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High-order Coverage of Smoothed Bayesian Bootstrap Intervals for Population Quantiles

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Abstract

We characterize the high-order coverage accuracy of smoothed and unsmoothed Bayesian bootstrap confidence intervals for population quantiles. Although the original (Rubin 1981) unsmoothed intervals have the same $O(n^{-1/2})$ coverage error as the standard empirical bootstrap, the smoothed Bayesian bootstrap of Banks (1988) has much smaller $O(n^{-3/2}[\log(n)]^3)$ coverage error and is exact in special cases, without requiring any smoothing parameter. It automatically removes an error term of order $1/n$ that other approaches need to explicitly correct for. This motivates further study of the smoothed Bayesian bootstrap in more complex settings and models.

Keywords: continuity correction, fractional order statistics.

1. Introduction

We study the frequentist coverage accuracy of certain Bayesian bootstrap confidence intervals for population quantiles. Specifically, we consider percentile method intervals using the Bayesian bootstrap (BB) of Rubin (1981) and the continuity-corrected Bayesian bootstrap (CCBB) of Banks (1988).

Although the BB has the same order of coverage error as the conventional nonparametric bootstrap, the CCBB is substantially more accurate. Specifically, the BB has $O(n^{-1/2})$ coverage error, whereas CCBB has $O(n^{-3/2}[\log(n)]^3)$. Because the nonparametric bootstrap shares the same $O(n^{-1/2})$ error as BB (e.g., Falk and Kaufmann 1991), and both are special cases of exchangeable weights bootstrap, we do not study nonparametric bootstrap, instead focusing on the large improvement of CCBB over BB. Unlike other smoothed bootstraps, the CCBB does not have any smoothing parameter, so this error rate depends only on iid sampling and mild smoothness conditions on the population distribution. Further, the CCBB is exact for intervals with order statistic endpoints or when the population distribution is uniform.

Although other confidence intervals for quantiles achieve the same accuracy, our results motivate further study of the CCBB in other settings to which it may generalize more readily. For quantiles, the accuracy is matched by Ho and Lee (2005) and Goldman and Kaplan (2017), who provide calibrated versions of the order statistic-based intervals in Beran and Hall (1993) and Hutson (1999), respectively. These calibrations explicitly remove an error term of order $1/n$ that the CCBB automatically avoids. Notwithstanding some extensions of fractional order statistic-based confidence intervals to more complex quantile-based objects of interest (Goldman and Kaplan 2018b,a), the CCBB may be more readily generalized to other objects of interest or non-iid sampling.

Extension to linear quantile regression remains an interesting open question. For nonparametric inference on conditional quantiles, the CCBB can be used as in Definition 3 of Goldman and Kaplan (2017), with theoretical properties matching those of their calibrated interval in their Theorem 6. Their framework defines a local sample based on the independent variables' values, after which only dependent variable observations are used, thus reducing the computation to unconditional scalar quantile analysis. In contrast, linear quantile regression must consider both dependent and independent variables together, so each observation remains a vector. BB extends naturally, but it is not clear how CCBB should extend to smoothing multivariate CDFs. Anderson (1966) proposes a way to construct multi-dimensional "statistically equivalent blocks," as noted by Banks (1988, Ex. 4, p. 677). These blocks satisfy a generalization of the probability integral transform, but they are not as closely related to the multivariate BB as the univariate CCBB and BB are to each other. There is also some sensitivity to the assumed support; such sensitivity is mostly absent from the univariate quantile setting because (central) quantiles are not sensitive to the extreme tails of the distribution, whereas linear quantile regression is indeed sensitive to the tails of the independent variables' distributions. Possibly such sensitivity disappears if using a type of regression more robust (to outliers) than quantile regression, like the least median of squares regression of Rousseeuw (1984). We have also considered smoothing over each region on which the BB CDF is flat, but this seems to make a first-order difference, whereas the univariate CCBB is a higher-order refinement of the BB.

Other papers have examined accuracy of CCBB and related intervals for quantiles, but without our theoretical results on coverage error. Examples include Breth (1979), Banks (1988), and Meeden (1993), who proposes a grid-based alternative to CCBB that maintains a Bayesian interpretation (unlike CCBB).

Section 2 introduces the intervals. Sections 3 and 4 contain theoretical results. Section 5 illustrates the theory with simulations. Appendix A contains proofs.

Notation Vectors are bold; e.g., the sample is $\mathbf{Y} = (Y_1, \ldots, Y_n)$. Also, $\mathbb{1}\{\cdot\}$ is the indicator function, $\mathrm{Q}_\tau(Y)$ is the τ-quantile of random variable Y whose CDF is $F_Y(\cdot)$, and $\mathrm{P}(\cdot)$ is probability; additional notation is defined as needed. Acronyms used include those for Bayesian bootstrap (BB), confidence interval (CI), continuity-corrected Bayesian bootstrap (CCBB), coverage probability (CP), cumulative distribution function (CDF), and probability density function (PDF). Let $F_\beta(p; a, b)$ and $f_\beta(p; a, b)$ respectively denote the CDF and PDF of a $\mathrm{Beta}(a, b)$ distribution evaluated at p.

2. Setup

2.1. Assumptions

Assumptions A1 and A2 describe the setting. Assumption A1 describes the sampling and object of interest and is used for all our results. Assumption A2 is an additional smoothness assumption required for our most general results. It is the same as Assumption A2 of Goldman and Kaplan (2017).

Assumption A1. Observations Y_i are iid realizations of random variable Y with continuous CDF $F_Y(\cdot)$, and interest is in the τ-quantile, $\mathrm{Q}_\tau(Y) \equiv \inf\{y : F_Y(y) \geq \tau\}$, for fixed $\tau \in (0, 1)$. The sample of size n contains $Y_1, \ldots, Y_n$.

Assumption A2. i) $F_Y'(\mathrm{Q}_\tau(Y)) > 0$; ii) $F_Y'''(\cdot)$ exists and is continuous in a neighborhood of $\mathrm{Q}_\tau(Y)$.

Notationally, let the order statistics (i.e., ordered sample values) be

$$Y_{n:1} \leq Y_{n:2} \leq \cdots \leq Y_{n:n}. \tag{1}$$

Given the continuity of $F_Y(\cdot)$ in A1, the inequalities become strict with probability 1. For notational completion, let $Y_{n:0}$ and $Y_{n:n+1}$ denote the lower and upper bounds of the support of Y, but these only affect CCBB inference on extreme quantiles, which we do not consider.

2.2. Bootstrap distributions

The bootstrap distributions are conditional on the data $\mathbf{Y} = (Y_1, \ldots, Y_n)$, with the randomness coming from a vector of weights. The standard (empirical) bootstrap that resamples with replacement can equivalently be seen as drawing a multinomial-distributed vector of weights (each of which is a non-negative integer) and applying the weights to the original $Y_1, \ldots, Y_n$, where the weights are independent of the sample values. Instead of focusing on the resampled values, we can think of the empirical distribution corresponding to such values. That is, instead of resampling a bootstrap dataset $Y_1^*, \ldots, Y_n^*$ and computing the corresponding statistic (like the τ-quantile), it can be interpreted as randomly drawing multinomial $(\tilde{W}_1, \ldots, \tilde{W}_n)$ and computing the statistic based on the weighted empirical CDF

$$\widehat{F}^*(y) = \frac{1}{n}\sum_{i=1}^{n} \tilde{W}_i \, \mathbb{1}\{Y_i \leq y\} = \sum_{i=1}^{n} W_i \, \mathbb{1}\{Y_i \leq y\}, \quad W_i \equiv \tilde{W}_i/n.$$

The BB replaces the multinomial-based weights W_i with Dirichlet-based weights. Given sample size n,

$$\mathbf{W} \equiv (W_1, \ldots, W_n) \sim \text{Dir}(1, \ldots, 1), \tag{2}$$

a Dirichlet distribution with all n parameters equal to 1, i.e., a uniform distribution over the unit $(n-1)$-simplex. The corresponding CDF is

$$\widehat{F}_{*u}(y) = \sum_{i=1}^{n} W_i \, \mathbb{1}\{Y_{n:i} \leq y\}, \tag{3}$$

where the u subscript stands for "unsmoothed." The $Y_{n:i}$ could equivalently be replaced by Y_i, but (3) connects better with the CCBB. For intuition, note $\widehat{F}_{*u}(Y_{n:k}) = \sum_{i=1}^{k} W_i$.

The CCBB applies Dirichlet probability weights to intervals instead of points. There are $n+1$ intervals, from $Y_{n:k-1}$ to $Y_{n:k}$ for $k = 1, \ldots, n+1$; and thus $n+1$ weights, $(W_1, \ldots, W_{n+1}) \sim \text{Dir}(1, \ldots, 1)$, the Dirichlet distribution with all $n+1$ parameters equal to 1, i.e., a uniform distribution over the unit n-simplex. Instead of weight W_k corresponding to the kth point $Y_{n:k}$, now W_k corresponds to the kth interval, and the probability is spread uniformly over the interval. Instead of (3), this yields

$$\widehat{F}_{*s}(y) = \sum_{i=1}^{n+1} \left[W_i \, \mathbb{1}\{Y_{n:i} \leq y\} + W_i \frac{y - Y_{n:i-1}}{Y_{n:i} - Y_{n:i-1}} \mathbb{1}\{Y_{n:i} > y > Y_{n:i-1}\} \right], \tag{4}$$

where subscript s stands for "smoothed." Note the bounds $Y_{n:0}$ and $Y_{n:n+1}$ do not affect $\widehat{F}_{*s}(y)$ as long as $Y_{n:1} \leq y \leq Y_{n:n}$. For intuition, evaluating (4) at an order statistic yields

$$\widehat{F}_{*s}(Y_{n:k}) = \sum_{i=1}^{k} W_i,$$

which is also true of the unsmoothed version in (3): $\widehat{F}_{*u}(Y_{n:k}) = \sum_{i=1}^{k} W_i$. Instead of having discrete jumps, the CDF in (4) linearly interpolates between such points; it is a linear spline with knots at the sample values, which Banks (1988) calls "histospline smoothing" in allusion to Wahba (1975).

Consider the BB and CCBB distributions of the τ-quantile. Let

$$\widehat{Q}^*_{\tau,u} \equiv \inf\{y : \widehat{F}_{*u}(y) \geq \tau\}, \quad \widehat{Q}^*_{\tau,s} \equiv \inf\{y : \widehat{F}_{*s}(y) \geq \tau\}, \tag{5}$$

the τ-quantiles of the distributions defined in (3) and (4). Since the BB distributions are discrete, $\widehat{Q}^*_{\tau,u}$ must equal a sample value Y_i. In contrast, the CCBB CDF $\widehat{F}_{*s}$ is continuous and strictly increasing (with probability 1), so $\widehat{Q}^*_{\tau,s} = \widehat{F}^{-1}_{*s}(\tau)$, with a continuous distribution of $\widehat{Q}^*_{\tau,s}$. Conditional on the sample $\mathbf{Y}$ (but not the Dirichlet weights), $\widehat{Q}^*_{\tau,u}$ and $\widehat{Q}^*_{\tau,s}$ are random variables with respect to the distribution of the weights.

