ADAPTIVE QUANTILE COMPUTATION FOR BROWNIAN BRIDGE IN CHANGE-POINT ANALYSIS

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ABSTRACT. As an example for the fast calculation of distributional parameters of Gaussian processes, we propose a new Monte Carlo algorithm for the computation of quantiles of the supremum norm of weighted Brownian bridges. As it is known, the corresponding distributions arise asymptotically for weighted CUSUM statistics for change-point detection. The new algorithm employs an adaptive (sequential) time discretization for the trajectories of the Brownian bridge. A simulation study shows that the new algorithm by far outperforms the standard approach, which employs a uniform time discretization.

1. INTRODUCTION

In statistical inference, asymptotics frequently leads to the distribution of nonlinear functionals of Gaussian processes. E.g., the construction of uniform asymptotic confidence bands for a regression function based on kernel estimates requires the study of the supremum of the absolute values of a certain Gaussian process, cf. Härdle (1990, Sec. 4.3). To mention another example, for testing the equality of mean functions in functional data analysis, a test statistic is used which under the hypothesis converges in distribution to an integral of the square of a Gaussian process, cf. Horváth and Kokoszka (2012, Sec. 5.1).

In some cases like the first example above, cf. Bickel and Rosenblatt (1973), the distribution of the nonlinear functional may be derived in a form which, in particular, allows for the calculation of quantiles for tests and confidence assessments. In many other cases, however, distributional characteristics have to be calculated numerically by Monte Carlo simulation. Even in rather simple cases where the Gaussian process is just a Wiener process or a Brownian bridge, using the standard approximation of a continuous-time Gaussian process by a corresponding discrete-time process on an equidistant grid may result in a severe computational load if a decent quality of approximation is required. We shall discuss this below in more detail for a specific case.

In this paper, we show that this problem can be overcome by using fast adaptive approximation methods for the strong (or pathwise) approximation of nonlinear functionals of Gaussian processes. Adaptive algorithms employ sequential strategies to construct the underlying discretization, which may therefore be adjusted to key features of the individual trajectories.

For illustrating our approach, we focus on weighted CUSUM tests for changepoints, which leads to the distribution of the supremum of a weighted reflecting Brownian bridge, i.e., the supremum norm of a weighted Brownian bridge. We stress that the basic idea can be transferred to other situations where, e.g., quantiles of nonlinear functionals of Gaussian processes have to be calculated by Monte Carlo simulation.

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Change-point tests are of interest in many areas of applications, e.g., in production monitoring, see Page (1957), on-line-monitoring of intensive-care patients, see Fried and Imhoff (2004), or global warming studies, see Gallagher, Lund, and Robbins (2013), to name just a few. The first publications about testing for a change in data go back to the 1950s, see, e.g., Page (1957), who has considered testing for a change in the mean and has used weighted cumulated sums of sample residuals, so called weighted CUSUM statistics. The corresponding weight function is given by

$$w(t) = (t \cdot (1-t))^{-1/2}$$

for 0 < t < 1, so that the weighted cumulated sums are variance stable. The distribution of those statistics is determined asymptotically in a variant of the Darling-Erdös Theorem, see Theorem 1, which immediately yields asymptotic quantiles.

To cope with performance problems regarding size and power, the standard weights of CUSUM statistics have been modified which results asymptotically in the distribution of the supremum of a weighted reflecting Brownian bridge. Those statistics have no size problems and better power against changes of the mean closer to the boundaries of the observation interval. Simulation studies using different weight functions and analyzing the power of the corresponding CUSUM-type tests for different positions of the change (early, middle and late) show the importance of the weight function, see Csörgő and Horváth (1997), Kirch and Tadjuidje Kamgaing (2016), and Schwaar (2016). An overview to such general CUSUM-type tests is given in Aue and Horváth (2013).

In the present paper we consider weight functions of the form

$$w_{\eta,\gamma}(t) = 1_{\eta,1-\eta}(t) \cdot (t \cdot (1-t))^{-\gamma}$$

for 0 < t < 1 with parameters $0 \le \eta < 1/2$ and $0 \le \gamma \le 1/2$, and the corresponding convergence result for $(\eta, \gamma) \ne (0, 1/2)$ is formulated in Theorem 2. Except for the extremal cases $\gamma = 0$ and $\gamma = 1/2$, there is no known method for analytically calculating quantiles or other characteristics of the limit distributions for these or more general weight functions. Hence, we have to use Monte Carlo simulation where a crucial part consists in generating paths of a Brownian bridge. This is in particular computationally very expensive if we are interested in calculating, e.g., extreme quantiles beyond the common levels 0.05 or 0.01 with a high precision up to 10^{-3} . Such extreme levels of confidence are common in many applications in industry or medicine where a high degree of reliability is required. Also, in view of the Bonferroni inequality, low *p*-values of tests are of interest in multiple testing situations including many hypotheses, see, e.g., Hochberg (1988).

