Concentration-based confidence intervals for U-statistics

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Abstract

Concentration inequalities have become increasingly popular in machine learning, probability, and statistical research. Using concentration inequalities, one can construct confidence intervals (CIs) for many quantities of interest. Unfortunately, many of these CIs require the knowledge of population variances, which are generally unknown, making these CIs impractical for numerical application. However, recent results regarding the simultaneous bounding of the probabilities of quantities of interest and their variances have permitted the construction of empirical CIs, where variances are replaced by their sample estimators. Among these new results are two-sided empirical CIs for U-statistics, which are useful for the construction of CIs for a rich class of parameters. In this article, we derive a number of new one-sided empirical CIs for U-statistics and their variances. We show that our one-sided CIs can be used to construct tighter two-sided CIs for U-statistics, than those currently reported. We also demonstrate how our CIs can be used to construct new empirical CIs for the mean, which provide tighter bounds than currently known CIs for the same number of observations, under various settings.

Key words: Bernstein inequality; concentration inequalities; confidence intervals; sample variance; Hoeffding inequality; U-statistics
1 Introduction

Let \( X_1, \ldots, X_n \in X \subseteq \mathbb{R}^d \) be an independent and identically distributed (IID) random sample from some data generating process (DGP), characterized by some probability distribution \( F \). Let \( h : X^m \to \mathbb{R} \) be a symmetric function, in the sense that

\[
h ( x_{\pi_1(1)}, \ldots, x_{\pi_1(m)} ) = h ( x_{\pi_2(1)}, \ldots, x_{\pi_2(m)} ),
\]

for all \( \pi_i^\top = (\pi_i(1), \ldots, \pi_i(m)) \in \Pi_m \) \((i \in \{1, 2\})\), where \( \Pi_m \) is the set of all permutations of the first \( m \) consecutive natural numbers. We say that \( h \) is an order \( m \) symmetric kernel. Assuming that the parameter

\[
\theta ( F ) = \mathbb{E}_F h ( X_1, \ldots, X_m ) = \int_X \cdots \int_X h ( x_1, \ldots, x_m ) \, dF ( x_1 ) \cdots dF ( x_m ),
\]

exists, we can unbiasedly estimate \( \theta ( F ) = \theta \) via the so-called U-statistic

\[
U_n = U ( X_1, \ldots, X_n ) = \binom{n}{m}^{-1} \sum_{\kappa \in \mathbb{K}_m} h ( X_{\kappa(1)}, \ldots, X_{\kappa(m)} ),
\]

where \( \kappa^\top = (\kappa(1), \ldots, \kappa(m)) \in \mathbb{K}_m \) and \( \mathbb{K}_m \) is the set of all \( n! / [(n - m)! m!] \) distinct combinations of \( m \) elements from the first \( n \) consecutive natural numbers.

The U-statistics were first studied in the landmark articles of Halmos (1946) and Hoeffding (1948). Since their introduction, a significant body of work has been produced on the topic. Comprehensive treatments of the topic can be found in Serfling (1980, Ch. 5), Lee (1990), Koroljuk & Borovskich (1994), and Bose & Chatterjee (2018).

In recent years, concentration inequalities have become an important research theme in the machine learning, probability, and statistics research, due to their range of practical and theoretical applications. The current state of the literature is well-reported in the volumes of Ledoux (2001), Massart (2007), Dubhashi & Panconesi (2009), Boucheron et al. (2013), and Bercu et al. (2015).

The first results regarding the concentration of \( U_n \) about its mean value \( \theta \) were those established in Hoeffding (1963). Assume that \( h \in [a, b] \) (for \( a, b \in \mathbb{R} \), such that \( a < b \)), and denote the variance
of h by \( \sigma^2 = \mathbb{V}_F h (X_1, \ldots, X_m) \). Then, for any \( \epsilon > 0 \) and \( m \leq n \), Hoeffding (1963) proved the one-sided inequalities

\[
\Pr (U_n - \theta \geq \epsilon) \leq \exp \left( -\frac{2 \lfloor n/m \rfloor \epsilon^2}{(b - a)^2} \right) \quad \text{and}
\]

\[
\Pr (U_n - \theta \geq \epsilon) \leq \exp \left( -\frac{\lfloor n/m \rfloor \epsilon^2}{2\sigma^2 + (2c/3) \epsilon} \right),
\]

where \( \lfloor z \rfloor = \max \{ \zeta \in \mathbb{Z} : \zeta \leq z \} \) is the floor function (cf. Arcones & Gine 1993, Prop. 2.3) and \( c = 2 \max \{ |a|, |b| \} \). It is procedural to demonstrate that the right-hand sides (RHSs) of (1) and (2) also upper bound \( \Pr (\theta - U_n) \), thus we have the absolute inequalities

\[
\Pr (|U_n - \theta| \geq \epsilon) \leq 2 \exp \left( -\frac{2 \lfloor n/m \rfloor \epsilon^2}{(b - a)^2} \right) \quad \text{and}
\]

\[
\Pr (|U_n - \theta| \geq \epsilon) \leq 2 \exp \left( -\frac{\lfloor n/m \rfloor \epsilon^2}{2\sigma^2 + (2c/3) \epsilon} \right),
\]

since \( \Pr (|U_n - \theta| \geq \epsilon) = \Pr (U_n - \theta \geq \epsilon) + \Pr (\theta - U_n \geq \epsilon) \).