Distributions of various sums of the W_i follow from the general order statistic results of Wilks (1962, pp. 236–238). The CCBB distribution of $(W_1, \ldots, W_{n+1})$ matches the sampling distribution of standard uniform order statistic "spacings,"

$$(U_{n:1}, U_{n:2} - U_{n:1}, \ldots, U_{n:n} - U_{n:n-1}, 1 - U_{n:n}) \sim \mathrm{Dir}(1, \ldots, 1), \tag{6}$$

where the $U_{n:k}$ are order statistics based on $U_i \overset{iid}{\sim} \mathrm{Unif}(0,1)$, $i = 1, \ldots, n$. Further,

$$\begin{aligned} \text{BB: } W_1 + \cdots + W_k &\sim \mathrm{Beta}(k, n-k), \\ \text{CCBB: } W_1 + \cdots + W_k &\sim \mathrm{Beta}(k, n+1-k). \end{aligned} \tag{7}$$

2.3. Bootstrap intervals

The percentile method confidence intervals' endpoints come directly from quantiles of the distributions of the random variables in (5). For a one-sided $1-\alpha$ confidence interval, the BB lower endpoint is the α-quantile of $\widehat{Q}^*_{\tau,u}$, and the CCBB lower endpoint is the α-quantile of $\widehat{Q}^*_{\tau,s}$. The one-sided upper endpoints would instead be the $(1-\alpha)$-quantiles. A two-sided (equal-tailed) $1-\alpha$ interval instead takes the $\alpha/2$ and $1-\alpha/2$ quantiles of either $\widehat{Q}^*_{\tau,u}$ (for BB) or $\widehat{Q}^*_{\tau,s}$ (for CCBB).

We consider percentile method confidence intervals for two reasons. First, interpreting the BB distribution as a Bayesian posterior given the model of Ferguson (1973) with an improper Dirichlet process prior, the corresponding Bayesian credible interval is exactly the percentile method confidence interval. Second, even for the standard bootstrap, Falk and Kaufmann (1991) show that percentile intervals (the "backward method") perform better for quantiles.

3. Results for order statistic endpoints

Theorem 1 characterizes the BB and CCBB probabilities associated with one-sided confidence intervals whose lower endpoint is an order statistic. The unsmoothed part of Theorem 1 is similar to a result from Efron (1982, p. 82, eqn. (10.23)). The proof uses the equivalence $Y_{n:k} < \widehat{Q}^*_{\tau,u} \iff \sum_{i=1}^{k} W_i < \tau$ along with (7).

Theorem 1. *Under Assumption A1, given (3)–(5), for $k = 1, \ldots, n$,*

$$\begin{aligned} \mathrm{P}(Y_{n:k} < \widehat{Q}^*_{\tau,u} \mid \mathbf{Y}) &= F_\beta(\tau; k, n-k) < \mathrm{P}(Y_{n:k} \leq \widehat{Q}^*_{\tau,u} \mid \mathbf{Y}) = F_\beta(\tau; k-1, n+1-k), \\ \mathrm{P}(Y_{n:k} < \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) &= \mathrm{P}(Y_{n:k} \leq \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) = F_\beta(\tau; k, n+1-k) = \mathrm{P}(Y_{n:k} \leq \mathrm{Q}_\tau(Y)). \end{aligned}$$

The main point of Theorem 1 is that the CCBB probability of $Y_{n:k} \leq \widehat{Q}^*_{\tau,s}$ under $\widehat{F}_{*s}$ (conditional on the data $\mathbf{Y}$) is identical to the probability of $Y_{n:k} \leq \mathrm{Q}_\tau(Y)$ under F_Y. Thus, if the α-quantile of the CCBB distribution of $\widehat{Q}^*_{\tau,s}$ is $Y_{n:k}$ for some k, then $Y_{n:k}$ is the lower endpoint of the one-sided $1-\alpha$ CCBB confidence interval for $\mathrm{Q}_\tau(Y)$, and it has exact finite-sample coverage because $\mathrm{P}(Y_{n:k} \leq \mathrm{Q}_\tau(Y)) = \mathrm{P}(Y_{n:k} \leq \widehat{Q}^*_{\tau,s} \mid \mathbf{Y})$. Further, this is not true for BB.

The probabilities in Theorem 1 extend readily to lower one-sided and two-sided intervals because, for either $\hat{Q}^*_\tau = \hat{Q}^*_{\tau,u}$ or $\hat{Q}^*_\tau = \hat{Q}^*_{\tau,s}$,

$$\begin{aligned} \mathrm{P}(Y_{n:k} \geq \hat{Q}^*_\tau \mid \mathbf{Y}) &= 1 - \mathrm{P}(Y_{n:k} < \hat{Q}^*_\tau \mid \mathbf{Y}), \\ \mathrm{P}(Y_{n:k} \leq \hat{Q}^*_\tau \leq Y_{n:r} \mid \mathbf{Y}) &= \mathrm{P}(Y_{n:k} \leq \hat{Q}^*_\tau \mid \mathbf{Y}) - \mathrm{P}(Y_{n:r} < \hat{Q}^*_\tau \mid \mathbf{Y}). \end{aligned} \tag{8}$$

Corollary 1.1 characterizes the difference between the BB and CCBB probabilities in Theorem 1.

Corollary 1.1. *Given Theorem 1,*

$$\begin{aligned} \mathrm{P}(Y_{n:k} \leq \hat{Q}^*_{\tau,u} \mid \mathbf{Y}) - \mathrm{P}(Y_{n:k} \leq \hat{Q}^*_{\tau,s} \mid \mathbf{Y}) &= \frac{1-\tau}{n} f_\beta(\tau; k, n+1-k), \\ \mathrm{P}(Y_{n:k} \geq \hat{Q}^*_{\tau,u} \mid \mathbf{Y}) - \mathrm{P}(Y_{n:k} \geq \hat{Q}^*_{\tau,s} \mid \mathbf{Y}) &= (\tau/n) f_\beta(\tau; k, n+1-k). \end{aligned}$$

If $c_1 \leq k/n \leq c_2$ for constants $0 < c_1 < c_2 < 1$ as $n \to \infty$, then both differences are $O(n^{-1/2})$.

Corollary 1.1 shows the benefit of smoothing. For intervals with an order statistic endpoint $Y_{n:k}$, the CCBB probability is exact, whereas the BB probability differs by $O(n^{-1/2})$ for central order statistics ($c_1 \leq k/n \leq c_2$). If τ and $1-\alpha$ are fixed, then asymptotically the endpoint will be a central order statistic. Further, the right-hand sides in Corollary 1.1 are positive, so the BB always reports a probability higher than the true coverage probability. All else equal, this pushes BB confidence intervals in the direction of overcoverage.

4. Results for fractional order statistics

We now more generally consider "fractional" order statistic endpoints. This is useful when the desired nominal level (like 95%) is not attainable at an integer order statistic. For integer k and interpolation weight $\epsilon \in [0,1)$, the $(k+\epsilon)$th fractional order statistic is

$$Y_{n:k+\epsilon} \equiv Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}). \tag{9}$$

The special case with $\epsilon = 0$ yields the usual (integer) order statistics.

Figure 1 illustrates the following intuition for the CCBB distribution of $\hat{Q}^*_{\tau,s}$. Given the piecewise linear CDF smoothing of CCBB, the τ-quantile given a particular Dirichlet draw of $\mathbf{W}$ is also linearly interpolated. Given $(W_1, \ldots, W_{n+1})$,

$$\hat{Q}^*_{\tau,s} = Y_{n:c} + \frac{(\tau - \sum_{i=1}^c W_i)}{W_{c+1}}(Y_{n:c+1} - Y_{n:c}), \quad c \equiv \max\{d : \sum_{i=1}^d W_i \leq \tau\}, \tag{10}$$

i.e., c is the largest integer such that $\sum_{i=1}^c W_i \leq \tau$. That is, since the CCBB CDF linearly interpolates between the points

$$\hat{F}_{*s}(Y_{n:c}) = \sum_{i=1}^c W_i \text{ and } \hat{F}_{*s}(Y_{n:c+1}) = \sum_{i=1}^{c+1} W_i,$$

the CCBB inverse CDF (quantile function) $\hat{F}^{-1}_{*s}(\cdot)$ linearly interpolates between

$$Y_{n:c} = \hat{F}^{-1}_{*s}(\sum_{i=1}^c W_i) \text{ and } Y_{n:c+1} = \hat{F}^{-1}_{*s}(\sum_{i=1}^{c+1} W_i).$$

By inspection, (10) has the same form as (9), with $k = c$ and $\epsilon = (\tau - \sum_{i=1}^c W_i)/W_{c+1}$. Equation (10) can also be interpreted as moving along the straight line in the quantile function with slope $(Y_{n:c+1} - Y_{n:c})/W_{c+1}$, starting at value $Y_{n:c}$ and moving to the right by $\tau - \sum_{i=1}^c W_i$.

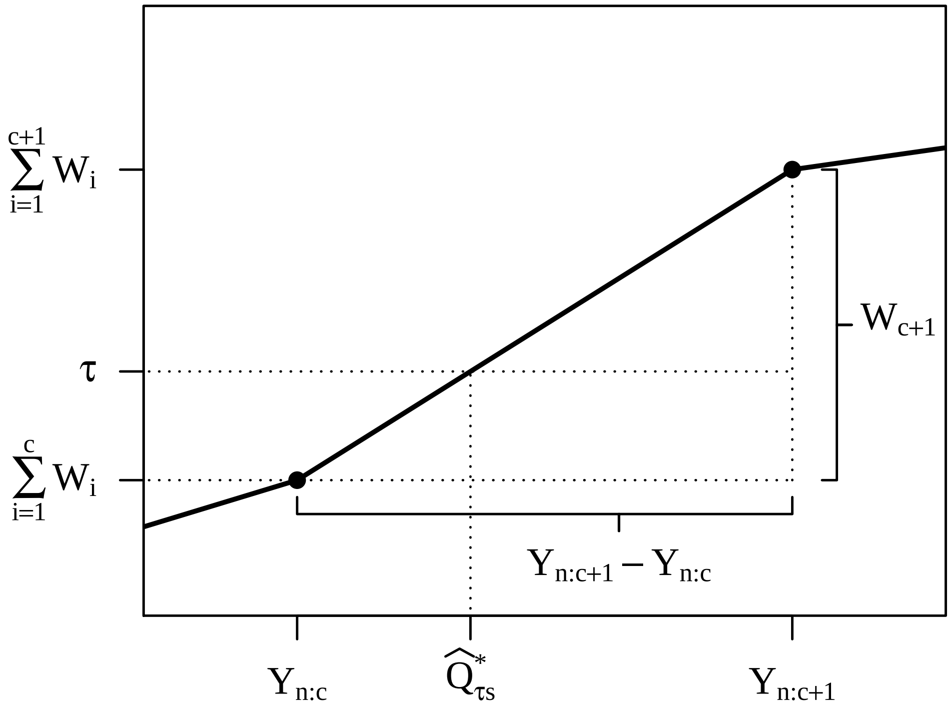

Figure 1: Illustration of (10).