In this paper, we propose an adaptive algorithm which reduces the computation time for calculating asymptotic quantiles of CUSUM test statistics with weight function $w_{\eta,\gamma}$ for $\gamma \notin \{0, 1/2\}$, where the reduction turns out to be dramatic in the more challenging situations. Consider, for instance, the task to compute the 0.95-quantile with accuracy 10^{-2} for the parameters $\eta = 0$ and $\gamma = 0.45$. On a common up-to-date processor the standard algorithm with an equidistant grid requires more than two hours of computation time, while the adaptive algorithm achieves the same goal within 12 seconds. The reason for this is, roughly speaking, that the adaptive algorithm allows to sample almost exactly from the correct limit distribution at a reasonable computational cost.

This paper is organized as follows. In Section 2 we give a brief sketch of the change-point application that is used as a demonstrator for our approach. In Sections 3 and 4 we consider the strong approximation of the supremum of the

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unweighted Brownian motion and of weighted reflecting Brownian bridges, respectively. For the former problem, Calvin, Hefter, and Herzwurm (2017) have constructed an adaptive algorithm that strikingly outperforms all non-adaptive algorithms, see Theorems 7 and 9. See also Calvin (1997, 2001, 2004) for related convergence results. No such result is known for weighted reflecting Brownian bridges, but still we construct a modification of the adaptive algorithm for these processes in Section 4.1. Numerical experiments reveal again the vast superiority of the adaptive algorithm over, at least, the standard algorithm that is based on an equidistant grid, see Section 4.2. In Section 5 we study quantile computation for the supremum of a weighted reflecting Brownian bridge. We present a new algorithm, with the adaptive algorithm from Section 4.1 as the key ingredient, that yields a quantile up to a user-specified error tolerance, see Section 5.1. Numerical experiments, which show the superiority of the new algorithm over the standard approach, are presented in Section 5.2.

2. The Statistical Problem: Change-Point Test

We are interested in detecting a structural change, specifically at most one change (AMOC), in a time series model, and for illustration we consider the following most simple model with a possible mean change. The model, which is one of the earliest change-point models analyzed, is given by

$$\xi_i = \begin{cases} \varepsilon_i, & \text{if } i \le m, \\ d + \varepsilon_i, & \text{if } i > m, \end{cases}$$

for i = 1, ..., n, where $n, m \in \mathbb{N}$ with $n \ge 2$ and

$$1 \le m = m(n) \le n,$$

and where $d \in \mathbb{R}$ with $d \neq 0$, see Page (1957). The residuals ε_i are assumed to be iid, each centered with finite second moment $\sigma^2 > 0$, which is assumed to be known for simplicity. If m < n, then a structural change is present, and m is called the change-point. A test is constructed for

$$H_0: m = n, \qquad \qquad H_1: m < n.$$

Based on the quasi likelihood ratio test, the weighted CUSUM statistic

$$T_n(w) = \max_{1 \le k < n} w(k/n) \cdot \frac{|T_{k,n}|}{\sqrt{n}}$$

with

$$T_{k,n} = \sum_{i=1}^{k} \xi_i - \frac{k}{n} \sum_{i=1}^{n} \xi_i$$

and with suitable weight functions $w : [0, 1[\rightarrow [0, \infty[$ has been derived. We add that under H_0 (no change)

$$T_{k,n} = \sum_{i=1}^{k} \varepsilon_i - \frac{k}{n} \sum_{i=1}^{n} \varepsilon_i = n \cdot \left(\frac{k}{n} \cdot \left(1 - \frac{k}{n}\right)\right) \cdot \left(\frac{1}{k} \sum_{i=1}^{k} \varepsilon_i - \frac{1}{n-k} \sum_{i=k+1}^{n} \varepsilon_i\right).$$

See Csörgő and Horváth (1997, Thm. 2.1.2) for the following result.

Theorem 1 (Darling-Erdös Theorem). Let

$$w(t) = (t \cdot (1-t))^{-1/2}$$

for 0 < t < 1, and assume that $\mathbb{E}(|\varepsilon_i|^{2+\delta}) < \infty$ for some $\delta > 0$. Under H_0 we have $\lim_{n \to \infty} P(\{T_n(w) \le c_n(\alpha)\}) = 1 - \alpha$ for $0 < \alpha < 1$ and

$$c_n(\alpha) = \frac{\sigma}{a(\log n)} \left(-\log\left(-\frac{1}{2}\log(1-\alpha)\right) + b(\log n) \right),$$

with

$$a(x) = \sqrt{2\log x}$$
 and $b(x) = 2\log x + \frac{1}{2}\log\log x - \frac{1}{2}\log \pi$.

Theorem 1 immediately yields an asymptotic level α test, see Remark 4. However, for small sample sizes n the convergence in the Darling-Erdös Theorem often leads to level distortion, see Kirch (2006). To overcome this problem modifications of the weight function w are considered, see, e.g., Csörgő and Horváth (1988). In this paper we study weight functions $w_{\eta,\gamma}$ of the form

(1)
$$w_{\eta,\gamma}(t) = 1_{]\eta,1-\eta[}(t) \cdot (t \cdot (1-t))^{-\gamma}$$

for 0 < t < 1, where

$$0 \le \eta < 1/2,$$
 $0 \le \gamma \le 1/2.$

Observe that Theorem 1 deals with the case $(\eta, \gamma) = (0, 1/2)$.

