Exponential finite sample bounds for incomplete U-statistics

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Abstract

Incomplete U-statistics have been proposed to accelerate computation. They use only a subset of the subsamples required for kernel evaluations by complete U-statistics. This paper gives a finite sample bound in the style of Bernstein’s inequality. Applied to complete U-statistics the resulting inequality improves over the bounds of both Hoeffding and Arcones. For randomly determined subsamples it is shown, that as soon as their number reaches the square of the sample-size, the same order bound is obtained as for the complete statistic.

1 Introduction

Let \( \mu \) be a probability measure on a measurable space \( \mathcal{X} \), \( m \) an integer and \( K : \mathcal{X}^m \rightarrow \mathbb{R} \) a measurable, symmetric, bounded kernel. We wish to estimate the parameter \( \theta = \theta(\mu) = \mathbb{E}[K(X_1, \ldots, X_m)] \) from a finite sample \( X = (X_1, \ldots, X_n) \sim \mu^n \), where the number \( n \) of independent observations is much larger than the degree \( m \) of the kernel. The standard estimator is the U-statistic

\[
U(X) = \left( \begin{array}{c} n \\ m \end{array} \right)^{-1} \sum_{1 \leq i_1 < \ldots < i_m \leq n} K(X_{i_1}, \ldots, X_{i_m}).
\]

The dependence on \( K \), which should be understood in most cases, will not be made explicit. We also introduce the shorthand

\[
U(X) = \left( \begin{array}{c} n \\ m \end{array} \right)^{-1} \sum_{W \subset [n], |W|=m} K(X^W),
\]

where \( K(X^W) = K(X_{i_1}, X_{i_2}, \ldots, X_{i_m}) \) where \((i_1, i_2, \ldots, i_m)\) is an enumeration of \( W \), which is arbitrary by the symmetry of \( K \).

The U-statistic is an unbiased estimator of \( \theta \), and it has minimal variance among all unbiased estimators of \( \theta \) (10). On the other hand computational requirements are excessive for large \( m \) and \( n \). Since the number of subsets scales as \( n^m \) for \( n = 10^4 \) and \( m = 5 \) the order of necessary kernel evaluations is already about \( 10^{18} \) and out of reach for present computing power.

Since the high degree of dependence between the terms suggests, that a smaller number of kernel evaluations will already lead to an acceptable estimation error with lowered computational burden, incomplete U-statistics were proposed. Let \( W = (W_1, \ldots, W_M) \in \{ W \subset [n] : |W| = m \}^M \) be a sequence of \( M \) subsets of \( \{1, \ldots, n\} \) of cardinality \( m \), and define the incomplete U-statistic

\[
U_W(X) = \frac{1}{M} \sum_{i=1}^M K(X^{W_i}).
\]

The sequence \( W \) is called the design (14) and may be chosen at random, for example by sampling from \( \{ W \subset [n] : |W| = m \} \). The number \( M \) of required kernel evaluations can be interpreted as a computational budget.
In this work we address the question how small $M$ can be and how $W$ has to be chosen to obtain with overwhelming probability an acceptable bound on the estimation error for a finite sample of given size $n$. We will give variance dependent exponential finite sample bounds, modeled after the classical Bernstein inequality. If applied to complete U-statistics, which are a special case of incomplete ones, these bounds improve over the classical result of Hoeffding \( \cite{11} \) and over the more recent one of Arcones \( \cite{2} \). If $W = (W_1, ..., W_m)$ is sampled with replacement from the uniform distribution on $\{ W \subseteq [n] : |W| = m \}$, we show that $M = \lfloor n^2 \rfloor$ samples suffice to obtain with high probability a bound of the same order.

We assume the kernel to be bounded throughout and set $K : \mathcal{X}^m \to [-1, 1]$ to simplify statements. Results for different values of $\|K\|_{\infty}$ follow from re-scaling. The next section introduces some notation and gives a brief historical review of literature on the subject. Section 3 states our results and Section 4 contains the proofs.

2 Preliminaries

The symbol $|.|$ is used both for the absolute value of real numbers and the cardinality of sets. We use lower-case letters for scalars, upper-case letters for random variables and bold letters for vectors. For $n \in \mathbb{N}$, $[n]$ denotes the set $\{1, ..., n\}$. If $\mathcal{X}$ is a set, $y, y' \in \mathcal{X}$ and $k \in [n]$ we introduce the partial difference operator

$$ D^k_{y,y'} f (x) = f (S^k_y x) - f (S^k_{y'} x). $$

Throughout this work $1 \leq m < n$ will be fixed integers, and $K$ will be a measurable kernel $K : \mathcal{X}^m \to [-1, 1]$. The kernel $K$ will be assumed permutation symmetric unless otherwise stated. $X = (X_1, ..., X_n)$ will be an iid vector distributed in $\mathcal{X}^n$, that is $X \sim \mu^n$, where $\mu$ is a probability measure on $\mathcal{X}$ and $\mathcal{X}'$ will be an independent copy of $X$. For $K : \mathcal{X}^m \to [-1, 1]$ and $k \in [m]$ the conditional variances are defined as $\sigma^2_k (K) = \text{Var} \left[ \mathbb{E} [K (X_1, ..., X_m) | X_1, ..., X_k] \right]$, where the dependence on $K$ is usually omitted.