Since the establishment of (3) and (4), there had been little progress in the derivation of fundamentally novel bounds for U-statistics. A major contribution in this direction was due to Arcones (1995). Assume that \( h \in [0, 1] \), and that \( \varsigma^2 = \mathbb{V}_F \mathbb{E}_F [h (X_1, \ldots, X_m) | X_1] < \infty \) exists. Then, for any \( \epsilon > 0 \) and \( m \leq n \), Arcones (1995) proved that

\[
\Pr (|U_n - \theta| \geq \epsilon) \leq 4 \exp \left( -\frac{\lfloor n/m \rfloor \epsilon^2}{2m\varsigma^2 + (2^{m+3}m^{m-1} + [2/3]m^{-2}) \epsilon} \right). \quad (5)
\]

In practice, only bounds of h tend to be known, regarding data from any arbitrary DGP. Thus, without knowledge of the variances \( \sigma^2 \) or \( \varsigma^2 \), the Bernstein-type bounds (2), (4), and (5) cannot be used numerically. In such situations, only the Hoeffding-type bounds (1) and (3) tend to see practical application.

Let \( X_1, \ldots, X_n \in [a, b] \) be independent random variables. If \( \Sigma_n^2 = n^{-1} \sum_{i=1}^n \mathbb{V} X_i \) and \( \bar{X}_n = \)
\[ n^{-1} \sum_{i=1}^{n} X_i, \] then for any \( \epsilon > 0 \), Bennett (1962) proved the classic Bernstein-type inequalities

\[
\Pr \left( \bar{X}_n - \mathbb{E}\bar{X}_n \geq \epsilon \right) \leq \exp \left( -\frac{n \epsilon^2}{\Sigma_n^2/2 + (2c/3) \epsilon} \right) \tag{6}
\]

and

\[
\Pr \left( \left| \bar{X}_n - \mathbb{E}\bar{X}_n \right| \geq \epsilon \right) \leq 2 \exp \left( -\frac{\epsilon^2}{\Sigma_n^2/2 + (2c/3) \epsilon} \right), \tag{7}
\]

where \( c = 2 \max \{|a|, |b|\} \). See also Bercu et al. (2015, Thm. 2.28). Similar to the U-statistics counterpart, the general inequalities (6) and (7) require knowledge of the variance \( \Sigma_n^2 \) to be of practical use.

A primary application of concentration inequalities is the construction of \((1 - \delta) \times 100\%\) confidence intervals (CIs) for some estimator of interest, where \( \delta \in (0, 1) \). Recently, empirical CIs based on the (6) and (7) forms, where \( \Sigma_n^2 \) is replaced by an estimator, have been constructed by Audibert et al. (2009) and Maurer & Pontil (2009). These results allow for the construction of CIs around the mean of data with known bounds, but unknown variances. Such bounds were applied to perform variance penalized estimation in Maurer & Pontil (2009) and for the analysis of multi-armed bandit problems in Audibert et al. (2009). Other examples of applications include racing-based online model selection (Mnih et al., 2008) and classifier boosting (Shivaswamy & Jebara, 2010).

In Peel et al. (2010), analogous results to Audibert et al. (2009) and Maurer & Pontil (2009) were obtained, for the specific context of U-statistics. That is, empirical two-sided CIs based on the Bernstein-type bounds (4) and (5) were constructed, where the variances \( \sigma^2 \) or \( \varsigma^2 \) were replaced by respective empirical estimators. These CIs have useful applications in racing-based online model selection (Peel et al., 2010), change detection (Sakthithasan et al., 2013), and optimal treatment allocation (Liang et al., 2018). Since the work of Peel et al. (2010), Loh & Nowozin (2013) also presented an empirical two-side CI, based on (5).

In this paper, we utilize inequalities (1) and (2) in order to construct empirical one-sided CIs for U-statistics. We demonstrate that these bounds are able to produce one-sided CIs that are analogous to the two-sided bounds of Peel et al. (2010). Furthermore, the two-sided form of our construction provides tighter bounds than those obtained by Peel et al. (2010). Using
our constructed CIs, we also demonstrate how one can obtain empirical CIs for the mean from a recently-derived variance-dependent improved Hoeffding-type concentration inequality of Bercu et al. (2015). Our work can be seen as an extension and refinement of the results of Peel et al. (2010) and as an addition to the literature on empirical variance-dependent bounds, as pioneered by Audibert et al. (2009) and Maurer & Pontil (2009). We make numerous comments regarding the relationship between our work and previously obtained outcomes in the final section of the article.

The paper proceeds as follows. In Section 2, we present the main results of the paper. New empirical CIs are derived in Section 3. Concluding remarks regarding our exposition and results are presented in Section 4.