For any real-valued stochastic process $X = (X(t))_{t \in [0,1[}$ we put

$$S(X) = \sup_{0 < t < 1} X(t).$$

Furthermore, $B = (B(t))_{t \in [0,1]}$ denotes a standard Brownian bridge on the unit interval. The process $|B| = (|B(t)|)_{t \in [0,1]}$ is called a reflecting Brownian bridge. The following theorem is a consequence of a general result from Kirch and Tadjuidje Kamgaing (2016) and Schwaar (2016), who study general weight functions under suitable regularity conditions.

Theorem 2. Let $w_{\eta,\gamma}$ be given by (1) with $(\eta,\gamma) \neq (0,1/2)$. Under H_0 we have

$$\frac{1}{\sigma} \cdot T_n(w_{\eta,\gamma}) \stackrel{d}{\longrightarrow} S(w_{\eta,\gamma}|B|).$$

Basically, Theorem 2 yields an asymptotic level α test. However, for application the quantiles of the supremum $S(w_{\eta,\gamma}|B|)$ of the weighted reflecting Brownian bridge $w_{\eta,\gamma}|B|$ are needed, i.e., they have to be known analytically or to be easily computed numerically, see Remark 4. In Schwaar (2020) besides data driven weighted change-point estimators, data driven weighted change-point tests are considered, where the parameter γ is replaced by an estimator and $\eta = 0$. Especially then knowledge about the quantiles for the weighted test statistic with non-extreme values is required.

For completeness we add that $S(w_{0,1/2}|B|) = \infty$ with probability one, which follows from the law of the iterated logarithm, and hence Theorem 2 implies $T_n(w_{0,1/2}) \xrightarrow{p} \infty$.

Remark 3. Consider the extremal cases $\gamma = 0$ and $\gamma = 1/2$. For $(\eta, \gamma) = (0, 0)$ the series representation of the c.d.f. of the Kolmogorov distribution may be used to compute the quantiles. More generally, for $\gamma = 0$ and $0 \leq \eta < 1/2$ a series representation of the c.d.f. of the supremum of a reflecting Brownian motion for given initial and terminal value, see Borodin and Salminen (2002, Eqn. (3.1.1.1.8)), may be used.

For $\gamma = 1/2$ and $0 < \eta < 1/2$ DeLong (1981) has studied the distribution of $S(w_{\eta,1/2}|B|)$ and related quantities, see also Yor (1984). The Mellin transform of a corresponding hitting time for a standard Brownian motion has been determined, and values of the c.d.f. have been obtained via numerical inversion.

To the best knowledge of the authors, no (semi-)analytic way to determine the quantiles is known beyond the extremal cases, i.e., for $0 < \gamma < 1/2$ and $0 \le \eta < 1/2$, cf. Salminen and Yor (2011, p. 76).

Remark 4. Let $c_{\eta,\gamma,n} > 0$. Consider the test that rejects H_0 if and only if

$$\frac{|T_{k,n}|}{\sqrt{n}} > c_{\eta,\gamma,n} \cdot \left(\frac{k}{n} \cdot \left(1 - \frac{k}{n}\right)\right)^{\gamma}$$

for some $k \in \mathbb{N}$ with

$$\eta \cdot n < k < (1 - \eta) \cdot n$$

To obtain an asymptotic level α test we proceed as follows. For $0 \leq \gamma < 1/2$ the critical value $c_{\eta,\gamma} = c_{\eta,\gamma,n}$ is determined by

$$P(\{S(w_{\eta,\gamma}|B|) \le c_{\eta,\gamma}/\sigma\}) = 1 - \alpha,$$

see Theorem 2, which may be solved semi-analytically if $\gamma = 0$ and numerically, using the algorithm presented in Section 5, if $0 < \gamma < 1/2$. For $\gamma = 1/2$ we may employ Theorem 1 to determine $c_{\eta,\gamma,n}$.

Example 5. We illustrate the role of the parameter γ in the case $\eta = 0$. Let $\sigma = 1$ and $\alpha = 0.05$. In Figure 1 the threshold function

$$f_{\gamma,n}(t) = c_{0,\gamma,n} \cdot (t \cdot (1-t))^{\gamma}$$

is presented for $\gamma = 0, 0.25, 0.45$, and for $\gamma = 0.5$ with $n = 10^2, 10^3$. The critical values are given numerically as follows. Remark 3 yields $c_{0,0.0} = 1.358$, and the adaptive algorithm $Q_{\varepsilon}^{\rm ad}(w,q)$ according to Section 5 with $\varepsilon = 10^{-2}$ yields $c_{0,0.25} = 1.99$ and $c_{0,0.45} = 2.91$. Furthermore, $c_{0,0.5,10^2} \approx 3.241$ and $c_{0,0.5,10^3} \approx 3.353$ due to Theorem 1.



FIGURE 1. Threshold function $f_{\gamma,n}$ from Example 5 for $\eta = 0$, $\sigma = 1$, and $\alpha = 0.05$.