2.1 A brief history

Hoeffding \( \cite{12} \) proved the following classical results on the variance and the asymptotic behavior of U-statistics.

**Theorem 2.1.** If $\sigma^2_m < \infty$

$$ \text{Var} [U (X)] = \left( \frac{n}{m} \right)^{-1} \sum_{k=1}^{m} \binom{m}{k} \binom{n-m}{k} \sigma^2_k K $$

$$ \text{Var} [U (X)] = \frac{m^2 \sigma^2_1}{n} + O (n^{-2}) $$

$$ n^{1/2} (U - \theta) \to \mathcal{N} (0, m^2 \sigma^2_1) \text{ in distribution as } n \to \infty. $$

In the degenerate case, when $\sigma^2_1 = 0$, the central limit theorem given does not provide much information, one has to normalize with $n$ instead of $n^{1/2}$ and the limiting distribution will be chi-squared. We will give no special consideration to the degenerate cases in this paper. Hoeffding also gives the following Bernstein-type inequality for U-statistics.

**Theorem 2.2.** \( \cite{11} \) If $\lfloor n/m \rfloor = n/m$ then $\forall t > 0$

$$ \text{Pr} \left\{ U (X) - \theta > t \right\} \leq \exp \left( \frac{-nt^2}{2m\sigma^2_m + 4mt/3} \right) $$

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The assumption that \( n \) is a multiple of \( m \) is made for convenience. Let \( M = n/m \) and \( \mathbf{W} = (\{X_1, \ldots, X_m\}, \{X_{m+1}, \ldots, X_{2m}\}, \ldots, \{X_{(R-1)m+1}, \ldots, X_{Rm}\}) \). Then the incomplete U-statistics \( U_{\mathbf{W}}(\mathbf{X}) \) is a sum of independent variables to which the standard form of Bernstein’s inequality can be applied and yields the above bound for \( \Pr \{ U_{\mathbf{W}}(\mathbf{X}) - \theta > t \} \). This is the basis of Hoeffding’s proof and provides a Bernstein-type inequality for incomplete U-statistics with budget \( n/m \). Hoeffding uses convexity of the moment generating function and the average of all permutations of the \( X_i \) to show that the bound holds also for the complete U-statistic. This type of argument has found many applications in particular to the expected suprema of U-processes, but we will not follow up on it any further.

Above inequality also gives

$$\Pr \left\{ n^{1/2} (U(\mathbf{X}) - \theta) > t \right\} \leq \exp \left( \frac{-t^2}{2m\sigma_m^2 + 4mn^{-1/2}/3} \right) \rightarrow \exp \left( \frac{-t^2}{2m\sigma_m^2} \right) \text{ as } n \rightarrow \infty.$$  

This does not match the CLT in Theorem 2.1. If we take an inequality of Bernstein-type as a template, we would prefer

$$\Pr \{ U(\mathbf{X}) - \theta > t \} \leq \exp \left( \frac{-nt^2}{2m^2\sigma_1^2 + o(n) + C(m)t} \right).$$

Such a result has been given by Arcones [2].

**Theorem 2.3.** \( \forall t > 0 \)

$$\Pr \{ U(\mathbf{X}) - \theta > t \} \leq 2 \exp \left( \frac{-nt^2}{2m^2\sigma_1^2 + (2m^2m + 2m^{-1}/3) t} \right).$$

Apart from the leading constant 2 this is consistent with Hoeffding’s CLT in Theorem 2.1. But from a practical point of view the bound is useless for large values of \( m \). Already for \( m = 5 \) we would need \( n \) to be at least \( 10^5 \) to give the right-hand-side a nontrivial value less than one. For a complete U-statistic, this would require at least \( 10^{25} \) kernel evaluations.

The proof of Theorem 2.3 is based on the consideration of decoupled U-statistics, where \( \mathbf{X} \) is given an independent copy for each argument of the kernel. The bounds for decoupled U-statistics is then related to the original U-statistic with the help of decoupling inequalities ([De la Peña (1992)]). While these techniques have led to qualitatively very sharp bounds for degenerate U-statistics ([3], [9], [1]), they are also responsible for the excessive size of the scale term in above inequality.