We focus on fractional order statistics that would be CI endpoints given τ. For central quantiles (asymptotically fixed τ), given n, Lemma 3 of Goldman and Kaplan (2017) characterizes the k and ϵ (or equivalently u) that achieve $1-\alpha$ coverage probability. Specifically, their Lemma 3 says that a $1-\alpha$ one-sided CI lower endpoint satisfies

$$u \equiv (k+\epsilon)/(n+1) = \tau - n^{-1/2} z_{1-\alpha}\sqrt{\tau(1-\tau)} + O(n^{-1}), \tag{11}$$

where $z_{1-\alpha}$ is the $(1-\alpha)$-quantile of the standard normal distribution. Thus, Theorem 2 focuses on $u = \tau - dn^{-1/2}$.

Theorem 2 shows that the CCBB probability of fractional order statistic intervals is identical to the coverage probability in certain special cases, and more generally it matches up to a $O(n^{-3/2}[\log(n)]^3)$ difference. Thus, the $Y_{n:k+\epsilon}$ that is the α-quantile of the CCBB distribution of $\widehat{Q}^*_{\tau,s}$ provides a confidence interval with coverage probability $1-\alpha+O(n^{-3/2}[\log(n)]^3)$. Theorem 2 also provides an analytic approximation to the CCBB probability based on the beta distribution, up to the same error term. The BB distribution in Theorem 2 follows immediately from Theorem 1 since the BB distributions have no probability strictly between order statistics. As in Section 3, the results for a lower endpoint CI translate to an upper endpoint and two-sided CIs by (8).

Theorem 2. *Let Assumption A1 and (3)–(5) and (9) hold in each of the following.*

(i) *If* $(k+\epsilon)/(n+1) = \tau - dn^{-1/2}$, *then*

$$\begin{aligned}
\mathrm{P}(Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \widehat{Q}^*_{\tau,u} \mid \mathbf{Y}) &= F_\beta(\tau; k, n-k), \\
\mathrm{P}(Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) &= \mathrm{P}(U_{n:k} + \epsilon(U_{n:k+1} - U_{n:k}) < \tau) \\
&= F_\beta(\tau; k+\epsilon, n+1-k-\epsilon) \\
&\quad + n^{-1}\frac{\epsilon(1-\epsilon)}{\tau(1-\tau)}\frac{d}{\sqrt{\tau(1-\tau)}}\phi\Big(d/\sqrt{\tau(1-\tau)}\Big) \\
&\quad + O(n^{-3/2}[\log(n)]^3),
\end{aligned}$$

where $\phi(\cdot)$ is the standard normal PDF and (6) is the joint distribution of the $U_{n:k}$.

(ii) *If $Y \sim Unif(a, b)$, or if $\epsilon = 0$, then the CCBB and coverage probabilities are identical:*

$$\mathrm{P}(Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) = \mathrm{P}(Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \mathrm{Q}_\tau(Y)).$$

(iii) *If Assumption A2 holds, then*

$$\mathrm{P}(Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) = \mathrm{P}(Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \mathrm{Q}_\tau(Y)) + O(n^{-3/2}[\log(n)]^3).$$

Theorem 2 shows the close connection between CCBB and the confidence intervals from Hutson (1999) and Goldman and Kaplan (2017). Hutson (1999) selects $k + \epsilon$ to set $F_\beta(\tau; k + \epsilon, n + 1 - k - \epsilon) = 1 - \alpha$. This is the same beta CDF as in Theorem 2(i). Goldman and Kaplan (2017, Thm. 4) show this leaves an error in coverage probability equal to the n^{-1} term and remainder in Theorem 2(i), and they suggest adjusting α to remove the n^{-1} term. Here, the CCBB probability automatically captures the n^{-1} term, as well as the beta CDF term. Section 5 illustrates cases where this improved theoretical accuracy translates to better simulation performance, and cases where it does not.

Corollary 2.1 characterizes the difference between the BB and CCBB probabilities with fractional central order statistics, which is again $O(n^{-1/2})$ as in Corollary 1.1.

Corollary 2.1. *The difference between the BB and CCBB probabilities in Theorem 2(i) is $O(n^{-1/2})$ if $c_1 \le k/n \le c_2$ for constants $0 < c_1 < c_2 < 1$ as $n \to \infty$.*

5. Simulations

To illustrate our results, we simulate the coverage probability (CP) of four types of one-sided confidence intervals: BB; CCBB; "HGK" intervals proposed by Hutson (1999) and studied by Goldman and Kaplan (2017); and "GKc," the calibration proposed by Goldman and Kaplan (2017). Code in R (R Core Team 2020) to replicate the results is on the first author's website.[1]

We consider one-sided intervals (lower endpoint) with nominal level $1 - \alpha = 0.95$, setting $n = 18$ and letting τ and F_Y vary.

The different τ are chosen to illustrate different types of situations. Some τ are chosen so that HGK has an (integer) order statistic endpoint, in which case it has exact finite-sample CP, regardless of the underlying distribution F_Y. In such cases, CCBB also has exact CP, per Theorem 2(ii) (up to simulation error). Other τ are chosen so the HGK endpoint is roughly halfway between order statistics. This makes HGK coverage error larger because the leading term is proportional to $\epsilon(1 - \epsilon)$ (Goldman and Kaplan 2017, Thm. 4(i)), which is maximized at $\epsilon = 0.5$. Yet other τ are very close to 1, again to make HGK coverage error larger because the leading term is also inversely proportional to $\tau(1 - \tau)$. Two particularly extreme τ ($n\tau > n - 1$) are chosen to test the limits of our central quantile results. Because we examine one-sided confidence intervals with a lower endpoint, τ cannot get too close to zero, otherwise even the lowest order statistic (sample minimum) cannot achieve the desired coverage. The lower endpoint results would be identical to upper endpoint results after flipping the data distributions and changing τ to $1 - \tau$.

The different F_Y are also chosen to illustrate our theoretical results. Theorem 2(ii) says CCBB should provide exact finite-sample CP when F_Y is uniform, regardless of n, τ, or $1-\alpha$. For comparison, normal, exponential, and Cauchy distributions are also used. Although no method's $k + \epsilon$ depends on F_Y, the CP does depend on F_Y if $\epsilon > 0$.

5.1. Endpoint comparison

Table 1 compares the lower endpoints chosen by each method for each τ. Specifically, each confidence interval has the form $[Y_{n:k+\epsilon}, \infty)$, with $Y_{n:k+\epsilon} = Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k})$ as in (9),

[1] https://kaplandm.github.io

so Table 1 shows the $k + \epsilon$ chosen by each method. This $k + \epsilon$ depends on τ, but not F_Y; it also depends on n and $1 - \alpha$, but these do not vary across simulations.

Table 1: Fractional order statistic indices $(k + \epsilon)$ for the lower endpoint

n	τ	BB	CCBB	HGK	GKc
18	0.1600	1.00	1.13	1.07	1.12
18	0.1700	2.00	1.30	1.18	1.28
18	0.2000	2.00	1.66	1.53	1.69
18	0.2500	2.00	2.24	2.16	2.25
18	0.4978	6.00	5.99	6.00	6.00
18	0.9000	14.00	14.58	14.44	14.77
18	0.9799	17.00	17.00	17.00	17.00
18	0.9900	17.00	17.77	17.49	18.00

Nominal coverage $1-\alpha = 0.95$; CCBB uses 300,000 Dirichlet draws.

BB always has $\epsilon = 0$ and sets k as the largest integer such that $F_\beta(\tau; k-1, n+1-k) \geq 1-\alpha$, using Theorem 1. That is, when equality is impossible, we have BB try to err on the conservative side (overcoverage). If instead k were chosen to minimize the absolute coverage error $|F_\beta(\tau; k-1, n+1-k) - (1-\alpha)|$, then the undercoverage would be even worse and appear in more cases. Note that due to discreteness, BB chooses the same endpoint $Y_{n:2}$ for all $\tau \in [0.17, 0.25]$, whereas the other methods' endpoints increase continuously over that range.

HGK and GKc also determine $k+\epsilon$ with a beta CDF. HGK sets $1-\alpha = F_\beta(k+\epsilon, n+1-k-\epsilon)$ exactly, per (7) and (8) in Hutson (1999) or (3) and (5) in Goldman and Kaplan (2017). GKc uses the same formula after replacing α with $\alpha + n^{-1} z_{1-\alpha}\phi(z_{1-\alpha})\epsilon(1-\epsilon)/[\tau(1-\tau)]$, per (8) in Goldman and Kaplan (2017). (If the resulting k is larger than the HGK k, then GKc sets $\epsilon = 0$.)

CCBB requires simulation. Per Theorem 2(i), it sets $1-\alpha = \mathrm{P}(U_{n:k} + \epsilon(U_{n:k+1} - U_{n:k}) < \tau)$, with probability simulated using (6) (see code for details). On a (sub)standard personal computer, it takes only a few seconds to compute the CCBB $k + \epsilon$ for all of Table 1.

Table 1 indirectly illustrates Theorems 1 and 2. First, BB is clearly different from the other three methods. Second, as Theorem 2 suggests, the other three methods are relatively similar to each other, especially CCBB and GKc. In special cases, all four methods are identical (up to CCBB simulation error). In other cases, CCBB is between HGK and GKc, usually closer to GKc; BB can be higher or lower than the other three.

5.2. Coverage probability

CP is simulated as follows. First, we simulate many samples of $U_i \stackrel{iid}{\sim} \mathrm{Unif}(0,1)$. Second, for the non-uniform F_Y, samples are generated using $Y_i = F_Y^{-1}(U_i)$; this helps isolate the effect of F_Y on CP. Third, for each method, the endpoint $Y_{n:k+\epsilon}$ is computed in each sample using the $k + \epsilon$ in Table 1. Finally, given a method's $Y_{n:k+\epsilon}$ endpoints, the simulated CP is the proportion of samples in which $Y_{n:k+\epsilon} \leq F_Y^{-1}(\tau)$. The CP does not depend on F_Y for intervals with $\epsilon = 0$, which is always true of BB and in special cases true of CCBB, HGK, and GKc (when Table 1 shows an integer value of $k + \epsilon$).