We observe from Figure 1 that the power of the test with a weight function having γ close to 1/2 is higher for early and late changes. In the case of a change in the middle, the test with $\gamma = 0$ has a higher power than the one with γ close to 1/2.

Remark 6. The construction of change-point tests in more complicated time series models, e.g., with a serial dependence, may also be based on CUSUM statistics and quantiles of S(X) for suitable processes X. See Aue and Horváth (2013) for models that lead to X = w|B| with weight functions w, or to $X = \sum_{j=1}^{\ell} B_j^2$ with independent standard Brownian bridges B_j . More generally, see Aue, Rice, and Sönmez (2018) for functional time series models that lead to $X = \sum_{j=1}^{\infty} \lambda_j B_j^2$ with non-negative scalars λ_j . Our approach in Section 5 can easily be adapted to these classes of processes.

3. Approximation of the Supremum of a Brownian Motion

In this section we discuss the strong (or pathwise) approximation of the supremum S(W) of a standard Brownian motion $W = (W(t))_{t \in [0,1]}$ on the unit interval. We consider algorithms A that evaluate W at a finite number of points $t_k \in [0,1]$ and approximate S(W) by the discrete maximum of W at these points. The error e(A) of any such measurable algorithm A is defined by

$$e(A) = \mathrm{E}\left(|S(W) - A(W)|\right).$$

We recall known results that demonstrate that suitable adaptive algorithms, i.e., algorithms that sequentially evaluate any trajectory of W, are far superior to non-adaptive algorithms, i.e., algorithms that are based on a fixed, a priori given discretization of [0, 1].

At first we consider the class of all non-adaptive algorithms that use n evaluations of W. The following result is due to Ritter (1990).

Theorem 7. There exist constants $c_1, c_2 > 0$ with the following properties for every $n \in \mathbb{N}$. The algorithm A_n^{eq} given by

$$A_n^{\rm eq}(W) = \max_{k=1,\dots,n} W(k/n)$$

satisfies

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(2)
$$e(A_n^{\text{eq}}) \le c_1 \cdot n^{-1/2}.$$

For every choice of $t_1, \ldots, t_n \in [0,1]$ the algorithm A_n^{non} given by

$$A_n^{\mathrm{non}}(W) = \max_{k=1,\dots,n} W(t_k)$$

satisfies

(3)
$$e(A_n^{\operatorname{non}}) \ge c_2 \cdot n^{-1/2}.$$

For the purpose of this paper the crucial part of Theorem 7 is the lower bound (3), which says that non-adaptive algorithms achieve at most the order of convergence 1/2. This lower bound is sharp, up to constants, as we have a matching upper bound (2), which is already achieved by an equidistant discretization.

Remark 8. We conjecture that the lower bound (3) is also valid for algorithms A_n^{non} of the form $A_n^{\text{non}}(W) = \zeta(W(t_1), \ldots, W(t_n))$, where $\zeta \colon \mathbb{R}^n \to \mathbb{R}$ is any measurable mapping. The conjecture is true at least if $t_k = k/n$, see Hefter and Herzwurm (2017, Prop. 2.1 and proof of Thm. 3.3), or if the L_2 -error of A_n^{non} is considered, instead of the L_1 -error $e(A_n^{\text{non}})$, see Calvin (2004, beginning of proof of Thm. 2.1).

The asymptotic distribution of the error $S(W) - A_n^{eq}(W)$ has been derived in Asmussen, Glynn, and Pitman (1995, Thm. 1).

An adaptive algorithm A_n^{ad} that uses *n* evaluations of the Brownian motion *W* is formally defined by a point $t_1 \in [0, 1]$ and Borel-measurable mappings

$$\chi_k \colon \mathbb{R}^{k-1} \to]0,1]$$

for k = 2, ..., n. Iteratively the algorithm computes $y_1 = W(t_1)$ and

$$y_k = W(\chi_k(y_1, \dots, y_{k-1}))$$

for $k = 2, \ldots, n$, and it yields the output

$$A_n^{\mathrm{ad}}(W) = \max_{k=1,\dots,n} y_k.$$

In this way the k-th evaluation site $\chi_k(y_1, \ldots, y_{k-1})$ may depend on the previously obtained values y_1, \ldots, y_{k-1} (and the corresponding evaluation sites). Of course, the non-adaptive algorithms, which are considered in Theorem 7, correspond to the particular case of constant mappings χ_k .

The following result is due to Calvin, Hefter, and Herzwurm (2017).

Theorem 9. There exists a sequence of adaptive algorithms A_n^{ad} with the following property. For every $\rho > 0$ there exists a constant c > 0 such that for every $n \in \mathbb{N}$

$$e(A_n^{\mathrm{ad}}) \le c \cdot n^{-\rho}.$$

We refer to Calvin, Hefter, and Herzwurm (2017) for the construction of the algorithms $A_n^{\rm ad}$ that are considered in Theorem 9; see also Section 4 for basic ideas.

According to Theorem 9 suitable adaptive algorithms achieve, roughly speaking, the polynomial order of convergence ∞ . Combining Theorems 7 and 9 we see that adaptive algorithms strikingly outperform all non-adaptive algorithms for the strong approximation of the supremum S(W) of a Brownian motion.