Using a general concentration inequality for functions of independent variables [17] essentially gives the following bound (slightly simplified and adapted to the scaling of \( K \) chosen here).

**Theorem 2.4.** \( \forall t > 0 \)

$$\Pr \{ U(\mathbf{X}) - \theta > t \} \leq \exp \left( \frac{-t^2}{2\text{Var}(U(\mathbf{X}))/n^2 + 8m^2/n^2 + 4 (m^2 + m/3) t/n} \right).$$

This bound is consistent with the CLT and avoids the exponential dependence of the scale term on \( m \). Here we give a similar inequality for incomplete U-statistics. We show that it leads to a refinement of Theorem 2.3 for complete U-statistics, and that it suffices to make \( n^2 \) kernel evaluations, regardless of the degree \( m \) of the kernel to get the same order bound.

The study of incomplete U-statistics seems to begin with the work of Blom [4]. This and several other works considered the question of choosing \( \mathbf{W} \) so as to minimize the variance of the incomplete statistic. [4] and Lee [15] consider balanced incomplete block designs, which require \( M = n^2 \) for any order of the kernel. Kong et al ([14]) propose a sophisticated design strategy, which also takes the values of the \( X_i \) into account. Their method is shown to be asymptotically efficient in the sense, that the quotients of the variances of the corresponding incomplete U-statistics and the complete U-statistic approaches one as the sample size \( n \) tends to infinity. All these results are either asymptotic, or they only give probabilistic guarantees via Chebychev’s inequality, while exponential bounds should be possible for bounded kernels.

Several authors ([7], [6], [5], [5]) consider the optimization of incomplete U-statistics over classes of kernels. These works give uniform finite sample bounds, but they are of the worst-case type and do not take variance information into account.
3 Results

The concentration properties of a statistic depend on its sensitivity to the modification of a small portion of the data. To state our results we define the relevant sensitivity properties of the design, and, separate from this, of the kernel.

For an incomplete U-statistic with design \( W = (W_1, ..., W_M) \) the modification of a datum \( X_k \) will only affect those kernel evaluations \( K(X_k, \cdot) \), for which \( k \in W_i \). This motivates the following definition.

**Definition 3.1.** For a design \( W = (W_1, ..., W_M) \in \{W \subset [n]: |W| = m\}^M \) and \( k, l \in \{1, ..., n\} \), \( k \neq l \) define
\[
R_k(W) \triangleq |\{i : k \in W_i\}| \text{ and } R_{k,l}(W) \triangleq |\{i : k, l \in W_i\}|
\]
\[
A(W) \triangleq \sum_{k=1}^n \frac{R_k^2(W)}{M^2}, \quad B(W) \triangleq \sum_{k,l \neq 1} \frac{R_{k,l}^2(W)}{M^2}
\]
and \( C(W) \triangleq \max_k \frac{R_k}{M} \).

When there is no ambiguity we omit the dependency on the design \( W \).

The crucial properties of the kernel are its response to mixed partial difference operations.

**Definition 3.2.** For a bounded kernel \( K : \mathcal{X}^m \rightarrow [-1, 1] \) and \( X_1, ..., X_m, X'_1, X'_2 \) iid with values in \( \mathcal{X} \) define
\[
\beta(K) = \mathbb{E} \left[ \left( D_{X_1,X'_1} D_{X_2,X'_2} K(X_1, X_2, ..., X_m) \right)^2 \right]
\]
\[
\gamma(K) = \sup_{x \in \mathcal{X}^m, y, y' \in \mathcal{X}} \mathbb{E} \left[ \left( D_{y,y'} D_{X_2,X'_2} K(x_1, x_2, x_3, ..., x_m) \right)^2 \right]
\]
\[
\alpha(K) = \left( \sqrt{\beta(K)} / 2 + \sqrt{\gamma(K)} \right).
\]
When there is no ambiguity we omit the dependency on the kernel \( K \).

Worst-case bounds for \( \beta, \gamma \) and \( \alpha \) are \( \beta \leq 8, \gamma \leq 8 \) and \( \alpha \leq 2 + \sqrt{8} \leq 5 \) (see Lemma 4.10 below).

The following is our main Bernstein-type inequality for incomplete U-statistics.