2 Main results

2.1 Technical preliminaries

We begin the presentation of our main results by providing a pair of lemmas that are used throughout the remainder of the paper.

Lemma 1 (Union bound). For random variables $X, Y, Z$,

$$\Pr (X > Z) \leq \Pr (X > Y) + \Pr (Y > Z).$$

Proof. For any events $\mathcal{A}, \mathcal{B}$, we have the union bound:

$$\Pr (\mathcal{A} \cup \mathcal{B}) \leq \Pr (\mathcal{A}) + \Pr (\mathcal{B}).$$

Consider that $(X > Z)$ is a subset of $(X > Y) \cup (Y > Z)$. Thus

$$\Pr (X > Z) \leq \Pr ((X > Y) \cup (Y > Z)) \leq \Pr (X > Y) + \Pr (Y > Z).$$

$\square$
Lemma 2 (Inequality reversal). Suppose that $X$ is a random variable, and let $A, B > 0$ and $C, D \geq 0$, such that for every $\epsilon > 0$,

$$\Pr(X \geq \epsilon) \leq A \exp \left(-\frac{B\epsilon^2}{C + D\epsilon}\right).$$

Then, with probability at least $1 - \delta$, we have

$$X \leq \sqrt{\frac{C}{B} \log \frac{A}{\delta} + \frac{D}{B} \log \frac{A}{\delta}}.$$ 

Proof. Let $\Pr(X \geq \epsilon) = \delta$, then we have

$$\delta \leq A \exp \left(-\frac{B\epsilon^2}{C + D\epsilon}\right),$$

which we can solve for $\epsilon$, to get

$$\epsilon \leq \frac{1}{2B} \left(D \log \frac{A}{\delta} + \sqrt{D^2 \log^2 \frac{A}{\delta} + 4BC \log \frac{A}{\delta}}\right).$$

We then apply the square root inequality $\sqrt{x + y} \leq \sqrt{x} + \sqrt{y}$ in order to obtain the desired result. \qed

Although the two preceding results appear elsewhere in the literature, we include them for the convenience of the reader. Lemma 2 appears as Lemma 1 in Peel et al. (2010).

2.2 Concentration of the variance

Let $X_1, \ldots, X_n \in \mathbb{R}$ be IID random variables and note that the symmetric kernel

$$h(x_1, x_2) = (x_1 - x_2)^2 / 2$$
corresponds to the U-statistic

\[ U_n = \left( \frac{n}{2} \right)^{-1} \sum_{\kappa \in \mathcal{K}_2} \frac{(X_{\kappa(1)} - X_{\kappa(2)})^2}{2} = (n - 1)^{-1} \sum_{i=1}^{n} (X_i - \bar{X}_n)^2 = S_n^2, \]

which is the unbiased estimator of the variance. That is \( \theta = \mathbb{E}_F S_n^2 = \mathbb{V}_F X \), where \( X \) arises from the same DGP as the sample \( X_1, \ldots, X_n \). Furthermore, assume that \( X \in [0,1] \), so that \( h(X_1, X_n) \in [0,1/2] \). Using (1), we can obtain our first result.

**Proposition 1.** If \( X_1, \ldots, X_n \in [0,1] \) are IID, then for any \( \epsilon > 0 \),

\[ \Pr \left( S_n^2 - \mathbb{V}_F X \geq \epsilon \right) \leq \exp \left( -8 \left\lfloor \frac{n}{2} \right\rfloor \epsilon^2 \right). \]  

(8)

Alternatively, with probability at least \( 1 - \delta \),

\[ S_n^2 - \mathbb{V}_F X \leq \sqrt{\frac{1}{8 \left\lfloor n/2 \right\rfloor} \log \frac{1}{\delta}}. \]  

(9)

Both (8) and (9) hold with \( S_n^2 - \mathbb{V}_F X \) replaced by \( \mathbb{V}_F X - S_n^2 \).

**Proof.** Result (8) is obtained by direct substitution \( S_n^2 \) into (1), and (9) arises via Lemma 2. \( \square \)

Assume the same hypothesis as Proposition 1. We consider instead a bound for \( S_n^2 \) using (2).

Since \( h(X_1, X_2) \leq 1/2 \), it is true that

\[ \mathbb{V}_FS_n^2 = \mathbb{E}_F \left[ S_n^4 \right] - \mathbb{E}_F \left[ S_n^2 \right] \leq \mathbb{E}_F S_n^2 = \mathbb{V}_F X, \]  

(10)

and thus, by direct substitution into (2), we obtain the bound

\[ \Pr \left( S_n^2 - \mathbb{V}_F X \geq \epsilon \right) \leq \exp \left( -\frac{\left\lfloor n/2 \right\rfloor \epsilon^2}{2\mathbb{V}_F X + (2/3)\epsilon} \right), \]

since \( c = \max \{0, 1\} = 1 \).