Of course, Theorems 7 and 9 are irrelevant for the computation of quantiles of S(W), since the distribution of S(W) is known explicitly. The theorems strongly suggest, however, that adaptive algorithms should be considered for quantile computation if (semi-)analytic methods are not available. The latter holds true for the processes $w_{\eta,\gamma}|B|$ with $\gamma \notin \{0, 1/2\}$, see Section 2.

4. Approximation of the Supremum of a Weighted Reflecting Brownian Bridge

For notational convenience we put

$$w = w_{\eta,\gamma},$$

where $(\eta, \gamma) \neq (0, 1/2)$.

4.1. The Adaptive Algorithm. In this section we present an adaptive algorithm for the strong approximation of the supremum S(w|B|) of the weighted reflecting Brownian bridge w|B|. This algorithm is a modification of the algorithm constructed in Calvin, Hefter, and Herzwurm (2017), which achieves the error bound in Theorem 9 for the strong approximation of the supremum S(W) of a standard Brownian motion W.

Both of these adaptive algorithms are greedy algorithms, and the basic idea in the construction is as follows. After the k-th step the algorithm has computed a partition of the interval [0, 1] into k subintervals together with the values of the underlying stochastic process at the boundary points of all these intervals. A score value is available for each subinterval, and the subinterval with the highest score will be split at the midpoint. Ideally, the score value should be the conditional probability that the corresponding subinterval contains a global maximizer of w|B|. Reasonable substitutes for these conditional probabilities are needed in the computation.

In the sequel we present the algorithm for the strong approximation of S(w|B|)in detail. Based on the weight function w we assign a weight $v(\ell, r)$ to any interval $[\ell, r] \subseteq [0, 1]$ with positive length in the following way. Let

$$c = \frac{\ell + r}{2}.$$

For a weight function w that is positive and differentiable with a 'small' derivative everywhere on]0, 1[it is reasonable to take $v(\ell, r) = w(c)$. Since these conditions are not met for $w = w_{\eta,\gamma}$, except for the trivial case $(\eta, \gamma) = 0$, we proceed differently. To avoid a too small score value we take

$$v(\ell, r) = \begin{cases} 0, & \text{if } [\ell, r] \subseteq [0, \eta] \cup [1 - \eta, 1], \\ (c \cdot (1 - c))^{-\gamma}, & \text{otherwise.} \end{cases}$$

In fact, observe that $v(\ell, r) \neq w(c)$ if and only if $c \leq \eta < r$ or $\ell < 1 - \eta \leq c$. If $v(\ell, r) \neq w(c)$, then w(c) = 0 while $v(\ell, r)$ may potentially be very large.

Suppose that $x = B(\ell)$ and y = B(r) are known, while no values of B are known inside of $]\ell, r[$. It is reasonable to compare $v(\ell, r) \cdot B(c)$ with a certain threshold m, e.g., with the largest value of w|B| known so far, under the conditional distribution of B(c). The latter is the normal distribution with mean (x + y)/2 and variance $(r - \ell)/4$. More precisely, we define the score function

$$\varphi \colon D \times \mathbb{R}^2 \times [0, \infty[\to [0, \infty[$$

by

$$\varphi(\ell, r, x, y, m) = \mathbf{E}\left((v(\ell, r) \cdot Z - m)^+\right) + \mathbf{E}\left((v(\ell, r) \cdot Z + m)^-\right),$$

where

$$D = \{(\ell, r) \in [0, 1]^2 : \ell < r\}$$

and

$$Z \sim N((x+y)/2, (r-\ell)/4).$$

Remark 10. The score function is easily computed as follows. Let Φ denote the distribution function of $Y \sim N(0, 1)$, and let $a \in \mathbb{R}$. Put

$$\psi(a) = \Phi'(a) + a \cdot \Phi(a).$$

Since $E((Y+a)^+) = \psi(a)$, we obtain

$$\begin{split} \varphi(\ell, r, x, y, m) \\ &= v(\ell, r) \cdot \frac{\sqrt{r-\ell}}{2} \cdot \left(\psi\left(\frac{x+y-2m/v(\ell, r)}{\sqrt{r-\ell}}\right) + \psi\left(-\frac{x+y+2m/v(\ell, r)}{\sqrt{r-\ell}}\right) \right) \end{split}$$

if $v(\ell, r) > 0$. Otherwise $\varphi(\ell, r, x, y, m) = 0$, since $m \ge 0$.

To avoid rounding errors in the evaluation of ψ one may use

$$\lim_{a \to \infty} \frac{\psi(a)}{a} = 1$$

and

$$\lim_{a \to -\infty} \frac{\psi(a)}{a^{-2} \cdot \Phi'(a)} = 1.$$

We use this asymptotic behavior for |a| > 3, i.e., we replace ψ by

$$\widetilde{\psi}(a) = \begin{cases} a, & \text{if } a > 3, \\ a^{-2} \cdot \Phi'(a), & \text{if } a < -3, \\ \psi(a), & \text{otherwise,} \end{cases}$$

in the computation of $\varphi(\ell, r, x, y, m)$.