**Theorem 3.3.** For fixed kernel \( K \) with values in \([-1, 1]\), design \( W \) and \( t > 0 \)
\[
\Pr \{ U_W(X) - \theta > t \} \leq \exp \left( -\frac{t^2}{2 A \sigma_t^2 + B \beta / 2 + (\sqrt{B} \gamma + 4 C / 3) t} \right),
\]
and for \( 0 < \delta \leq 1/e \) with probability at least \( 1 - \delta \)
\[
U_W(X) - \theta \leq \sqrt{2 A \sigma_t^2 \ln(1/\delta)} + \left( \alpha \sqrt{B} + 4 C / 3 \right) \ln(1/\delta).
\]

The proof will be given in the next section. Since \( \alpha, \beta \) and \( \gamma \) are invariant under \( K \leftrightarrow -K \) the same bound holds for \( \theta - U_W(X) \).

As a first application we give a refinement of Theorem 2.4.

**Corollary 3.4.** For \( K \) with values in \([-1, 1]\) and \( t > 0 \)
\[
\Pr \{ U(X) - \theta > t \} \leq \exp \left( -\frac{t^2}{2 m^2 \sigma_t^2 + m^4 \beta / (2n) + (m^2 \sqrt{7} + (4 / 3) m) t} \right),
\]
and for \( 0 < \delta \leq 1/e \) with probability at least \( 1 - \delta \)
\[
U(X) - \theta \leq \sqrt{2 m^2 \sigma_t^2 \ln(1/\delta)} + \left( \alpha m^2 + 4 m / 3 \right) \ln(1/\delta).
\]
Proof. For U-statistics \( M = \binom{n}{m}, R_k = \binom{n-1}{m-1} \) and for \( k \neq l, R_{kl} = \binom{n-2}{m-2} \). Thus \( A = m^2/n, B = \frac{m^2(m-1)^2}{n(n-1)} \leq \frac{m^4}{n^4} \) and \( C = m/n \). Substitute in Theorem 3.3.

This result is a slight improvement of Theorem 2.4 in two ways. First since

\[
\frac{m^2 \sigma^2}{n} \leq \text{Var}(U(X))
\]

and second since the coefficients \( \beta \) and \( \gamma \) can be substantially smaller than their worst-case bounds. If, for example \( X \) is a metric space and the kernel is separately Lipschitz \( L \) in each argument. Then \( \beta \) and \( \gamma \) can be bounded by \( L \text{Var}(X_1) \). Moreover, if mixed second partial differences of the kernel are of \( O\left(\frac{1}{m}\right) \), then \( \alpha = O\left(\frac{1}{m}\right) \) and meaningful bounds result for U-statistics of growing order as long as \( m = o(n) \).

For comparison to the bound of Arcones (Theorem 2.3) we substitute the worst case values for \( \beta \) and \( \gamma \) in Corollary 3.4 to obtain

\[
\Pr \left\{ U(X) - \theta > t \right\} \leq \exp \left( \frac{-nt^2}{2m^2 \sigma^2 + 4m^4/n + \left( \sqrt{8m^2 + (4/3)m} \right)t} \right)
\]

and assume \( \sigma^2 = 0 \). If the bound in Theorem 2.3 was less than or equal to (2) it would have to be nontrivial, so \( nt^2 > \left(2m^2 \sigma^2 + (2m^2 m^2 + 2m-1) t/n \right) \ln 2, \) which implies \( nt > 2^{m^2} m^2 \ln 2 \). On the other hand, even ignoring the factor 2 in Theorem 2.3, we would also need

\[
\frac{4m^4}{(2m^2 m^2 - (m^2 \sqrt{8} + (4/3)m))} \geq nt.
\]

This implies

\[
\frac{m^4}{(2m^2 m^2 - (m^2 \sqrt{8} + (4/3)m))} \geq 2^{m^2} m^2 \ln 2,
\]

which is easily seen to be false for all positive integers \( m \). The bound in Corollary 3.4 is therefore smaller than the one in Theorem 2.3 for all values of \( m, n \in \mathbb{N} \) and \( t > 0 \).

The second application of Theorem 3.3 concerns random designs, where the design \( \mathbf{W} \) is sampled with replacement from the uniform distribution on the set \( \{ \mathbf{W} \subset [n] : |\mathbf{W}| = m \} \), independent of \( \mathbf{X} \).

**Theorem 3.5.** Under random sampling of \( \mathbf{W} = (W_1, ..., W_M) \) if \( M \geq \ln^2 n, \) then with \( \delta_1 > 0 \) and probability at least \( 1 - (\delta_1 + \delta_2) \)

\[
U_{\mathbf{W}}(X) - \theta \leq \sqrt{\frac{2m^2 \sigma^2 \ln (1/\delta_1)}{n}} + \frac{am^2 + (4/3) m}{n} \ln (1/\delta_1) + \frac{5am^2 + 9 \sqrt{m} + 4}{\sqrt{M}} \ln^2 (3/\delta_2).
\]

**Remarks:**

1. The first two terms of the bound match the bound (1) for complete U-statistics given above, apart from the factor \( \ln (1/\delta_1) \) instead of \( \ln (1/\delta) \), which arises from a union bound. The remaining terms bound the error incurred by incompleteness.