Using Lemma 2, we have, with probability at least \( 1 - \delta \),
\[
S_n^2 - \mathbb{V}_F X \leq \sqrt{\frac{2\mathbb{V}_F X}{[n/2]} \log \frac{1}{\delta} + \frac{2}{3[n/2]} \log \frac{1}{\delta}},
\]
which we can complete the square to obtain
\[
S_n^2 \leq \left[ \sqrt{\mathbb{V}_F X} + \frac{1}{2} \sqrt{\frac{2}{[n/2]} \log \frac{1}{\delta}} \right]^2 + \frac{1}{6[n/2]} \log \frac{1}{\delta},
\]
(11)
Taking the square root, and applying the square root inequality to both sides of (11) yields
\[
\sqrt{S_n^2} + \sqrt{\frac{1}{6[n/2]} \log \frac{1}{\delta}} \leq \sqrt{\mathbb{V}_F X} + \sqrt{\frac{2}{4[n/2]} \log \frac{1}{\delta}}
\]
\[
\leq \sqrt{\mathbb{V}_F X} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{6} \right) \sqrt{\frac{1}{[n/2]} \log \frac{1}{\delta}}.
\]
From (2), we also have, with probability at least 1 - \(\delta\),
\[
\mathbb{V}_F X - S_n^2 \leq \sqrt{\frac{2\mathbb{V}_F X}{[n/2]} \log \frac{1}{\delta} + \frac{1}{3[n/2]} \log \frac{1}{\delta}},
\]
which rearranges to
\[
\mathbb{V}_F X - \sqrt{\frac{2\mathbb{V}_F X}{[n/2]} \log \frac{1}{\delta} - \frac{1}{3[n/2]} \log \frac{1}{\delta}} \leq S_n^2
\]
and we can again complete the square to obtain
\[
\left[ \sqrt{\mathbb{V}_F X} - \frac{1}{2} \sqrt{\frac{2}{[n/2]} \log \frac{1}{\delta}} \right]^2 \leq S_n^2 + \frac{7}{6[n/2]} \log \frac{1}{\delta}.
\]
By the square root inequality, we have
\[
\sqrt{\mathbb{V}_F X} \leq \sqrt{S_n^3} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{42}}{6} \right) \sqrt{\frac{1}{[n/2]} \log \frac{1}{\delta}}.
\]
We therefore have the following empirical one-sided CIs.
Proposition 2. If $X_1, \ldots, X_n \in [0, 1]$ are IID, then with probability at least $1 - \delta$,

\[
\sqrt{S_n^2} \leq \sqrt{\mathbb{V}_F X} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{6} \right) \sqrt{\frac{1}{\lceil n/2 \rceil}} \log \frac{1}{\delta} \quad \text{and} \quad (12)
\]

\[
\sqrt{\mathbb{V}_F X} \leq \sqrt{S_n^2} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{42}}{6} \right) \sqrt{\frac{1}{\lceil n/2 \rceil}} \log \frac{1}{\delta}, \quad (13)
\]

where $\sqrt{2}/2 + \sqrt{6}/6 \leq 1.116$ and $\sqrt{2}/2 + \sqrt{42}/6 \leq 1.788$.

2.3 Variance of a U-statistic

Assume that $h \in [0, 1]$. Following Peel et al. (2010), we introduce a new kernel of order $2m$:

\[
\eta(x_1, \ldots, x_{2m}) = [h(x_1, \ldots, x_m) - h(x_{m+1}, \ldots, x_{2m})]^2/2.
\]

We note that $\eta$ can either be symmetric or otherwise. If $\eta$ is not symmetric, then we can define a symmetric version of $\eta$, in the form

\[
\tilde{\eta}(x_1, \ldots, x_{2m}) = \frac{1}{(2m)!} \sum_{\pi \in \Pi_{2m}} \eta(x_{\pi(1)}, \ldots, x_{\pi(2m)}),
\]

where $\mathbb{E}_F [\eta(X_1, \ldots, X_{2m})] = \mathbb{E}_F [\tilde{\eta}(X_1, \ldots, X_{2m})]$ (cf. Serfling 1980, Ch. 5). Furthermore, we can inspect that

\[
\mathbb{E}_F \eta = \frac{1}{2} \mathbb{E}_F [h(X_1, \ldots, X_m) - h(X_{m+1}, \ldots, X_{2m})]^2
\]

\[
= \frac{1}{2} \left[ \mathbb{E}_F h^2 - 2 \mathbb{E}_F h \mathbb{E}_F h + \mathbb{E}_F h^2 \right]
\]

\[
= \mathbb{E}_F h^2 - [\mathbb{E}_F h]^2 = \mathbb{V}_F h = \sigma^2,
\]

and note also that $h \in [0, 1]$ implies $\eta \in [0, 1/2]$.