We are ready to define the adaptive algorithm, which will be denoted by $A_n^{\mathrm{ad}}(w, \cdot)$. The algorithm will sequentially evaluate any trajectory of B, and the relevant information about the corresponding partition of [0, 1] after k steps is represented by a set \mathcal{I}_k as follows. There are k elements in \mathcal{I}_k , which correspond to the k subintervals in this partition. More precisely, $(\ell, r, x, y, s) \in \mathcal{I}_k$ represents a subinterval $[\ell, r]$ with boundary values $x = B(\ell)$ and y = B(r) and with score value s. Furthermore, $m_k \geq 0$ denotes the discrete maximum of w|B| after k steps. In the first step we put

$$m_1 = 0,$$
 $\mathcal{I}_1 = \{(0, 1, 0, 0, \varphi(0, 1, 0, 0, m_1))\}.$

In the k-th step with $2 \leq k \leq n$ we choose any $I = (\ell, r, x, y, s) \in \mathcal{I}_{k-1}$ with the maximal value of s among all elements of \mathcal{I}_{k-1} , i.e., with the largest score value (this choice needs not to be unique), and we evaluate B at the midpoint of the corresponding subinterval, i.e., we compute

$$z = B(c)$$

The new discrete maximum of w|B| is given by

$$m_k = \max\left(m_{k-1}, w(c) \cdot |z|\right),$$

and the new partition is represented by

$$\mathcal{I}_k = (\mathcal{I}_{k-1} \setminus \{I\}) \cup \{I_1, I_2\}$$

with

$$I_1 = (\ell, c, x, z, \varphi(\ell, c, x, z, m_k)), \qquad I_2 = (c, r, z, y, \varphi(c, r, z, y, m_k)).$$

After n steps the adaptive algorithm returns the output

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$$A_n^{\mathrm{ad}}(w,B) = m_n$$

Remark 11. We discuss the computational cost to simulate $A_n^{\mathrm{ad}}(w, B)$. First of all, we use a max-priority queue for storing the elements of the sets $\mathcal{I}_1, \ldots, \mathcal{I}_n$. This allows to choose $(\ell, r, x, y, s) \in \mathcal{I}_{k-1}$ with the maximal value of s at a cost of order $\ln(k)$ in the k-th step, see Cormen, Leiserson, Rivest, and Stein (2003, Sec. 6.5). Thereafter B(c) may be simulated at a constant cost, independently of k, under the conditional distribution. By definition, no updates of the score values are computed for the elements in $\mathcal{I}_k \cap \mathcal{I}_{k-1}$, although m_k may be larger than m_{k-1} . It follows that the total cost to simulate $A_n^{\mathrm{ad}}(w, B)$ is of the order $n \ln(n)$.

4.2. Numerical Experiments. We compare the adaptive algorithm $A_n^{\text{ad}}(w, \cdot)$ and the non-adaptive algorithm $A_n^{\text{eq}}(w, \cdot)$ given by

$$A_n^{\text{eq}}(w, B) = \max_{k=1,...,n-1} w(t_k) \cdot |B(t_k)|$$

with $t_k = k/n$, which has been used by, e.g., Eastwood and Eastwood (1998) and Orasch and Pouliot (2004), and for a similar problem by Akashi, Dette, and Liu (2018).

Analogously to Section 3 we consider the error

(4)
$$e(A_n(w, \cdot)) = \operatorname{E}\left(|S(w|B|) - A_n(w, B)|\right)$$

for $A_n(w, \cdot) = A_n^{\mathrm{ad}}(w, \cdot)$ and $A_n(w, \cdot) = A_n^{\mathrm{eq}}(w, \cdot)$. We add that exact values or upper or lower bounds of the error are not available for any of these algorithms. Therefore we determine the error via a Monte Carlo simulation, where we replace S(w|B|) in (4) by $A_{n_0}^{\mathrm{ad}}(w, B)$ or $A_{n_0}^{\mathrm{eq}}(w, B)$, respectively, with n_0 being 10 times larger than the largest value of n that is considered in the numerical experiment. Simultaneously, we determine the average run-time of both algorithms. For each value of n we use 10^3 Monte Carlo replications.



FIGURE 2. Average run-time vs. number n of discretization points for the strong approximation of S(w|B|).

All programs are written in C++, and the computations are performed on a single Intel Xeon Gold 6126 processor. All results are presented together with asymptotic confidence intervals with confidence level 0.95. In the numerical experiments we consider $\eta = 0$ and $\gamma = 0.25$ or $\gamma = 0.45$, cf. Example 5.

In Figure 2 we relate the average run-time to the number n of discretization points. For $n \leq 10^4$ the computational overhead due to adaption is moderate, as the non-adaptive algorithm is at most 10 times faster than the adaptive algorithm in this range. Furthermore, the average run-times for both algorithms are in line with the worst case behavior, namely, order $n \ln(n)$ for $A_n^{\rm ad}(w, \cdot)$, see Remark 11, and order n for $A_n^{\rm eq}(w, \cdot)$. Finally, we see that the average run-time does not depend on γ .