Table 2: Simulated coverage probability

n	τ	F_Y	BB	CCBB	HGK	GKc
18	0.1600	Unif(0, 1)	0.956	0.950	0.953	0.951
18	0.1600	N(0, 1)	0.956	0.951	0.953	0.951
18	0.1600	Exp(1)	0.956	0.949	0.953	0.950
18	0.1600	Cauchy	0.956	0.952	0.954	0.952
18	0.1700	Unif(0, 1)	0.836	0.949	0.957	0.951
18	0.1700	N(0, 1)	0.836	0.952	0.958	0.953
18	0.1700	Exp(1)	0.836	0.948	0.956	0.950
18	0.1700	Cauchy	0.836	0.955	0.959	0.956
18	0.2000	Unif(0, 1)	0.900	0.950	0.961	0.946
18	0.2000	N(0, 1)	0.900	0.956	0.965	0.953
18	0.2000	Exp(1)	0.900	0.947	0.959	0.944
18	0.2000	Cauchy	0.900	0.963	0.969	0.961
18	0.2500	Unif(0, 1)	0.960	0.950	0.954	0.949
18	0.2500	N(0, 1)	0.960	0.951	0.954	0.950
18	0.2500	Exp(1)	0.960	0.949	0.953	0.948
18	0.2500	Cauchy	0.960	0.952	0.955	0.952
18	0.4978	Unif(0, 1)	0.950	0.951	0.950	0.950
18	0.4978	N(0, 1)	0.950	0.951	0.950	0.950
18	0.4978	Exp(1)	0.950	0.951	0.950	0.950
18	0.4978	Cauchy	0.950	0.951	0.950	0.950
18	0.9000	Unif(0, 1)	0.972	0.951	0.959	0.934
18	0.9000	N(0, 1)	0.972	0.947	0.956	0.929
18	0.9000	Exp(1)	0.972	0.945	0.954	0.927
18	0.9000	Cauchy	0.972	0.939	0.949	0.923
18	0.9799	Unif(0, 1)	0.950	0.950	0.950	0.950
18	0.9799	N(0, 1)	0.950	0.950	0.950	0.950
18	0.9799	Exp(1)	0.950	0.950	0.950	0.950
18	0.9799	Cauchy	0.950	0.950	0.950	0.950
18	0.9900	Unif(0, 1)	0.986	0.950	0.974	0.835
18	0.9900	N(0, 1)	0.986	0.898	0.954	0.835
18	0.9900	Exp(1)	0.986	0.890	0.946	0.835
18	0.9900	Cauchy	0.986	0.862	0.898	0.835

Nominal coverage $1 - \alpha = 0.95$; 300,000 replications.

Table 2 shows the simulated coverage probabilities that illustrate our theoretical results. As a general summary of Theorem 2, Corollary 2.1, and Goldman and Kaplan's (2017) Theorem 4: for central quantiles (fixed τ as $n \to \infty$), BB intervals have CP different from the nominal level by $O(n^{-1/2})$, HGK by $O(n^{-1})$ and tending toward over-coverage, and GKc and CCBB by $O(n^{-3/2}[\log(n)]^3)$. Simulation error seems to be ± 0.001, so we ignore such differences in the discussion below.

First, per Theorem 2(ii), Table 2 verifies that CCBB has exact CP when $\epsilon = 0$ (i.e., for the third and fifth τ values, for which the $k + \epsilon$ value in Table 1 is an integer), which is also true of HGK and GKc (Goldman and Kaplan 2017, p. 333). This is true regardless of F_Y. (Somewhat coincidentally, CP is also 0.95 in these cases for BB, even though the BB simulated probability of the interval is strictly above 0.95, per Corollary 1.1.)

Second, also per Theorem 2(ii), CCBB has exact CP when F_Y is uniform. This is true even for the most challenging $\tau = 0.99$.

Third, CCBB is more accurate than BB. For all but the largest (most extreme) $\tau = 0.99$, CCBB has CP between 0.939 and 0.963, whereas BB's CP goes as high as 0.972 and as low as 0.836. With $\tau = 0.99$, CCBB is exact when F_Y is uniform, but otherwise CCBB has CP below 0.90, whereas BB has 0.986 CP. This illustrates how our central quantile results in Theorem 2 are less accurate for extreme τ (here $n\tau = 17.82 > n - 1$).

Fourth, CCBB is generally more accurate than HGK, as well as GKc, although there are important caveats. It is somewhat unfair to compare them when F_Y is uniform because we picked the uniform distribution precisely because CCBB is exact in that case. Nonetheless, CCBB usually has CP somewhat closer to nominal with the other F_Y's, too. For all but the largest (most extreme) τ, for normal and exponential F_Y, CCBB has CP in the range $[0.945, 0.956]$, while the HGK range is $[0.950, 0.965]$, and GKc is $[0.927, 0.953]$. When also including Cauchy F_Y, the CCBB, HGK, and GKc ranges become $[0.939, 0.963]$, $[0.949, 0.969]$, and $[0.923, 0.961]$, respectively. As noted by Goldman and Kaplan (2017), HGK rarely undercovers because the leading n^{-1} term in its coverage error is always positive (regardless of F_Y, interval type, and τ), whereas CCBB and GKc can have CP above or below the nominal level. This is particularly notable with the most extreme $\tau = 0.99$, where CCBB significantly undercovers (for the non-uniform F_Y) and GKc undercovers even more, whereas HGK has CP in the range $[0.946, 0.974]$ for the three non-Cauchy F_Y and less undercoverage for the Cauchy F_Y. Again, results for $\tau = 0.99$ are partly explained by the central quantile asymptotic framework breaking down at such an extreme quantile.

5.3. Length and power

Because all four methods use a fractional order statistic endpoint $Y_{n:k+\epsilon}$, it is straightforward to compare confidence interval lengths. Specifically, if one method's $k + \epsilon$ (as reported in Table 1) is larger than another's, then its $Y_{n:k+\epsilon}$ is also larger in every dataset, so its interval $[Y_{n:k+\epsilon}, \infty)$ is always shorter. For the same reason, its coverage probability must be lower. Put differently: there always exists some $k + \epsilon$ such that $[Y_{n:k+\epsilon}, \infty)$ achieves exact $1 - \alpha$ coverage; any smaller $k + \epsilon$ generates an excessively long confidence interval, and any larger $k + \epsilon$ suffers undercoverage. Thus, in Table 2, in any given row, larger CP corresponds to a longer interval.

Similarly, the size and power of the corresponding hypothesis tests are straightforward to compare across these four methods. That is, the null hypothesis is $H_0\colon F_Y^{-1}(\tau) \leq q$, which is rejected at level α in favor of $H_1\colon F_Y^{-1}(\tau) > q$ if the $1 - \alpha$ confidence interval $[Y_{n:k+\epsilon}, \infty)$ excludes q, i.e., if $Y_{n:k+\epsilon} > q$. The size of such a test is $\mathrm{P}(Y_{n:k+\epsilon} > F_Y^{-1}(\tau))$, which is simply one minus CP and can be computed from Table 2. For $q < F_Y^{-1}(\tau)$, the power $\mathrm{P}(Y_{n:k+\epsilon} > q)$ is an increasing function of $k + \epsilon$. Thus, as with interval length, relative power among the four methods can be compared using Table 1.

Figure 2 illustrates these points through simulated power curves corresponding to certain rows in Table 2. The horizontal axis "Deviation" is $F_Y^{-1}(\tau) - q$. Within a given graph, none of the power curves ever cross, and they all share a similar shape. Because this is simply a consequence of all methods using a fractional order statistic, with only the $k + \epsilon$ differing, it holds true equally at $\tau = 0.17, 0.9, 0.99$, as seen.

Additional power curves are shown in Appendix B. Theoretical results on higher-order power are beyond our scope; first-order power is all the same and equal to the power of a test based on asymptotic normality, as in Theorem 4(iv) of Goldman and Kaplan (2017).

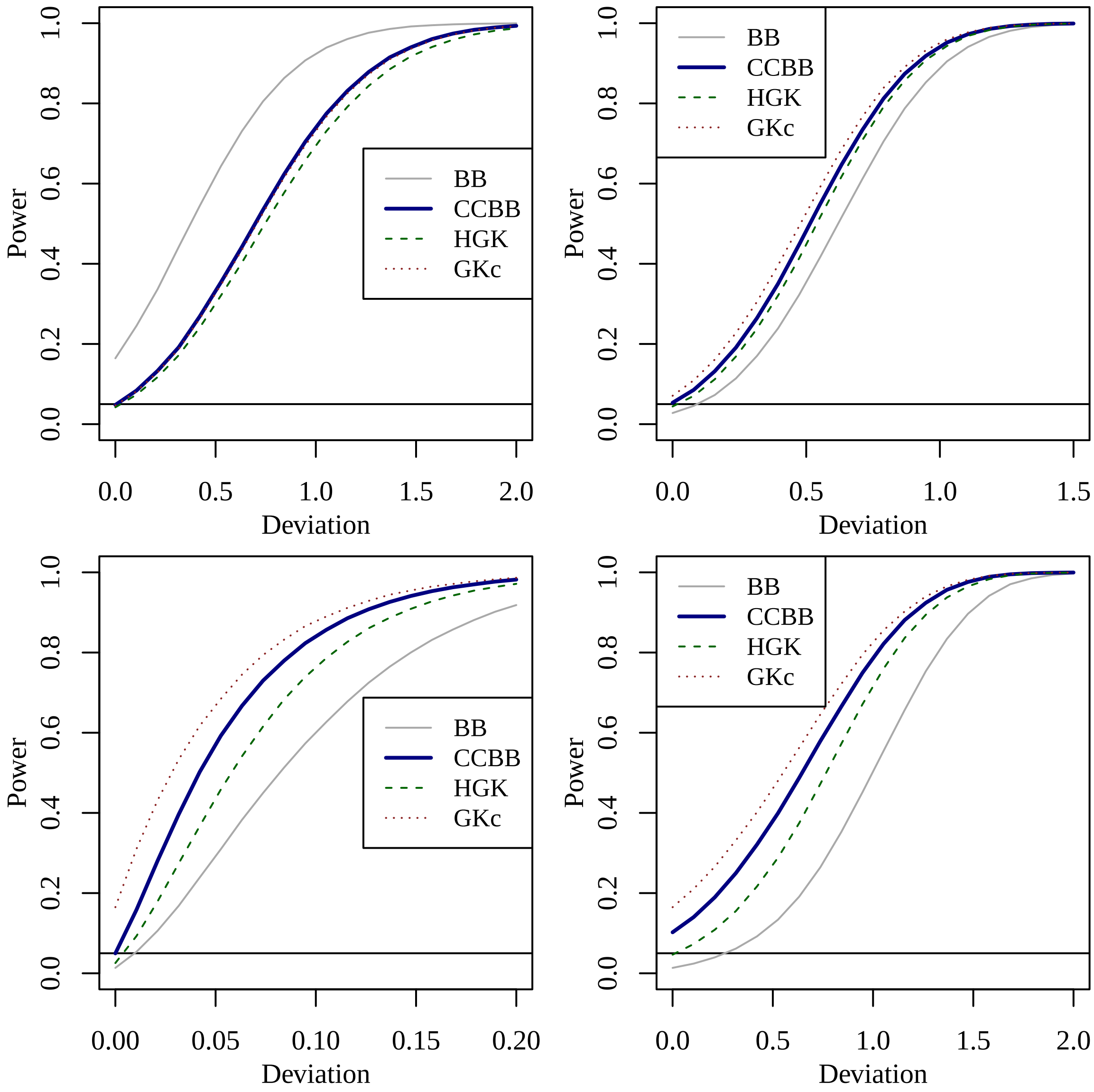

Figure 2: Power curves; $\tau = 0.17$ (top left), $\tau = 0.9$ (top right), $\tau = 0.99$ (bottom row); normal population except bottom left (uniform).