2. If \( M = O\left(n^{1+\epsilon}\right) \) for any \( \epsilon > 0 \), let \( \delta_1 = (1-n^{-\epsilon}) \delta \) and \( \delta_2 = n^{-\epsilon} \delta \), with \( \delta = \exp \left(-t^2/(2m^2 \sigma^2)\right) \). Then as \( n \to \infty \)

\[
\Pr \left\{ \sqrt{n} (U_{\mathbf{W}}(X) - \theta) > t \right\} \to \exp \left( -\frac{t^2}{2m^2 \sigma^2} \right).
\]

For random designs with computational budget \( M = n^{1+\epsilon} \) the bound is consistent with the CLT for the complete U-statistic.

3. For \( M = n^2 \) we recover the order \( 1/n \) of the subexponential term of the complete statistic in Corollary 3.4. This is no help for kernels of order 2, as they frequently occur in applications, but for kernels of order 3 it already gives a significant advantage.
For positive bounded kernels we give a sub-Gaussian bound on the lower tail, which can be used to obtain empirical, variance-dependent bounds.

**Theorem 3.6.** For fixed kernel $K$ with values in $[0, 1]$, design $W$ and $t > 0$

$$\Pr \{ \mathbb{E} [U_W (X)] - U_W (X) > t \} \leq \exp \left( \frac{-t^2}{8mC \mathbb{E} [U_W (X)]} \right).$$

For $0 < \delta$ we have

$$\Pr \left\{ \sqrt{\mathbb{E} [U_W (X)]} > \sqrt{U_W (X)} + \sqrt{8mC \ln (1/\delta)} \right\} \leq \delta.$$

These inequalities do not require permutation invariance of the kernel.

### 4 Proofs

In this section we prove the above results. Necessary auxiliary results are introduced as needed.

#### 4.1 Incomplete U-statistics

**Definition 4.1.** For $f : X^n \to \mathbb{R}$ define

$$ES_X (f) := \frac{1}{2} \sum_{k=1}^{n} \mathbb{E} \left[ \left( D_{X_k}^k f (X) \right)^2 \right]$$

and

$$H_X (f) := \sum_{k,l,k \neq l} \mathbb{E} \left[ \left( D_{X_l}^l D_{X_k}^k f (X) \right)^2 \right].$$

The first of these is the Efron-Stein estimate of the variance. These quantities are related to the variance of $f (X)$ and a lower bound on the variance as follows.

**Theorem 4.2.** \cite{8, 13}:

$$\sum_{k=1}^{n} \operatorname{Var} [\mathbb{E} [f (X) | X_k]] \leq \operatorname{Var} [f (X)] \leq ES_X (f) \leq \sum_{k=1}^{n} \operatorname{Var} [\mathbb{E} [f (X) | X_k]] + \frac{1}{4} H_X (f),$$

The second inequality is the well-known Efron-Stein inequality. The above chain of inequalities bounds the bias of the Efron-Stein estimate. If $f$ is a sum of independent component functions, then $D_{X_l}^l D_{X_k}^k f (X)$ is almost surely zero, so $H_X (f)$ vanishes and all the inequalities become identities. We also need the following concentration inequality from \cite{17}.

**Theorem 4.3.** For $f : X^n \to \mathbb{R}$, if $\forall k, f (X) - \mathbb{E} [f (X) | X^k] < b$ then for $t > 0$

$$\Pr \{ f (X) - \mathbb{E} [f (X)] > t \} \leq \exp \left( \frac{-t^2}{2ES_X (f) + (J_X (f) + 2b/3)t} \right),$$

where $J_X (f)$ is the interaction-functional

$$J_X (f) := \left( \sup_{x \in X^n} \sum_{k,l,k \neq l} \sup_{y,y' \in X} \mathbb{E} \left[ \left( D_{y,y'}^l D_{X_k}^k f (x) \right)^2 \right] \right)^{1/2}.$$

Again, if $f$ is a sum then $J_X$ vanishes and $ES_X (f)$ becomes equal to $\operatorname{Var} [f (X)]$, so the inequality reduces to the classical Bernstein inequality for sums (e.g. \cite{13}). For more general functions, however, $ES_X (f)$ overestimates the variance, so the inequality is not quite a proper Bernstein inequality. Theorem 4.2 above allows us to bound this overestimation. These results and the next simple lemma provide a proof of Theorem 3.3.
Lemma 4.4. For $N \in \mathbb{N}$, $i \in [N]$ let $F_i : \mathcal{Y} \times Z \rightarrow \mathbb{R}$ with $Z$ a random variable with values in $Z$. Then

$$\sup_y \mathbb{E} \left[ \left( \sum_{i=1}^{N} F_i (y, Z) \right)^2 \right] \leq N^2 \max_i \sup_y \mathbb{E} \left[ F_i (y, Z)^2 \right].$$

