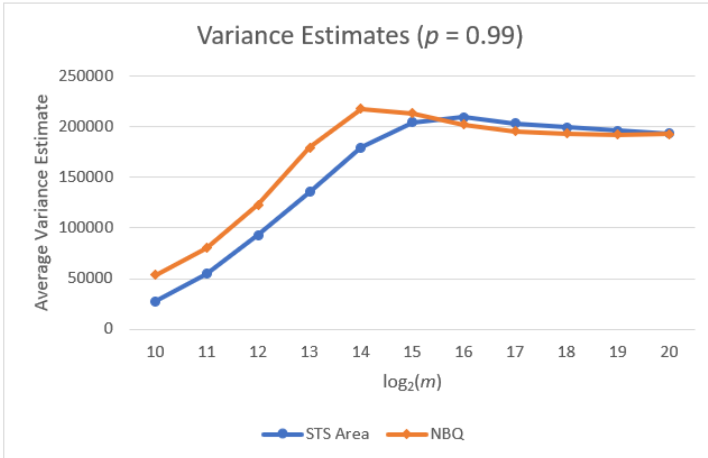

Figure 2: Average variance estimates for the marginal 0.99-quantile of a stationary waiting-time process in an M/M/1 queueing system with traffic intensity $\rho = 0.8$. All estimates are based on 2500 independent replications with $b = 32$ batches and batch sizes $m = 2^{\ell}$, $\ell = 10, 11, \ldots, 20$.

5 CONCLUSIONS AND FUTURE RESEARCH

In this paper, we developed the theoretical foundations for nonoverlapping batch-based STS point and CI estimators for marginal quantiles arising from steady-state simulation output. The theory and several generalizations are the subjects of ongoing work, where we: (i) provide all proofs in a complete, self-contained form; (ii) provide more details on point estimator properties; (iii) study area estimators based on various weight functions; (iv) consider other STS estimators besides the area estimator, e.g., the Cramér–von Mises (CvM) estimator; (v) offer an extensive Monte Carlo study so as to better depict empirical estimator performance; and (vi) study overlapping versions of the area and CvM estimators. Our ultimate goal is the devise automated sequential procedures for delivering CIs for steady-state quantiles satisfying both absolute and relative precision requirements, as motivated by the effectiveness of the SPSTS method for the steady-state mean in Alexopoulos et al. (2016).

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