Consider the U-statistics

\[
W_n = \left( \frac{n}{2m} \right)^{-1} \sum_{\kappa \in \mathbb{K}_{2m}} \eta(X_{\kappa(1)}, \ldots, X_{\kappa(2m)})
\]
and
\[ \tilde{W}_n = \left( \frac{n}{2m} \right)^{-1} \sum_{\kappa \in \mathcal{K}_{2m}} \tilde{\eta}(X_{\kappa(1)}, \ldots, X_{\kappa(2m)}) . \]

Using \( W_n \) and \( \tilde{W}_n \), we seek to obtain \((1 - \delta) \times 100\% \) one-sided CIs for the comparison of the quantities \( \nabla_F h \) and \( W_n \).

Assume that \( \eta \) is a symmetric kernel. As in Section 2.2, we may use (11) to obtain the following result, analogous to Proposition 1.

**Proposition 3.** If \( X_1, \ldots, X_n \in \mathcal{X} \) are IID, \( h \in [0, 1] \), and \( \eta \) is symmetric, then for any \( \epsilon > 0 \),

\[
\Pr \left( W_n - \sigma^2 \geq \epsilon \right) \leq \exp \left( -8 \left\lfloor n / (2m) \right\rfloor \epsilon^2 \right). \tag{14}
\]

Alternatively, with probability at least \( 1 - \delta \),

\[
W_n - \sigma^2 \leq \sqrt{\frac{1}{8 \left\lfloor n / (2m) \right\rfloor} \log \frac{1}{\delta}}. \tag{15}
\]

Both (14) and (15) hold with \( W_n - \sigma^2 \) replaced by \( \sigma^2 - W_n \).

Unfortunately, we cannot always assume that \( \eta \) is symmetric. However, by definition, \( \tilde{\eta} \) is always symmetric and has the same range as \( \eta \). That is, if \( h \in [0, 1] \), then \( \tilde{\eta} \in [0, 1/2] \). Thus, we have the following Proposition.

**Proposition 4.** If \( X_1, \ldots, X_n \in \mathcal{X} \) are IID and \( h \in [0, 1] \), then all of the conclusions from Proposition 3 hold with \( W_n \) replaced by \( \tilde{W}_n \).

In order to obtain Bernstein bound analogs of Proposition 3 and Proposition (4), we require the following versions of inequality (10):

\[
V_F \eta = \mathbb{E}_F \left[ \eta^2 \right] - \left[ \mathbb{E}_F \eta \right]^2 \leq \mathbb{E}_F \left[ \eta^2 \right] \leq \mathbb{E}_F \eta = \sigma^2 \text{ and}
\]

\[
V_F \tilde{\eta} = \mathbb{E}_F \left[ \tilde{\eta}^2 \right] - \left[ \mathbb{E}_F \tilde{\eta} \right]^2 \leq \mathbb{E}_F \left[ \tilde{\eta}^2 \right] \leq \mathbb{E}_F \tilde{\eta} = \sigma^2 .
\]

In the same manner in which Proposition 2 was obtained, we may prove the following result.
Proposition 5. If $X_1, \ldots, X_n \in \mathbb{X}$ are IID, $h \in [0, 1]$, and $\eta$ is symmetric, then with probability at least $1 - \delta$,\[ \sqrt{W_n} \leq \sqrt{\sigma^2} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{6} \right) \sqrt{\frac{1}{[n/(2m)]}} \log \frac{1}{\delta} \] and\[ \sqrt{\sigma^2} \leq \sqrt{W_n} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{42}}{6} \right) \sqrt{\frac{1}{[n/(2m)]}} \log \frac{1}{\delta}, \] where $\sqrt{2}/2 + \sqrt{6}/6 \leq 1.116$ and $\sqrt{2}/2 + \sqrt{42}/6 \leq 1.788$. More generally, (16) and (17) also hold with $W_n$ replaced by $\tilde{W}_n$.

2.4 Empirical confidence intervals

Assume that $X_1, \ldots, X_n \in \mathbb{X}$ are IID and $h \in [0, 1]$. Via inequality (2) and Lemma 2 we have\[ U_n - \theta > \sqrt{\frac{2\sigma^2}{[n/m]}} \log \frac{2}{\delta} + \frac{4}{3} \left[ \frac{1}{[n/(2m)]} \right] \log \frac{2}{\delta}, \] with probability at most $\delta/2$. If $\eta$ is symmetric, then Proposition 3 and Proposition 4 imply that\[ \sigma^2 > W_n + \sqrt{\frac{1}{8 \left[ n/(2m) \right]}} \log \frac{2}{\delta}, \] with probability at most $\delta/2$. We may apply Lemma 1 along with the square root inequality in order to prove that\[ U_n - \theta \leq \sqrt{\frac{2W_n}{[n/m]}} \log \frac{2}{\delta} + \sqrt{\frac{1}{[n/m]}} \left[ \sqrt{\frac{1}{2 \left[ n/(2m) \right]}} \log^{3/2} \left( \frac{2}{\delta} \right) \right] + \frac{4}{3} \left[ \frac{1}{[n/m]} \right] \log \frac{2}{\delta}, \] with probability at least $1 - \delta$. Inequality (20) also holds with $U_n - \theta$ replaced by $\theta - U_n$. Furthermore, (20) also holds with $W_n$ replaced by $\tilde{W}_n$.