6. Conclusion

For population quantiles of a continuous distribution, we have established the high-order accuracy of confidence intervals from the smoothed Bayesian bootstrap of Banks (1988), using recent developments in fractional order statistic theory. Further, we have established exact finite-sample coverage in special cases including when the population is uniform. The general high-order accuracy is achieved by capturing a term of order n^{-1} automatically, which in other approaches needs to be explicitly removed by calibration (Goldman and Kaplan 2017). The accuracy is orders of magnitude better than that of the unsmoothed Bayesian bootstrap (Rubin 1981), which equals the accuracy of the conventional nonparametric bootstrap, and which provides overly optimistic assessments of a given interval's coverage.

These results motivate future study of the smoothed Bayesian bootstrap. Most immediately, extensions to non-iid sampling or other quantile-based objects of interest would be valuable. An extension to multivariate data would further unlock applications like quantile regression.

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A. Proofs

Proof of Theorem 1. First, for either $\widehat{Q}^*_\tau = \widehat{Q}^*_{\tau,u}$ or $\widehat{Q}^*_\tau = \widehat{Q}^*_{\tau,s}$,

$$Y_{n:k} < \widehat{Q}^*_\tau \iff \sum_{i=1}^{k} W_i < \tau.$$

Thus,

$$\mathrm{P}(Y_{n:k} < \widehat{Q}^*_\tau \mid \mathbf{Y}) = \mathrm{P}(\sum_{i=1}^{k} W_i < \tau \mid \mathbf{Y}).$$

For the BB, by (7), $\sum_{i=1}^{k} W_i \mid \mathbf{Y} \sim \mathrm{Beta}(k, n-k)$. Since the beta distribution is continuous,

$$\mathrm{P}(\sum_{i=1}^{k} W_i < \tau \mid \mathbf{Y}) = \mathrm{P}(\sum_{i=1}^{k} W_i \le \tau \mid \mathbf{Y}) = F_\beta(\tau; k, n-k). \tag{12}$$

Since the BB $\widehat{F}_{*u}(\cdot)$ includes only discrete distributions with support $\{Y_i\}_{i=1}^n$,

$$Y_{n:k} \le \widehat{Q}^*_{\tau,u} \iff Y_{n:k-1} < \widehat{Q}^*_{\tau,u}.$$

Combining this with (12),

$$\mathrm{P}(Y_{n:k} \le \widehat{Q}^*_{\tau,u} \mid \mathbf{Y}) = \mathrm{P}(Y_{n:k-1} < \widehat{Q}^*_{\tau,u} \mid \mathbf{Y}) = F_\beta(\tau; k-1, n-(k-1)).$$

For the CCBB, the same steps hold as for (12), but with $\sum_{i=1}^{k} W_i \mid \mathbf{Y} \sim \mathrm{Beta}(k, n+1-k)$ from (7), so

$$\mathrm{P}(Y_{n:k} < \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) = \mathrm{P}(\sum_{i=1}^{k} W_i < \tau \mid \mathbf{Y}) = \mathrm{P}(\sum_{i=1}^{k} W_i \le \tau \mid \mathbf{Y}) = F_\beta(\tau; k, n+1-k).$$

Since the CCBB distribution of $\widehat{Q}^*_{\tau,s}$ is continuous, $\mathrm{P}(Y_{n:k} < \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) = \mathrm{P}(Y_{n:k} \le \widehat{Q}^*_{\tau,s} \mid \mathbf{Y})$. With continuous $F_Y(\cdot)$, using Wilks (1962, **8.7.4**),

$$\mathrm{P}(Y_{n:k} \le \mathrm{Q}_\tau(Y)) = \mathrm{P}(F_Y(Y_{n:k}) \le \tau) = F_\beta(\tau; k, n+1-k) = \mathrm{P}(Y_{n:k} \le \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}). \qquad \square$$

Proof of Corollary 1.1. The connection between beta and binomial distributions is used below. The PDF of a Beta(a, b) distribution is (Abramowitz and Stegun 1972, **6.2.2**, **26.1.33**)

$$f_\beta(p; a, b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} p^{a-1}(1-p)^{b-1},$$

where $\Gamma(\cdot)$ is the gamma function. If m is an integer, then $\Gamma(m) = (m-1)!$ (Abramowitz and Stegun 1972, **6.1.6**). Thus, if a and b are integers,

$$f_\beta(p; a, b) = \frac{(a+b-1)!}{(a-1)!(b-1)!} p^{a-1}(1-p)^{b-1}.$$

The probability mass function of a Binomial(m, p) distribution is (Abramowitz and Stegun 1972, **26.1.20**)

$$f_B(d; m, p) = \binom{m}{d} p^d (1-p)^{m-d} = \frac{m!}{d!(m-d)!} p^d (1-p)^{m-d}.$$

With $d = k-1$, $m = n-1$, and $p = \tau$,

$$f_B(k-1; n-1, \tau) = \frac{(n-1)!}{(k-1)!(n-k)!} \tau^{k-1}(1-\tau)^{n-k}.$$

With $p = \tau$, $a = k$, and $b = n+1-k$,

$$f_\beta(\tau; k, n+1-k) = \frac{n!}{(k-1)!(n-k)!} \tau^{k-1}(1-\tau)^{n-k} = n f_B(k-1; n-1, \tau). \tag{13}$$

The beta and binomial CDFs can both be written in terms of the regularized incomplete beta function I. The beta CDF is $F_\beta(p; a, b) = I_p(a, b)$ (David and Nagaraja 2003, eqn. (1.3.2)). Applying **26.5.24** in Abramowitz and Stegun (1972),

$$1 - F_B(d; m, p) = \overbrace{\sum_{s=d+1}^{m} f_B(s; m, p) = I_p(d+1, m-d)}^{\text{from } \mathbf{26.5.24}} = F_\beta(p; d+1, m-d). \tag{14}$$

From Theorem 1, applying (14) with $p = \tau$ and either $(d = k-2, m = n-1)$ or $(d = k-1, m = n)$,

$$\begin{aligned}
&\mathrm{P}(Y_{n:k} \le \hat{Q}^*_{\tau,u} \mid \mathbf{Y}) - \mathrm{P}(Y_{n:k} \le \hat{Q}^*_{\tau,s} \mid \mathbf{Y}) \\
&= F_\beta(\tau; k-1, n+1-k) - F_\beta(\tau; k, n+1-k) \\
&= [1 - F_B(k-2; n-1, \tau)] - [1 - F_B(k-1; n, \tau)] \\
&= F_B(k-1; n, \tau) - F_B(k-2; n-1, \tau).
\end{aligned}$$

The two binomial CDFs may be expressed in terms of $B_i \overset{iid}{\sim} \text{Bernoulli}(\tau)$:

$$F_B(k-2; n-1, \tau) = \mathrm{P}(\sum_{i=1}^{n-1} B_i \le k-2), \quad F_B(k-1; n, \tau) = \mathrm{P}(\sum_{i=1}^{n} B_i \le k-1).$$

Since $\sum_{i=1}^{n} B_i = B_n + \sum_{i=1}^{n-1} B_i$ and $B_n \le 1$,

$$\sum_{i=1}^{n-1} B_i \le k-2 \implies B_n + \sum_{i=1}^{n-1} B_i \le 1 + k - 2 \implies \sum_{i=1}^{n} B_i \le k-1.$$

Thus, the CDF difference equals the probability that the latter inequality holds but the former does not, which only occurs when $\sum_{i=1}^{n-1} B_i = k-1$ and $B_n = 0$:

$$\begin{aligned}
F_B(k-1; n, \tau) - F_B(k-2; n-1, \tau) &= \mathrm{P}(\sum_{i=1}^{n} B_i \le k-1 \text{ and } \sum_{i=1}^{n-1} B_i > k-2) \\
&= \overbrace{\mathrm{P}(\sum_{i=1}^{n-1} B_i = k-1 \text{ and } B_n = 0)}^{\text{use } \{B_i\}_{i=1}^{n-1} \perp\!\!\!\perp B_n} \\
&= \mathrm{P}(\sum_{i=1}^{n-1} B_i = k-1)\, \mathrm{P}(B_n = 0) \\
&= \overbrace{f_B(k-1; n-1, \tau)}^{\text{apply (13)}}(1-\tau) \\
&= n^{-1} f_\beta(\tau; k, n+1-k)(1-\tau).
\end{aligned}$$

The other probability difference is derived using the same steps. From Theorem 1, applying (14) with $p = \tau$ and either $(d = k-1, m = n)$ or $(d = k-1, m = n-1)$, and again using the B_i defined earlier,

$$\begin{aligned}
\mathrm{P}(Y_{n:k} \ge \widehat{Q}^*_{\tau,u} \mid \mathbf{Y}) - \mathrm{P}(Y_{n:k} \ge \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) &= 1 - \mathrm{P}(Y_{n:k} < \widehat{Q}^*_{\tau,u} \mid \mathbf{Y}) - [1 - \mathrm{P}(Y_{n:k} < \widehat{Q}^*_{\tau,s} \mid \mathbf{Y})] \\
&= \mathrm{P}(Y_{n:k} < \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) - \mathrm{P}(Y_{n:k} < \widehat{Q}^*_{\tau,u} \mid \mathbf{Y}) \\
&= F_\beta(\tau; k, n-k+1) - F_\beta(\tau; k, n-k) \\
&= [1 - F_B(k-1; n, \tau)] - [1 - F_B(k-1; n-1, \tau)] \\
&= F_B(k-1; n-1, \tau) - F_B(k-1; n, \tau) \\
&= \mathrm{P}(\sum_{i=1}^{n-1} B_i \le k-1) - \mathrm{P}(\sum_{i=1}^{n} B_i \le k-1) \\
&= \mathrm{P}(\sum_{i=1}^{n-1} B_i = k-1 \text{ and } B_n = 1) \\
&= \mathrm{P}(\sum_{i=1}^{n-1} B_i = k-1)\, \mathrm{P}(B_n = 1) \\
&= f_B(k-1; n-1, \tau)\tau \\
&= \frac{\tau}{n} f_\beta(\tau; k, n+1-k).
\end{aligned}$$