Proof. With Jensen’s inequality

$$\sup_y \mathbb{E} \left[ \left( \sum_{i=1}^{N} F_i (y, Z) \right)^2 \right] = N^2 \sup_y \mathbb{E} \left[ \left( \frac{1}{N} \sum_{i=1}^{N} F_i (y, Z) \right)^2 \right] \leq N^2 \sup_y \frac{1}{N} \sum_{i=1}^{N} \mathbb{E} \left[ F_i (y, Z)^2 \right] \leq N^2 \max_i \sup_y \mathbb{E} \left[ F_i (y, Z)^2 \right].$$

Proof of Theorem 3.3. By the bound on $K$ we have for all $k$

$$U_{W} (X) - \mathbb{E} \left[ U_{W} (X) \mid X^{\backslash k} \right] = \frac{1}{M} \sum_{i=1}^{M} K (X^{W_i}) - \mathbb{E} \left[ K (X^{W_i}) \mid X^{\backslash k} \right] = \frac{1}{M} \sum_{i,k \in W_i} K (X^{W_i}) - \mathbb{E} \left[ K (X^{W_i}) \mid X^{\backslash k} \right] \leq \frac{2R_k}{M} \leq 2C. \quad (3)$$

If $|W| = m$, $k \neq l$ and not both $k$ and $l$ are members of $W$ then $D_{z,y, z', y'}^{l} K (x^W) = 0$. Thus for any $k,l \in [n], k \neq l$

$$\sup_{x \in \mathcal{X}^n, y, y' \in \mathcal{X}} \mathbb{E} \left[ \left( \sum_{i=1}^{M} D_{y,y'}^{l} D_{X_k, X'_k}^{k} K (x^{W_i}) \right)^2 \right] = \sup_{x \in \mathcal{X}^n, y, y' \in \mathcal{X}} \mathbb{E} \left[ \left( \sum_{i \neq \{k,l\} \in W_i} D_{y,y'}^{l} D_{X_k, X'_k}^{k} K (x^{W_i}) \right)^2 \right] \leq (R_{kl})^2 \max_{i \neq \{k,l\} \in W_i} \sup_{x \in \mathcal{X}^n, y, y' \in \mathcal{X}} \mathbb{E} \left[ D_{y,y'}^{l} D_{X_k, X'_k}^{k} K (x^{W_i}) \right] \leq (R_{kl})^2 \gamma.$$
The first inequality follows Lemma 4.4. The last step follows from permutation symmetry of the kernel and the definition of $\gamma$. Thus
\[
J_X^2(UW) = \frac{1}{M^2} \sup_{x \in X^n} \sum_{k,l,k \neq l} \sup_{y,y' \in X} \mathbb{E} \left[ \sum_{i=1}^M D_{y,y'}^i D_{X_k,X_{k'}}^i K(x^{W_i}) \right]^2 \leq \frac{1}{M^2} \sum_{k,l,k \neq l} R_{kl}^2 \leq 1.
\]
In exactly the same way one proves that $H_X(UW) \leq B \beta$.

From the general Bernstein inequality Theorem 4.3 and the bound on $J_X^2(UW)$ we obtain
\[
\Pr \{ U_W(X) - \mathbb{E}[U_W(X)] > t \} \leq \exp \left( -\frac{t^2}{2ES_X(UW) + (\sqrt{B\gamma} + 4C/3) t} \right). \tag{4}
\]
It remains to bound the Efron-Stein term $ES_X(UW)$. Again using Lemma 4.4
\[
\text{Var} \left[ \sum_{i=1}^M \mathbb{E} [K(X^{W_i}) | X_k] \right] = \frac{1}{2M} \mathbb{E} \left[ \left( \sum_{i \in W_i} \mathbb{E} [K(X^{W_i}) | X_k] - \mathbb{E} [K(X^{W_i}) | X_k] \right)^2 \right] \leq \frac{R_k^2}{2} \max \mathbb{E} \left[ \left( \mathbb{E} [K(X^{W_i}) | X_k] - \mathbb{E} [K(X^{W_i}) | X_k] \right)^2 \right] = R_k^2 \sigma^2.
\]
The last step follows since $\mathbb{E} [K(X^{W_i}) | X_k]$ is identically distributed to $\mathbb{E} [K(X_1, ..., X_m) | X_1]$, so
\[
\sum_{k=1}^n \text{Var} \left[ \mathbb{E}[U_W(X) | X_k] \right] = \frac{1}{M^2} \sum_{k=1}^n \text{Var} \left[ \sum_{i=1}^M \mathbb{E} [K(X^{W_i}) | X_k] \right] \leq A \sigma^2. \tag{5}
\]
From Theorem 4.2 and the bound on $H_X(UW)$ we get
\[
ES_X(UW) \leq \sum_{k=1}^n \text{Var} \left[ \mathbb{E}[U_W(X) | X_k] \right] + \frac{1}{4} H_X(UW) \leq A \sigma^2 + \beta/4.
\]
Substitution in (4) completes the proof of the first inequality. The second assertion follows from equating the bound on the probability to $\delta$, solving for $t$ and using the fact that $0 \leq \delta \leq 1/e$ implies $\sqrt{\ln(1/\delta)} \leq \ln (1/\delta)$.