From Proposition 3 we have\[ \sqrt{\sigma^2} > \sqrt{W_n} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{42}}{6} \right) \sqrt{\frac{1}{[n/(2m)]}} \log \frac{2}{\delta}, \]
with probability at most \( \delta/2 \), for symmetric \( \eta \). Using Lemma 1 in combination with (18), we obtain the bound

\[
U_n - \theta \leq \sqrt{2W_n} \frac{2}{n/m} \log \frac{2}{\delta} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{42}}{6} \right) \sqrt{\frac{2}{n/m} \frac{n}{n/(2m)}} \log \frac{2}{\delta} + \frac{4}{3\lfloor n/m \rfloor \log \frac{2}{\delta}} + 4 \frac{\lfloor n/m \rfloor \log \frac{2}{\delta}}{3}
\]

with probability at least \( 1 - \delta \). Generally, (21) also holds when we replace \( U_n - \theta \) by \( \theta - U_n \) or \( W_n \) by \( \tilde{W}_n \), or both simultaneously. We summarize the results of this section in the following theorem.

**Theorem 1.** If \( X_1, \ldots, X_n \in \mathbb{X} \) are IID, \( h \in [0, 1] \), and \( \eta \) is symmetric, then inequalities (20) and (21) hold with probability at least \( 1 - \delta \). More generally, both (20) and (21) hold with probability at least \( 1 - \delta \) when \( U_n - \theta \) is replaced by \( \theta - U_n \), when \( W_n \) is replaced by \( \tilde{W}_n \), or when both quantities are substituted, simultaneously.

### 3 Empirical confidence intervals based on an improved Hoeffding inequality

For independent random variables \( X_1, \ldots, X_n \in [a, b] \), the inequalities

\[
\Pr \left( \bar{X}_n - \mathbb{E} \bar{X}_n \geq \epsilon \right) \leq \exp \left( -\frac{2n\epsilon^2}{(b-a)^2} \right) \quad \text{and} \quad \Pr \left( \bar{X}_n - \mathbb{E} \bar{X}_n \right) \geq \epsilon \leq 2 \exp \left( -\frac{2n\epsilon^2}{(b-a)^2} \right)
\]

were proved, for any \( \epsilon > 0 \), in [Hoeffding, 1963]. In [Bercu et al., 2015], an interesting improvement to the Hoeffding inequality of form (22) was reported. We present the IID expectation form of the inequality below, and note that the more general summation form appears as Theorem 2.47 in [Bercu et al., 2015].

**Theorem 2** (Bercu et al., 2015). If \( X_1, \ldots, X_n \in [a, b] \) are IID random variables, then

\[
\Pr \left( \bar{X}_n - \mathbb{E}_F X \geq \epsilon \right) \leq \exp \left( -\frac{3n\epsilon^2}{(b-a)^2 + 2\mathbb{V}_F X} \right).
\]
Furthermore, (24) also holds when $\bar{X}_n - \mathbb{E}_F X$ is replaced by $\mathbb{E}_F X - \bar{X}_n$.

Without loss of generality, suppose that $[a, b] = [0, 1]$. Then, we obtain

$$
\Pr(\bar{X}_n - \mathbb{E}_F X \geq \epsilon) \leq \exp\left(-\frac{3n\epsilon^2}{1 + 2\mathbb{V}_F X}\right)
$$

and, with probability at least $1 - \delta$,

$$
\bar{X}_n - \mathbb{E}_F X \leq \sqrt{\frac{1 + 2\mathbb{V}_F X}{3n}} \log \frac{1}{\delta},
$$

via Lemma 2. Thus, with probability at most $\delta/2$,

$$
\bar{X}_n - \mathbb{E}_F X > \sqrt{\frac{1 + 2\mathbb{V}_F X}{3n}} \log \frac{2}{\delta}. \quad (25)
$$

Similar to (19), we have

$$
\mathbb{V}_F X > S_n^2 + \sqrt{\frac{1}{8 \lceil n/2 \rceil}} \log \frac{2}{\delta}, 
$$

with probability at most $\delta/2$, via (9).

Combining (25) and (26) via Lemma 1 and the square root inequality then yields

$$
\bar{X}_n - \mathbb{E}_F X \leq \sqrt{\frac{1 + 2S_n^2}{3n}} \log \frac{2}{\delta} + \sqrt{\frac{1}{12n}} \sqrt{\frac{8}{\lceil n/2 \rceil}} \log^{3/2} \left(\frac{2}{\delta}\right), \quad (27)
$$

with probability at least $1 - \delta$. Given the symmetry of (24), we may also switch $\bar{X}_n - \mathbb{E}_F X$ with $\mathbb{E}_F X - \bar{X}_n$ in (27).