The mode of a Beta(a, b) distribution is $(a-1)/(a+b-2)$ for $a, b > 1$. Thus for $1 < k < n$, the mode of a Beta$(k, n+1-k)$ distribution is $(k-1)/(n-1)$, i.e.,

$$\arg\sup_{0 \le t \le 1} f_\beta(t; k, n+1-k) = (k-1)/(n-1).$$

Thus, the maximum value of the beta PDF is $f_\beta((k-1)/(n-1); k, n+1-k)$. Applying the Stirling-type approximation

$$m! = \sqrt{2\pi} m^{m+(1/2)} e^{-m} e^{r_m}, \quad \frac{1}{12m+1} < r_m < \frac{1}{12m} \tag{15}$$

of Robbins (1955) and evaluating (13) at the mode $\tau = (k-1)/(n-1)$,

$$
\begin{aligned}
&f_\beta((k-1)/(n-1); k, n+1-k) \\
&= \frac{n!}{(k-1)!(n-k)!}[(k-1)/(n-1)]^{k-1}\overbrace{[1-(k-1)/(n-1)]}^{=[n-1-(k-1)]/(n-1)}{}^{n-k} \\
&= \frac{n[(n-1)!]}{(k-1)!(n-k)!}[(k-1)/(n-1)]^{k-1}[(n-k)/(n-1)]^{n-k} \\
&= n\frac{(n-1)!}{(k-1)!(n-k)!}(k-1)^{k-1}(n-k)^{n-k}[1/(n-1)]^{(k-1)+(n-k)} \\
&= n\frac{(n-1)!}{(n-1)^{n-1}}\frac{(k-1)^{k-1}}{(k-1)!}\frac{(n-k)^{n-k}}{(n-k)!} \\
&= n\frac{\sqrt{2\pi}(n-1)^{1/2}e^{-(n-1)}e^{r_{n-1}}}{2\pi(k-1)^{1/2}(n-k)^{1/2}e^{-(k-1)}e^{-(n-k)}e^{r_{k-1}}e^{r_{n-k}}} \\
&= n(2\pi)^{-1/2}\sqrt{\frac{n-1}{(k-1)(n-k)}}\underbrace{\exp\{\overbrace{-(n-1)+(k-1)+(n-k)}^{=0}\}}_{=1}\exp\{r_{n-1}-r_{k-1}-r_{n-k}\}.
\end{aligned}
$$

For the approximation error, since $r_{k-1}, r_{n-k} > 0$,

$$\exp\{r_{n-1}-r_{k-1}-r_{n-k}\} \le \exp\{r_{n-1}\} \le \exp\{1/[12(n-1)]\} = 1 + O(n^{-1}).$$

Thus,

$$f_\beta((k-1)/(n-1); k, n+1-k) \le n(2\pi)^{-1/2}\sqrt{\frac{n-1}{(k-1)(n-k)}}[1+O(n^{-1})]. \tag{16}$$

If $c_1 \le k/n \le c_2$ for constants $0 < c_1 < c_2 < 1$ as $n \to \infty$, i.e., if k is of order n, then the upper bound rate of (16) simplifies further. Specifically, this implies $k - 1 \ge c_1 n - 1$ and $n - k \ge n - c_2 n = n(1 - c_2)$, so

$$\sqrt{\frac{n-1}{(k-1)(n-k)}} \le \sqrt{\frac{n}{(c_1 n-1)n(1-c_2)}} = [(c_1 n - 1)(1-c_2)]^{-1/2} = O(n^{-1/2}). \tag{17}$$

Replacing $n(2\pi)^{-1/2}$ with $O(n)$ in (16), the probability difference is

$$n^{-1}\overbrace{f_\beta((k-1)/(n-1); k, n+1-k)}^{\text{use (16)}} = n^{-1}O(n)O(n^{-1/2})[1+O(n^{-1})] = O(n^{-1/2}).$$

If k is not required to have rate n, then this bound on the difference is larger. If k or $n-k$ is fixed as $n \to \infty$ (i.e., $Y_{n:k}$ is an "extreme order statistic"), then (17) becomes $O(1)$ instead of $O(n^{-1/2})$, so the overall difference becomes $O(1)$ instead of $O(n^{-1/2})$. If $c_1 n^r \le k \le c_2 n^r$ for $0 < r < 1$, then (17) becomes

$$\sqrt{\frac{n-1}{(k-1)(n-k)}} \le \sqrt{\frac{n}{(c_1 n^r - 1)(n - c_2 n^r)}} = O(n^{-r/2}).$$

The same holds if instead $c_1 n^r \le n - k \le c_2 n^r$. In either case, the overall difference also becomes $O(n^{-r/2})$. □

Proof of Theorem 2. For Theorem 2(i), the BB result follows immediately from Theorem 1 since

$$\mathrm{P}(Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \hat{Q}^*_{\tau,u} \mid \mathbf{Y}) = \mathrm{P}(Y_{n:k} < \hat{Q}^*_{\tau,u} \mid \mathbf{Y}).$$

For the CCBB result in Theorem 2(i), first we show that (conditional on $\mathbf{Y}$)

$$\overbrace{Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \widehat{Q}^*_{\tau,s}}^{\text{event } A} \iff \overbrace{\sum_{i=1}^{k} W_i + \epsilon W_{k+1} < \tau}^{\text{event } B}\,. \tag{18}$$

Write $\widehat{Q}^*_{\tau,s}$ with $c \equiv \max\{d : \sum_{i=1}^{d} W_i \le \tau\}$ as in (10). We show (18) holds for $c < k$, $c > k$, and $c = k$. If $c < k$, implying $\sum_{i=1}^{k} W_i > \tau$, then neither A nor B occurs:

$$\text{for } A,\quad \overbrace{\widehat{Q}^*_{\tau,s} < Y_{n:c+1}}^{\text{by (10)}} \le \underbrace{Y_{n:c+1} \le Y_{n:k}}_{\text{by } c<k} \le \overbrace{Y_{n:k} \le Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k})}^{\text{by } \epsilon\ge 0};$$

$$\text{for } B,\quad \overbrace{\sum_{i=1}^{k} W_i + \epsilon W_{k+1} \ge \sum_{i=1}^{k} W_i}^{\text{by } \epsilon\ge 0} \underbrace{\sum_{i=1}^{k} W_i > \tau}_{\text{implied by } c<k}\,.$$

If $c > k$, implying $c \ge k+1$ and thus $\sum_{i=1}^{k+1} W_i \le \tau$, then both A and B occur:

$$\text{for } A,\quad \overbrace{\widehat{Q}^*_{\tau,s} \ge Y_{n:c}}^{\text{by (10)}} \ge \underbrace{Y_{n:c} \ge Y_{n:k+1}}_{\text{by } c>k} \overbrace{Y_{n:k+1} > Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k})}^{\text{by } \epsilon<1};$$

$$\text{for } B,\quad \overbrace{\sum_{i=1}^{k} W_i + \epsilon W_{k+1} < \sum_{i=1}^{k+1} W_i}^{\text{by } \epsilon<1} \underbrace{\sum_{i=1}^{k+1} W_i \le \tau}_{\text{implied by } c>k}\,.$$

If $c = k$, then event A in (18) becomes

$$\overbrace{Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \widehat{Q}^*_{\tau,s}}^{\text{event } A \text{ in (18)}} \underbrace{\widehat{Q}^*_{\tau,s} = Y_{n:k} + \frac{(\tau - \sum_{i=1}^{k} W_i)}{W_{k+1}}(Y_{n:k+1} - Y_{n:k})}_{\text{from (10) with } c=k}$$

$$\iff \epsilon < \frac{\tau - \sum_{i=1}^{k} W_i}{W_{k+1}}$$

$$\iff \underbrace{\sum_{i=1}^{k} W_i + \epsilon W_{k+1} < \tau}_{\text{event } B \text{ in (18)}}\,.$$

Since $A \iff B$ in (18), the corresponding CCBB probabilities are equal:

$$\mathrm{P}\{\overbrace{Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \widehat{Q}^*_{\tau,s}}^{A} \mid \mathbf{Y}\} = \mathrm{P}\{\overbrace{\sum_{i=1}^{k} W_i + \epsilon W_{k+1} < \tau}^{B} \mid \mathbf{Y}\}. \tag{19}$$

The right-hand side of (19) can then be approximated by Theorem 2(i) of Goldman and Kaplan (2017). Their theorem concerns the distribution of (linear combinations of) fractional order statistics. Recall from (6) that the joint Dirichlet distribution of $(W_1, \ldots, W_{n+1})$ is the same as the joint sampling distribution of standard uniform order statistic spacings

$(U_{n:1}, U_{n:2} - U_{n:1}, \dots, 1 - U_{n:n})$ given iid sampling. The sum of the first k spacings is $U_{n:k}$, and the $(k+1)$th spacing is $U_{n:k+1} - U_{n:k}$, so the CCBB distribution of $\sum_{i=1}^{k} W_i + \epsilon W_{k+1}$ equals the sampling distribution of $U_{n:k+\epsilon} \equiv U_{n:k} + \epsilon(U_{n:k+1} - U_{n:k})$, i.e., the fractional $(k+\epsilon)$th order statistic. That is, for any value $0 \le r \le 1$,

$$\mathrm{P}(\sum_{i=1}^{k} W_i + \epsilon W_{k+1} \le r \mid \mathbf{Y}) = \mathrm{P}\{U_{n:k} + \epsilon(U_{n:k+1} - U_{n:k}) \le r\}. \tag{20}$$

Theorem 2(i) of Goldman and Kaplan (2017) approximates the right-hand side of (20).