### 4.2 Random design

In this section we assume that $W = (W_1, ..., W_M)$ is sampled independent of $X$ and with replacement from the uniform distribution on $\{W \subset \{1, ..., n\} : |W| = m\}$. The quantities $A(W), B(W)$ and $C(W)$ are now random variables.

For $k, l \in \{1, ..., n\}$ and $k \neq l$ define for $i \in [M]$ the Bernoulli variables $Z_{i}^k = 1_{\{k \in W_i\}}$ and $Z_{i}^{kl} = 1_{\{k,l \in W_i\}}$. For fixed $k$ and $l$ the $Z_{i}^k$ are iid variables and so are the $Z_{i}^{kl}$. It is easy to see that $\mathbb{E}[Z_{i}^k] = m/n$ and $\mathbb{E}[Z_{i}^{kl}] = m (m-1) / (n (n-1))$. Also $R^k = \sum_i Z_{i}^k$ and $R^{kl} = \sum_i Z_{i}^{kl}$. Then
\[
A(W) = \frac{1}{M^2} \sum_{k=1}^n \left( \sum_{i=1}^M Z_{i}^k \right)^2, \quad B(W) = \frac{1}{M^2} \sum_{k,l \neq l} \left( \sum_{i=1}^M Z_{i}^{kl} \right)^2, \quad C(W) = \frac{1}{M} \max_{k=1}^n \sum_{i=1}^M Z_{i}^k.
\]
To prove Theorem 3.5, we will give high probability bounds for $A$, $B$ and $C$.

**Lemma 4.5.** If $\sqrt{M} \geq \ln n$, then for $\delta \in (0, 1)$ with probability at least $1 - \delta/4$

$$C(W) \leq \frac{m}{n} + \frac{\sqrt{2m + 3}}{\sqrt{M}} \ln (4/\delta).$$

**Proof.** The variance of $Z_i^k$ is less than its expectation, which is $m/n$. Therefore by Bernstein’s inequality for fixed $k \in [n]$ with probability at least $1 - \delta/4$

$$\frac{1}{M} \sum_{i=1}^{M} Z_i^k \leq \frac{m}{n} + \sqrt{\frac{2m \ln (4/\delta)}{nM}} + \frac{2 \ln (4/\delta)}{3M}.$$

$$\Pr \left\{ \frac{1}{M} \sum_{i=1}^{M} Z_i^k > \frac{m}{n} + t \right\} \leq \exp \left( -\frac{-Mt^2}{2m/n + 2t/3} \right)$$

$$\Pr \left\{ C(W) > \frac{m}{n} + t \right\} \leq n \exp \left( -\frac{-Mt^2}{2m/n + 2t/3} \right)$$

A union bound over $k \in [n]$ gives with probability at least $1 - \delta/4$

$$C(W) \leq \frac{m}{n} + \frac{\sqrt{2m + 3}}{\sqrt{M}} \ln (4/\delta),$$

where the last inequality follows from $n \geq \ln n$, $n \geq m$, $\sqrt{M} \geq \ln n$ and $\ln (4/\delta) \geq 1$. \hfill \Box

Bounds for $A$ and $B$ could easily be given by bounding $R_k = \sum_i Z_i^k$ (or $R_{kl} = \sum_i Z_i^{kl}$) with high probability, extending to all $k$ (or all pairs $k, l$) with a union bound and summing the squares. Unfortunately the union bound would incur a logarithmic factor in $n$. To avoid this we estimate the expectations of $A$ and $B$ and the probability to deviate from these expectations.