The relation between the error and the average run-time, which is most important, is presented in Figure 3. First of all, we observe a polynomial order of convergence ∞ for the adaptive algorithm, in contrast to a polynomial order of convergence of only about 1/2 for the non-adaptive algorithm. This is in line with the corresponding theoretical results for Brownian motion, see Theorem 7 and Theorem 9. We add that the confidence intervals regarding time are rather small and therefore not visible. As to be expected, a stronger singularity of the weight function, i.e., a larger value of γ , deteriorates the speed of convergence for both algorithms. For the same average run-time of 10^{-2} seconds the adaptive algorithm achieves an error of less than 10^{-8} for both values of γ , while the error of the non-adaptive algorithm is about 10^{-2} . For quantile computation we may therefore sample almost from the correct distribution by means of the adaptive algorithm with a reasonable average run-time, while this is impossible by means of the non-adaptive algorithm.

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FIGURE 3. Error given by (4) vs. average run-time for the strong approximation of S(w|B|).

5. QUANTILE COMPUTATION FOR A WEIGHTED REFLECTING BROWNIAN BRIDGE

In this section we present an algorithm for the computation of the q-quantile of S(w|B|). The inputs of this algorithm, which will be denoted by $Q_{\varepsilon}^{\mathrm{ad}}(w,q)$, are the weight w, i.e., η and γ , as well as 0 < q < 1 and an error tolerance $\varepsilon > 0$. The key ingredient is the algorithm $A_n^{\mathrm{ad}}(w, \cdot)$ from Section 4. Our construction is rather ad hoc and many improvements are possible. We mainly want to demonstrate the potential of using an adaptive algorithm as the building block for quantile computation.

5.1. The Algorithm. The algorithm $Q_{\varepsilon}^{\mathrm{ad}}(w,q)$ starts with a precomputing step in order to ideally determine the minimal integer $n_0 \in \mathbb{N}$ such that

$$e(A_{n_0}^{\mathrm{ad}}(w,\cdot)) \leq \varepsilon.$$

Due to the fast convergence of $A_n^{\mathrm{ad}}(w, B)$ towards the supremum S(w|B|), which has been observed in the numerical experiments in Section 4, we use $E(\Delta_n)$ with

$$\Delta_n = |A_{2n}^{\mathrm{ad}}(w, B) - A_n^{\mathrm{ad}}(w, B)|$$

as an approximation to $e(A_n^{\mathrm{ad}}(w, \cdot))$. Moreover, we use a simple Monte Carlo algorithm $X_n^{(m)}$ with *m* independent samples of Δ_n to approximate the expectation $E(\Delta_n)$. In the precomputing step we take

$$m = 10^3$$
,

and we compute the minimal integer $n_0 \in \mathbb{N}$ of the form

$$n_0 = 10 \cdot 2^i$$

with $i \in \mathbb{N}_0$ such that

 $X_{n_0}^{(m)} \le \varepsilon.$

If no such n_0 exists, then the output of the algorithm $Q_{\varepsilon}^{\mathrm{ad}}(w,q)$ is undefined. We add that this happens with probability zero if, as we conjecture, $\Delta_n \xrightarrow{p} 0$.

In the second step we generate a certain number k_0 of independent samples of $A_{n_0}^{\rm ad}(w, B)$, which are independent from the precomputing step, too. The choice of this number is motivated by the following fact.

Remark 12. Consider iid random variables Y_1, Y_2, \ldots with a continuous density function f. Assume that $f(F^{-1}(q)) > 0$ for the q-quantile $F^{-1}(q)$ of Y_1 , and let $Z_{q,k}$ denote the $\lceil q \cdot k \rceil$ -th order statistic of Y_1, \ldots, Y_k . Then

$$c_q \cdot \sqrt{k} \cdot (Z_{q,k} - F^{-1}(q)) \xrightarrow{d} Z$$

with $Z \sim N(0, 1)$ and

$$c_q = \frac{f(F^{-1}(q))}{\sqrt{q \cdot (1-q)}},$$

see, e.g., David and Nagaraja (2003, Thm. 10.3).

Replacing the unknown constant c_q from Remark 12 by one, we take

$$k_0 = \lceil \varepsilon^{-2} \rceil$$

samples of $A_{n_0}^{\mathrm{ad}}(w, B)$, and the algorithm $Q_{\varepsilon}^{\mathrm{ad}}(w, q)$ returns the $\lceil q \cdot k_0 \rceil$ -th order statistic of these samples.

The following fact may be used to compute confidence intervals for the q-quantile of $A_{n_0}^{\mathrm{ad}}(w, B)$, which yields a quality control for the second step. Observe, however, that the precomputing step does not yield a rigorous link to the q-quantile of S(w|B|).

Remark 13. Consider iid random variables Y_1, \ldots, Y_k , and let $Y_{(i)}$ the corresponding *i*-th order statistic. Furthermore, let $0 < \alpha < 1$, and assume that $a, b \in \{1, \ldots, k\}$ with a < b satisfy

$$P(\{Z \in \{a, \dots, b-1\}\}) \ge 1 - \alpha,$$

where Z is binomially distributed with parameters k and q. Then $[Y_{(a)}, Y_{(b)}]$ is a (conservative) confidence interval for the q-quantile of Y_1 with confidence level $1 - \alpha$, see, e.g., David and Nagaraja (2003, Sec. 7.1).