The following shows specifically how to apply Theorem 2(i) of Goldman and Kaplan (2017) to $U_{n:k+\epsilon}$. Their Assumption 1 is iid sampling, as in our case. In their notation, $J = 1$, $\psi_1 = 1$, and $F(\cdot)$ is the standard uniform CDF: for $0 \le t \le 1$, $F(t) = t$, $F^{-1}(t) = t$, and PDF $f(t) = 1$. Thus, their Assumption 2 is satisfied for any $0 < u < 1$ since $f(u) > 0$ and $f''(u) = 0$ is continuous in u. Their u_1 and ϵ_1 are the same as u and ϵ here. So far, this makes their general fractional L-statistic L^L equal to our $U_{n:k+\epsilon}$. Also, their $\mathbb{X}_0$ equals our u, and their $\mathcal{V}_{\boldsymbol{\psi}}$ equals our $u(1-u)$. Their L^I follows a $\text{Beta}((n+1)u, (n+1)(1-u)) = \text{Beta}(k+\epsilon, n+1-k-\epsilon)$ distribution. Thus, setting their $\mathbb{X}_0 + n^{-1/2}K$ equal to our τ, their Theorem 2(i) says in their notation that

$$\mathrm{P}(L^L < \mathbb{X}_0 + n^{-1/2}K) - \mathrm{P}(L^I < \mathbb{X}_0 + n^{-1/2}K) = O(n^{-1}),$$

which in our notation is

$$\mathrm{P}(U_{n:k+\epsilon} < \tau) - F_{\beta}(k+\epsilon, n+1-k-\epsilon) = O(n^{-1}). \tag{21}$$

Theorem 2(i) of Goldman and Kaplan (2017) further provides an analytic expression for the n^{-1} term. In their notation, setting $\mathbb{X}_0 = u$ and $\mathbb{X}_0 + n^{-1/2}K = \tau$, solving for their K yields $K = \sqrt{n}(\tau - u)$. Given $u = \tau - dn^{-1/2}$, $K = \sqrt{n}(\tau - u) = d$. Plugging into their Theorem 2(i) yields, first in their notation and then translated into ours with $K = d$, $\mathcal{V}_{\boldsymbol{\psi}} = u(1-u)$, $\psi_1 = 1$, and $\epsilon_1 = \epsilon$,

$$\begin{aligned}
&\mathrm{P}(U_{n:k+\epsilon} < \tau) - F_{\beta}(k+\epsilon, n+1-k-\epsilon) \\
&= n^{-1} \frac{K \exp\{-K^2/(2\mathcal{V}_{\boldsymbol{\psi}})\}}{\sqrt{2\pi\mathcal{V}_{\boldsymbol{\psi}}^3}} \overbrace{\psi_1}^{=1} \overbrace{\epsilon_1(1-\epsilon_1)}^{=\epsilon(1-\epsilon)} \overbrace{[f(F^{-1}(u))]^{-2}}^{=1} + O(n^{-3/2}[\log(n)]^3) \\
&= n^{-1} \frac{d \exp\{-d^2/[2u(1-u)]\}}{\sqrt{2\pi[u(1-u)]^3}} \epsilon(1-\epsilon) + O(n^{-3/2}[\log(n)]^3) \\
&= n^{-1} \frac{\epsilon(1-\epsilon)}{u(1-u)} \frac{d}{\sqrt{u(1-u)}} \frac{1}{\sqrt{2\pi}} \exp\{-(1/2)[d/\sqrt{u(1-u)}]^2\} + O(n^{-3/2}[\log(n)]^3) \\
&= n^{-1} \frac{\epsilon(1-\epsilon)}{\tau(1-\tau)} \frac{d}{\sqrt{\tau(1-\tau)}} \phi\Big(d/\sqrt{\tau(1-\tau)}\Big) + O(n^{-3/2}[\log(n)]^3),
\end{aligned} \tag{22}$$

using the fact that $u = \tau + O(n^{-1/2})$ and writing $\phi(\cdot)$ as the standard normal PDF.

For Theorem 2(ii), the $\epsilon = 0$ result follows immediately from Theorem 1 and the result from Wilks (1962) that $F_Y(Y_{n:k}) \stackrel{d}{=} U_{n:k} \sim \text{Beta}(k, n+1-k)$ if $F_Y(\cdot)$ is continuous, so

$$\mathrm{P}(Y_{n:k} < \mathrm{Q}_{\tau}(Y)) = \mathrm{P}\{F_Y(Y_{n:k}) < F_Y(\mathrm{Q}_{\tau}(Y))\} = \mathrm{P}\{U_{n:k} < \tau\} = F_{\beta}(\tau; k, n+1-k).$$

The other result comes from (20), which directly gives the equivalence for $\text{Unif}(0,1)$ that can be extended to $\text{Unif}(a,b)$ as follows. Let $V_i \stackrel{iid}{\sim} \text{Unif}(a,b)$, with order statistics $V_{n:k}$ and

$\mathrm{Q}_\tau(V) = a + (b-a)\tau$. Then, $(V_i - a)/(b-a) \stackrel{iid}{\sim} \mathrm{Unif}(0,1)$, and

$$\begin{aligned}
&\mathrm{P}\{V_{n:k} + \epsilon(V_{n:k+1} - V_{n:k}) < a + (b-a)\tau\} \\
&= \mathrm{P}\{V_{n:k} - a + \epsilon[(V_{n:k+1} - a) - (V_{n:k} - a)] < (b-a)\tau\} \\
&= \mathrm{P}\left\{\frac{V_{n:k} - a}{b-a} + \epsilon\left[\frac{V_{n:k+1} - a}{b-a} - \frac{V_{n:k} - a}{b-a}\right] < \tau\right\} \\
&= \mathrm{P}\{U_{n:k} + \epsilon(U_{n:k+1} - U_{n:k}) < \tau\}.
\end{aligned}$$

For Theorem 2(iii), plugging $d = z_{1-\alpha}\sqrt{\tau(1-\tau)} + O(n^{-1/2})$ from (11) into (22),

$$\begin{aligned}
&\mathrm{P}\{Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}\} - F_\beta(k+\epsilon, n+1-k-\epsilon) \\
&= n^{-1}\frac{\epsilon(1-\epsilon)}{\tau(1-\tau)}\frac{d}{\sqrt{\tau(1-\tau)}}\phi\Big(d/\sqrt{\tau(1-\tau)}\Big) + O(n^{-3/2}[\log(n)]^3) \\
&= n^{-1}\frac{\epsilon(1-\epsilon)z_{1-\alpha}}{\tau(1-\tau)}\phi(z_{1-\alpha}) + O(n^{-3/2}[\log(n)]^3),
\end{aligned}$$

for any $0 < \alpha < 1$. This matches the coverage probability in Theorem 4(i) from Goldman and Kaplan (2017), noting that their p is our τ. That is, their Theorem 4(i) says that if A1 and A2 and (11) hold, then

$$\begin{aligned}
&\mathrm{P}\{Y_{n:k} + \epsilon(Y_{n:k+1} - Y_{n:k}) < \mathrm{Q}_\tau(Y)\} - F_\beta(k+\epsilon, n+1-k-\epsilon) \\
&\qquad = n^{-1}\frac{\epsilon(1-\epsilon)z_{1-\alpha}}{\tau(1-\tau)}\phi(z_{1-\alpha}) + O(n^{-3/2}[\log(n)]^3).
\end{aligned}$$

More directly, the n^{-1} term in their Theorem 4(i) does not depend on the underlying distribution (other than satisfying A2). Since by Theorem 2(ii) the CCBB probability equals the coverage probability when the underlying distribution is uniform, it also equals the coverage probability given any other distribution satisfying A2 up to the $O(n^{-3/2}[\log(n)]^3)$ remainder. □

Proof of Corollary 2.1. For $\epsilon = 0$, Corollary 1.1 gives the $O(n^{-1/2})$ difference. The difference cannot be smaller over the larger range of $\epsilon \in [0,1)$; below we show it is not bigger, either.

For $0 < \epsilon < 1$, the CCBB probability is bounded by

$$\mathrm{P}(Y_{n:k+1} \le \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) < \mathrm{P}(Y_{n:k+\epsilon} \le \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) < \mathrm{P}(Y_{n:k} \le \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}).$$

From Theorems 1 and 2, this implies

$$F_\beta(\tau; k+1, n-k) < \mathrm{P}(Y_{n:k+\epsilon} \le \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) < F_\beta(\tau; k, n+1-k). \tag{23}$$

The difference between the unsmoothed BB probability $F_\beta(\tau; k, n-k)$ and the bounds in (23) can be computed using Corollary 1.1. The upper bound difference comes directly from Corollary 1.1:

$$F_\beta(\tau; k+1, n-k) - F_\beta(\tau; k, n-k) = \frac{\tau}{n} f_\beta(\tau; k, n+1-k). \tag{24}$$

Replacing k with $k+1$ in Theorem 1 yields

$$\mathrm{P}(Y_{n:k+1} \le \widehat{Q}^*_{\tau,u} \mid \mathbf{Y}) = F_\beta(\tau; k, n-k), \quad \mathrm{P}(Y_{n:k+1} \le \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) = F_\beta(\tau; k+1, n-k). \tag{25}$$

Further applying Corollary 1.1 after replacing k with $k+1$,

$$F_\beta(\tau; k, n-k) - F_\beta(\tau; k+1, n-k) = \frac{1-\tau}{n} f_\beta(\tau; k+1, n-k). \tag{26}$$

This is the difference between the BB probability and the lower bound in (23).

As ϵ goes from 0 to 1, the CCBB probability goes from the upper bound to the lower bound in (23). Thus, the BB–CCBB difference goes from

$$-\frac{\tau}{n} f_\beta(\tau; k, n+1-k) \text{ to } \frac{1-\tau}{n} f_\beta(\tau; k+1, n-k). \quad (27)$$

That is,

$$-\frac{\tau}{n} f_\beta(\tau; k, n+1-k) \le \mathrm{P}(Y_{n:k+\epsilon} \le \widehat{Q}^*_{\tau,u} \mid \mathbf{Y}) - \mathrm{P}(Y_{n:k+\epsilon} \le \widehat{Q}^*_{\tau,s} \mid \mathbf{Y}) \le \frac{1-\tau}{n} f_\beta(\tau; k+1, n-k). \quad (28)$$

Since the lower bound is negative and the upper bound positive, and the difference varies continuously with ϵ, there is some magic ϵ for which the BB and CCBB actually agree. However, since ϵ is determined by the nominal level and sample size (i.e., not chosen independently), in general the difference is larger. As stated in Corollary 1.1, with $c_1 \le k/n \le c_2$, the bounds in (28) are $O(n^{-1/2})$. □

B. Additional simulations

Figures 3–5 show additional power curves as discussed in Section 5.3.