Next, (13) implies that

$$
\sqrt{\mathbb{V}_F X} > \sqrt{S_n^2} + \left(\frac{\sqrt{2}}{2} + \frac{\sqrt{42}}{6}\right) \sqrt{\frac{1}{\lceil n/2 \rceil}} \log \frac{2}{\delta} \quad (28)
$$

with probability at most $\delta/2$. Combining with (28) via Lemma 1 and the square root inequality then yields
\[ \hat{X}_n - \mathbb{E}_F X \leq \sqrt{\frac{1}{3n}} \log \frac{2}{\delta} + \sqrt{\frac{2S_n^2}{3n}} \log \frac{2}{\delta} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{42}}{6} \right) \sqrt{\frac{2}{3 \lceil n/2 \rceil}} \log \frac{2}{\delta}, \]  

(29)

with probability at least \(1 - \delta\). Again, the inequality (29) holds if we switch \(\hat{X}_n - \mathbb{E}_F X\) with \(\mathbb{E}_F X - \hat{X}_n\).

Finally, note that we can obtain two-sided versions of (27) and (29) by considering the union of lower bounds on \(\hat{X}_n - \mathbb{E}_F X\), \(\mathbb{E}_F X - \hat{X}_n\), and \(\sqrt{V_F} X\), simultaneously. We then obtain, with probability at least \(1 - \delta\),

\[ |\hat{X}_n - \mathbb{E}_F X| \leq \sqrt{\frac{1 + 2S_n^2}{3n}} \log \frac{4}{\delta} + \frac{1}{12n} \sqrt{\frac{8}{\lceil n/2 \rceil}} \log^{3/2} \left( \frac{3}{\delta} \right) \]

and

\[ |\hat{X}_n - \mathbb{E}_F X| \leq \sqrt{\frac{1}{3n}} \log \frac{3}{\delta} + \sqrt{\frac{2S_n^2}{3n}} \log \frac{3}{\delta} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{42}}{6} \right) \sqrt{\frac{2}{3 \lceil n/2 \rceil}} \log \frac{3}{\delta}. \]

4 Concluding remarks

Remark 1. Inequalities (2), (4), (6), and (7) are often stated with either the additional assumption that \(\mathbb{E}_F h = 0\) or that \(\mathbb{E}\hat{X}_n = 0\) (see, e.g., Arcones & Gine, 1993, Prop. 2.3, Arcones (1995), and Bercu et al., 2015, Thm. 2.28). As such, the constant \(c\) is usually defined as \(\max \{|a|, |b|\}\). However we define \(c = 2 \max \{|a|, |b|\}\), since we allow for cases where \(\mathbb{E}_F h \neq 0\) or \(\mathbb{E}\hat{X}_n \neq 0\), and due to the fact that \(|X - \mathbb{E}X| \leq |X| + |\mathbb{E}X| \leq 2 \max \{|a|, |b|\}\), for any \(X \in [a,b]\).

Remark 2. To the best of our knowledge, Propositions 1 and 3 and Proposition 4 do not appear elsewhere in the literature. Proposition 2 is a special case of Proposition 5, where we use the order one kernel \(h = x\). Proposition 2 can be viewed as a refinement of intermediate results from the proof of Peel et al. (2010, Thm. 3). Our refinements are as follows: we correctly differentiated the cases where \(\eta\) is symmetric or where we must replace it by \(\hat{\eta}\); we constructed our CIs using the inequality (2) instead of the two-sided version (4), and thus obtained better constants; we obtained one-sided CIs for both \(\sqrt{W_n} - \sqrt{\sigma^2}\) and \(\sqrt{\sigma^2} - \sqrt{W_n}\) (and when \(W_n\) is replaced by \(\hat{W}_n\), whereas Peel et al. (2010) only considered the CI for \(\sqrt{\sigma^2} - \sqrt{W_n}\); and lastly, we make no assumptions on
the divisibility of \( n \), whereas Peel et al. (2010) assumes that \( n \) is divisible by both 2 and \( m \) in their presentation.

**Remark 3.** We may compare Proposition 2 directly to Theorem 10 of Maurer & Pontil (2009), which cannot be obtained within the U-statistics framework. Under the same conditions as Proposition 2 Maurer & Pontil (2009, Thm. 10) states that, with probability at least \( 1 - \delta \),

\[
\sqrt{S_n^2} \leq \sqrt{V_F X} + \sqrt{\frac{2}{n - 1} \log \frac{1}{\delta}} \quad \text{and} \quad (30)
\]

\[
\sqrt{V_F X} \leq \sqrt{S_n^2} + \sqrt{\frac{2}{n - 1} \log \frac{1}{\delta}}. \quad (31)
\]

It is easy to see that the CIs of Maurer & Pontil (2009, Thm. 10) achieve the same rates with respect to \( n \) and \( \delta \) as Proposition 2. Furthermore, for large \( n \), (30) and (31) provide tighter bounds than (12) and (13), respectively, for almost all values of \( n \). We note that the only exception is when \( n = 2 \) or \( 4 \), where (12) is tighter than (30).