5.2. Numerical Experiments. We compare the algorithm $Q_{\varepsilon}^{\mathrm{ad}}(w,q)$ and an algorithm $Q_{\varepsilon}^{\mathrm{eq}}(w,q)$ that is constructed as $Q_{\varepsilon}^{\mathrm{ad}}(w,q)$, but instead of $A_n^{\mathrm{ad}}(w,\cdot)$ the non-adaptive algorithm $A_n^{\mathrm{eq}}(w,\cdot)$ is used as the building block. Furthermore, in the precomputing step of $Q_{\varepsilon}^{\mathrm{eq}}(w,q)$ we fully use the findings from Figures 2 and 3 for free in order to determine the value of n_0 . This comes very close to choosing exactly and at no computational cost the minimal integer $n_0 \in \mathbb{N}$ such that $e(A_{n_0}^{\mathrm{eq}}(w,\cdot)) \leq \varepsilon$, and thus is very much in favor of $Q_{\varepsilon}^{\mathrm{eq}}(w,q)$ compared to of $Q_{\varepsilon}^{\mathrm{ad}}(w,q)$.

We consider the error

(5)
$$e(Q_{\varepsilon}(w,q)) = \mathbf{E}\left(\left|F^{-1}(w,q) - Q_{\varepsilon}(w,q)\right|\right)$$

for $Q_{\varepsilon}(w,q) = Q_{\varepsilon}^{\mathrm{ad}}(w,q)$ and $Q_{\varepsilon}(w,q) = Q_{\varepsilon}^{\mathrm{eq}}(w,q)$, where $F^{-1}(w,q)$ denotes the q-quantile of S(w|B|).

We proceed as in the previous section. The only difference is that a deterministic quantity, $F^{-1}(w,q)$, instead of a random variable, S(w|B|), is unknown in the definition of the error.

The error $e(Q_{\varepsilon}(w,q))$ and the average run-time are determined via a Monte Carlo simulation, where we use 10^2 replications for each value of ε , and the results are presented together with asymptotic confidence intervals as before. We also use the same set of parameters η and γ , the same hardware system, and the same programming language as before. The value of q is chosen as q = 0.95. In the Monte Carlo simulation we replace $F^{-1}(w,q)$ by a highly accurate approximation, namely 2.0008 for $\gamma = 0.25$ and 2.9222 for $\gamma = 0.45$. The latter is obtained as the $\lceil q \cdot k_0 \rceil$ -th order statistic of k_0 samples of $A_{n_0}^{\rm ad}(w,B)$, where $n_0 = 10^3$ and where k_0 is close to $4 \cdot 10^8$. According to the findings from Section 4 the distributions of $A_{n_0}^{\rm ad}(w,B)$ and S(w|B|) should almost coincide for this value of n_0 . Furthermore, using Remark 13 with confidence level 0.99, we have obtained the confidence intervals [2.0006, 2.0010] for $\gamma = 0.25$ and [2.9220, 2.9224] for $\gamma = 0.45$. We add that this master computation has required a run-time of about three weeks for each value of γ .

In Figure 4 we relate the actual error to the error tolerance ε . We see that both algorithms almost perfectly achieve the computational goal, namely, an error close to the input ε .



FIGURE 4. Error given by (5) vs. error tolerance ε for the quantile approximation of S(w|B|) with q = 0.95.

As for the strong approximation, the relation between the error and the average run-time is most important, see Figure 5 for the results. For $Q_{\varepsilon}^{\rm ad}(w,q)$ we observe a polynomial order of convergence of about 1/2, while the corresponding order for $Q_{\varepsilon}^{\rm eq}(w,q)$ is only about 1/4. This corresponds to the findings from Section 4 and to Remark 12: The orders of convergence of $A_n^{\rm ad}(w,\cdot)$ and $A_n^{\rm eq}(w,\cdot)$ for the strong approximation of S(w|B|) are given by ∞ and 1/2, respectively, see Figure 3, and the order of convergence for the quantile approximation should be 1/2, see Remark 12.

The algorithm $Q_{\varepsilon}^{\mathrm{ad}}(w,q)$ achieves an error 10^{-2} in 5 seconds for $\gamma = 0.25$ and in 12 seconds for $\gamma = 0.45$, and even an error 10^{-3} in less than 15 or 35 minutes, respectively. The algorithm $Q_{\varepsilon}^{\mathrm{eq}}(w,q)$ achieves the error 10^{-2} in 2 minutes for $\gamma =$ 0.25 and (based on a extrapolation beyond the range of our numerical experiment) in more than 2 hours for $\gamma = 0.45$; the corresponding run-times for the error 10^{-3} are 6 days and 6 years, respectively.



FIGURE 5. Error given by (5) vs. average run-time for the quantile approximation of S(w|B|) with q = 0.95.

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