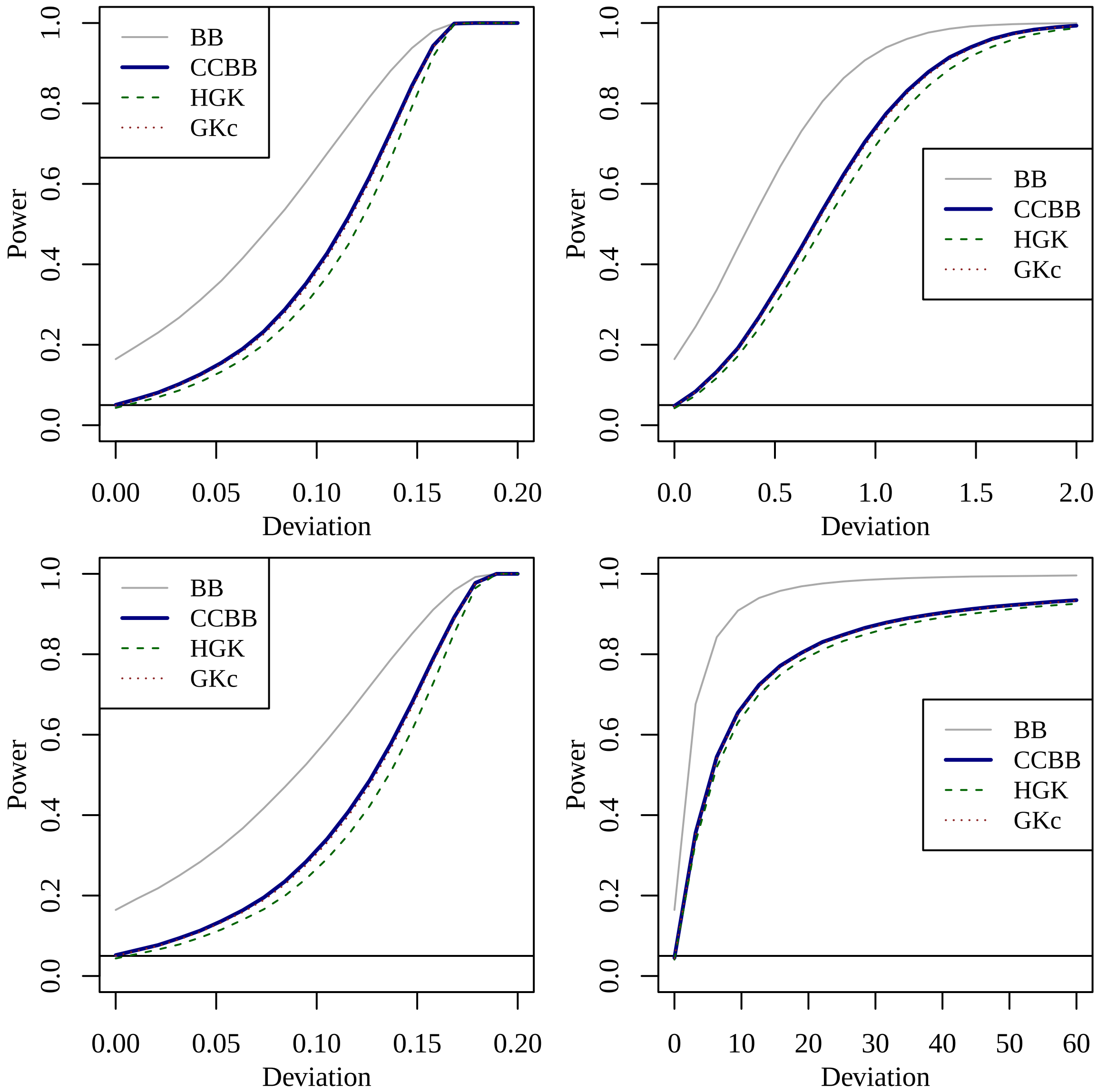

Figure 3: Power curves, $\tau = 0.17$; uniform (top left), normal (top right), exponential (bottom left), and Cauchy (bottom right) populations.

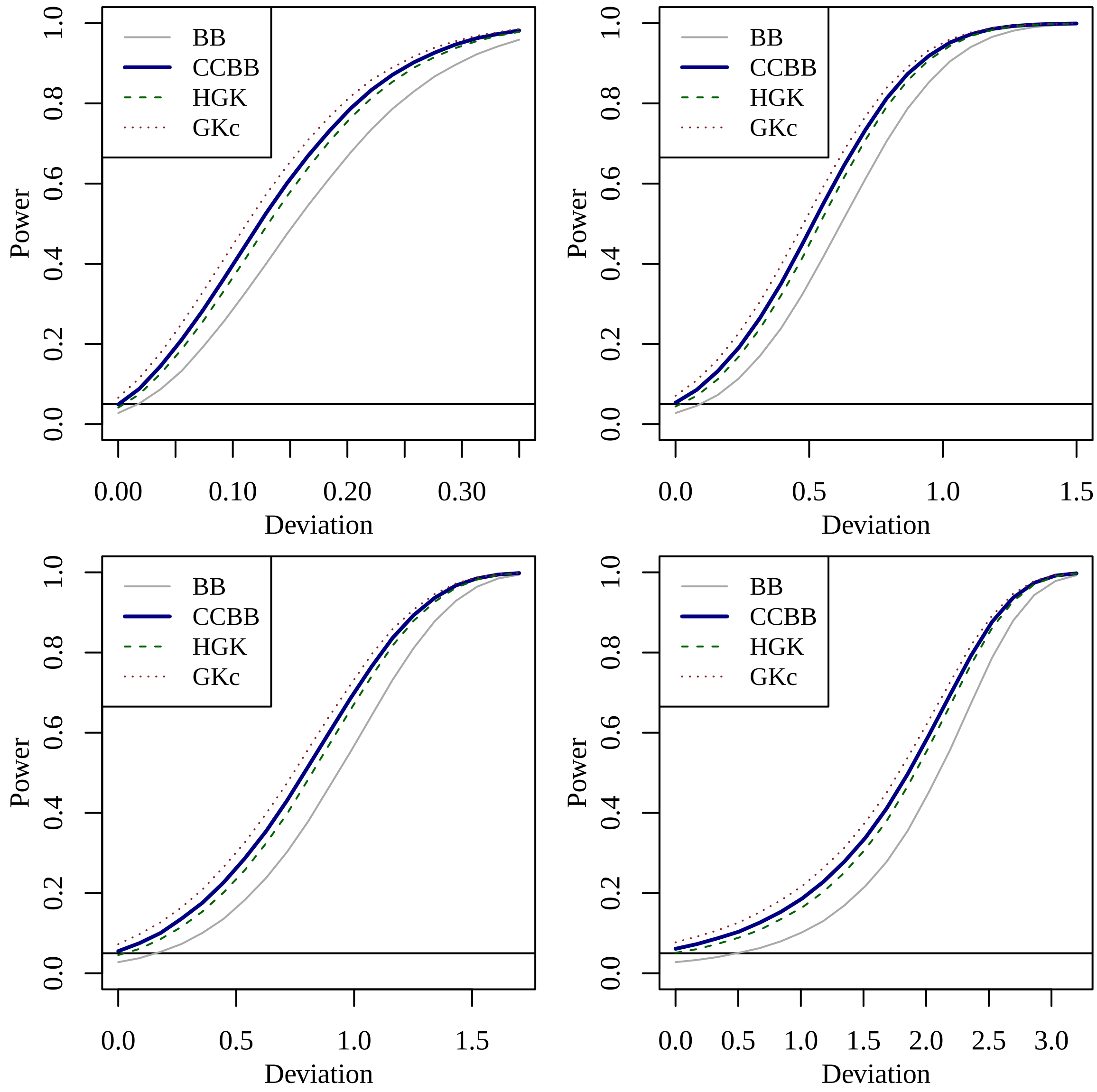

Figure 4: Power curves, $\tau = 0.9$; uniform (top left), normal (top right), exponential (bottom left), and Cauchy (bottom right) populations.

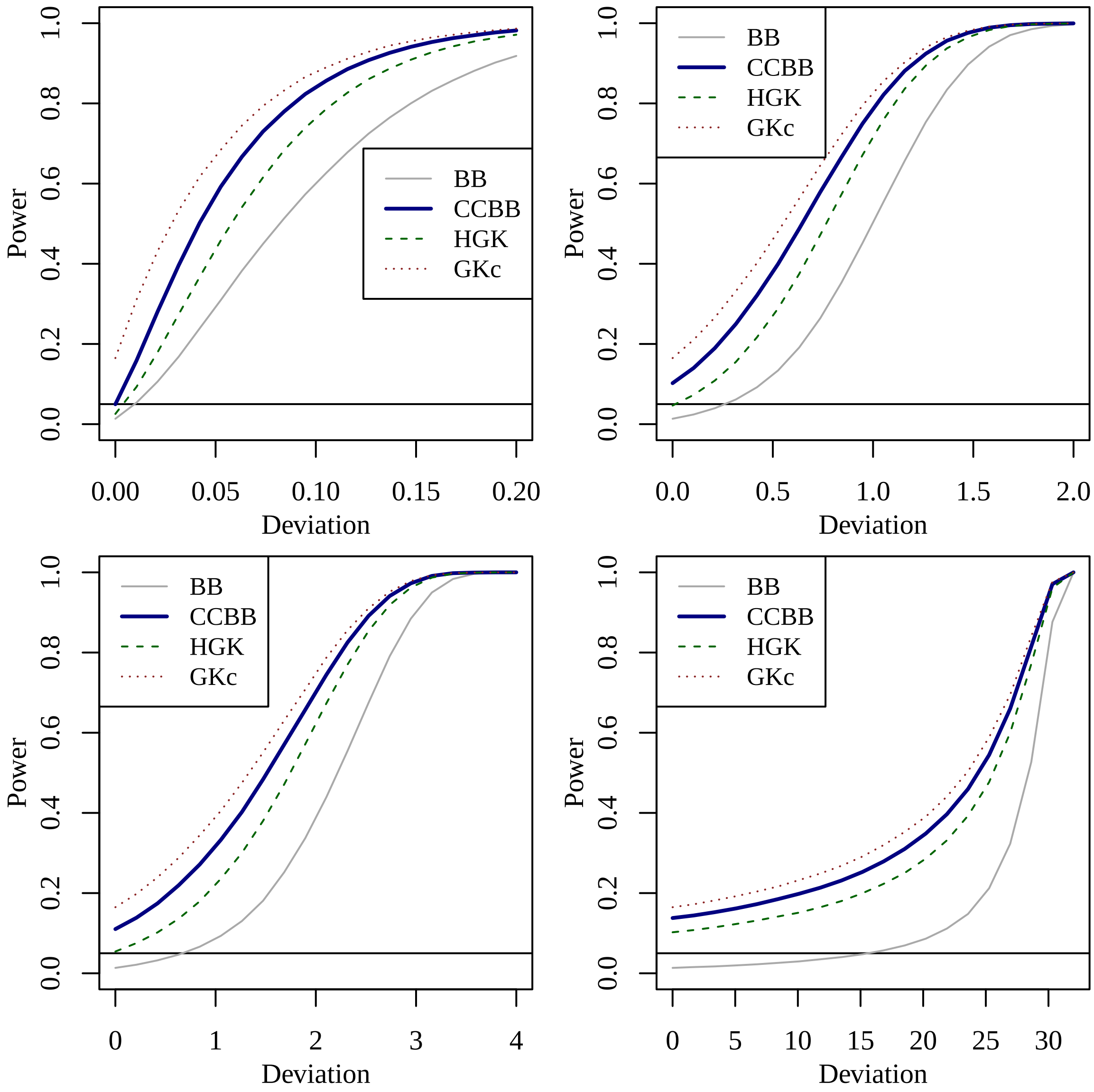

Figure 5: Power curves, $\tau = 0.99$; uniform (top left), normal (top right), exponential (bottom left), and Cauchy (bottom right) populations.

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