**Remark 4.** By considering the lower bounds of \( U_n - \theta, \theta - U_n \) and \( \sqrt{\sigma^2} \), simultaneously, we may obtain the two-sided version of (21):

\[
|U_n - \theta| \leq \sqrt{\frac{2W_n}{[n/m]}} \log \frac{3}{\delta} + \left( \sqrt{\frac{2}{2}} + \sqrt{\frac{\sqrt{42}}{6}} \right) \sqrt{\frac{2}{[n/m] \lfloor n / (2m) \rfloor}} \log \frac{3}{\delta} + \frac{4}{3 \lfloor n/m \rfloor} \log \frac{3}{\delta}, \quad (32)
\]

with probability at least \( 1 - \delta \). We may compare this directly with Peel et al. (2010, Thm. 3), which for symmetric \( \eta \) and under the assumption that \( n \) is divisible by 2 and \( m \), implies that

\[
|U_n - \theta| \leq \sqrt{\frac{2mW_n}{n}} \log \frac{4}{\delta} + \frac{5m}{n} \log \frac{4}{\delta},
\]

with probability at least \( 1 - \delta \). Under the same assumptions regarding the divisibility of \( n \), we can write (32) as

\[
|U_n - \theta| \leq \sqrt{\frac{2mW_n}{n}} \log \frac{3}{\delta} + \left( 4 + \sqrt{2} \lfloor 3 + \sqrt{21} \rfloor \right) \frac{m}{3n} \log \frac{3}{\delta},
\]

where \( \left( 4 + \sqrt{2} \lfloor 3 + \sqrt{21} \rfloor \right) / 3 \leq 4.908 \). Thus, (32) is tighter than the CI of Peel et al. (2010, Thm. 3).
Remark 5. As noted in Bercu et al. (2015, Sec. 2.5.4), (24) is a strict improvement of (22) since \((b - a)^2 \geq 4V_F X\). Furthermore, it is provable that \((b - a)^2 \geq 4V_F X\) for all random variables \(X \in [a, b]\), except for binary \(X \in \{a, b\}\), where \(Pr(X = a) = Pr(X = b) = 1/2\).

Remark 6. CIs (27) and (29) may be compared directly to the empirical Bernstein-type inequalities of Audibert et al. (2009) and Maurer & Pontil (2009). Under the same conditions as those under which (27) and (29) are established, with probability at least \(1 - \delta\), we have

\[
\bar{X}_n - E_F X \leq \sqrt{\frac{2(n - 1)S_n^2}{n^2} \log \left( \frac{2}{\delta} \right)} + \frac{3}{n} \log \left( \frac{2}{\delta} \right)
\]

and

\[
\bar{X}_n - E_F X \leq \sqrt{\frac{2S_n^2}{n} \log \left( \frac{2}{\delta} \right)} + \frac{7}{3} \frac{\log \left( \frac{2}{\delta} \right)}{\log \left( \frac{2}{\delta} \right)},
\]

via Audibert et al. (2009, Thm. 1) and Maurer & Pontil (2009, Thm. 4), respectively. A visual comparison of the logarithms of the RHSs of (27), (29), (33), and (34) is provided in Figure 1. We compare the four bounds for \(S_n^2 \in \{0.05, 0.25\}\) and \(\delta \in \{0.01, 0.1\}\). It is observable that (27) was uniformly tighter than (29). For smaller values of \(S_n^2\), (33) and (34) were tighter than (27), for larger \(n\). For larger \(S_n^2\), (27) was tighter than (33) and (34) over a middle range of \(n\), however (29) remained uncompetitive. Changing \(\delta\) did not tend to alter the relative performance of the bounds. As noted by Maurer & Pontil (2009), (34) has better constants than (33) and thus provided tighter bounds for larger values of \(n\). We finally note that (29) can be improved by using (31) in the place of (13) in its derivation. This was not pursued because we wished for the derivation to be self-contained within the U-statistics framework.

Remark 7. For \(k, n \in \mathbb{N}\), such that \(k < n\), we have \(|n/k| > (n - k + 1)/k\). Thus, we may remove the floor operator in each of the inequalities where it appears by upper bounding its multiplicative inverse. For instance,

\[
\sqrt{\frac{2mW_n}{n - m + 1} \log \frac{3}{\delta}} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{42}}{6} \right) \sqrt{\frac{4m^2}{(n - m + 1)(n - 2m + 1)} \log \frac{3}{\delta}} + \frac{4m}{3(n - m + 1) \log \frac{3}{\delta}}
\]

is an upper bound for the RHS of (32).
A: $S^2 = 0.05$ and delta = 0.01

B: $S^2 = 0.25$ and delta = 0.01

C: $S^2 = 0.05$ and delta = 0.1

D: $S^2 = 0.25$ and delta = 0.1

Figure 1: Logarithms of the upper bounds of the CIs (27), (29), (33), and (34), as a function of \( n \), for \( S_n^2 \) and \( \delta \) set at various levels. Each subplot A–D visualizes the relative performances of the four bounds, for the values \( S_n^2 \) and \( \delta \) that are displayed in the title. The labels Improved Hoeffding 1 and 2 correspond to (27) and (29), respectively, whereas Audibert and Maurer correspond to (33) and (34), respectively.
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