**Lemma 4.6.**

$$\mathbb{E} [A(W)] \leq \frac{m^2}{n} + \frac{m}{M} \quad \text{and} \quad \mathbb{E} [B(W)] \leq \frac{m^4}{n^2} + \frac{m^2}{M}$$

**Proof.** Using independence

$$\mathbb{E} \left[ \left( \sum_{i=1}^{M} Z_i^k \right)^2 \right] = \sum_i \mathbb{E} [Z_i^k] + \sum_{i \neq j} \mathbb{E} [Z_i^k Z_j^k]$$

$$= \frac{Mm}{n} + \frac{M(M - 1)m^2}{n^2}.$$ 

The first identity follows from multiplication with $n/M^2$. The second one follows similarly using $\mathbb{E} [Z_i^{kl}] = \frac{m(m-1)}{n(n-1)}$. \hfill \Box
To give high-probability deviation bounds for $A$ and $B$ we now use a concentration inequality from [16], which is particularly well suited for expressions involving the squares of random variables. For any $\mathcal{X}$ and functions $f: \mathcal{X}^N \to \mathbb{R}$ define an operator $D^2$ by

$$D^2 f(x) = \sum_{k=1}^{N} \left( f(x) - \inf_{y \in \mathcal{X}} S_{y}^{k} f(x) \right)^2.$$  

**Theorem 4.7.** Suppose $f: \mathcal{X}^N \to \mathbb{R}$ satisfies for some $a > 0$

$$D^2 f(x) \leq a f(x), \forall x \in \mathcal{X}^N,$$

and let $x = (X_1, ..., X_N)$ be a vector of independent variables. Then for all $t > 0$

$$\Pr \{ f(x) - E[f] > t \} \leq \exp \left( \frac{-t^2}{2aE[f] + at} \right).$$

If in addition $f(x) - \inf_{y \in \mathcal{X}} S_{y}^{k} f(x) \leq 1$ for all $k \in \{1, ..., N\}$ and all $x \in \mathcal{X}^N$ then

$$\Pr \{ f(x) - E[f] > t \} \leq \exp \left( \frac{-t^2}{2 \max \{a, 1\} E[f]} \right).$$

**Corollary 4.8.** If $f: \mathcal{X}^N \to \mathbb{R}$ satisfies (6) and for some $b > 0$ $f(x) - \inf_{y \in \mathcal{X}} S_{y}^{k} f(x) \leq b$ for all $k \in \{1, ..., N\}$ and all $x \in \mathcal{X}^N$ then

$$\Pr \{ E[f] - f(x) > t \} \leq \exp \left( \frac{-t^2}{2 \max \{a, b\} E[f]} \right).$$

Also for all $\delta > 0$ with probability at least $1 - \delta$

$$\sqrt{f(x)} - \sqrt{2a \ln \left( \frac{1}{2\delta} \right)} \leq \sqrt{E[f]} \leq \sqrt{f(x)} + \sqrt{2 \max \{a, b\} \ln \left( \frac{1}{\delta} \right)}.$$

For a one-sided bound $2/\delta$ can be replaced by $1/\delta$.

**Proof.** If $f(x) - \inf_{y \in \mathcal{X}} S_{y}^{k} f(x) \leq b$ then $(f(x)/b) - \inf_{y \in \mathcal{X}} S_{y}^{k} (f(x)/b) \leq 1$ and (6) implies $D^2 \left( f(x)/b \right) \leq (a/b) \left( f(x)/b \right)$, so by the second conclusion of Theorem 4.7

$$\Pr \{ E[f] - f(x) > t \} = \Pr \{ f(x)/b - E[f/b] > t/b \} \leq \exp \left( \frac{-(t/b)^2}{2 \max \{a/b, 1\} E[f/b]} \right) = \exp \left( \frac{-t^2}{2 \max \{a, b\} E[f]} \right).$$

(this is really an alternative formulation of the second conclusion of Theorem 4.7). Equating the R.H.S. to $\delta$ solving for $t$ and elementary algebra then give with probability at least $1 - \delta$ that

$$\sqrt{E[f]} \leq \sqrt{f(x)} + \sqrt{2 \max \{a, b\} \ln \left( \frac{1}{\delta} \right)}.$$

In a similar way the first conclusion of Theorem 4.7 gives with probability at least $1 - \delta$ that

$$\sqrt{f(x)} - \sqrt{2a \ln \left( \frac{1}{\delta} \right)} \leq \sqrt{E[f]}.$$

A union bound concludes the proof. \hfill \Box

For the random design we use only the upper tail bound above. The lower tail bound will be used for the sub-Gaussian bound Theorem 3.6.

**Lemma 4.9.** For $\delta > 0$

$$\Pr \left\{ \sqrt{A(W)} > \sqrt{\frac{m^2}{n}} + \left( 1 + 4 \sqrt{\ln (1/\delta)} \right) \sqrt{\frac{m}{M}} \right\} \leq \delta$$

$$\Pr \left\{ \sqrt{B(W)} > \sqrt{\frac{m^2}{n}} + \left( 1 + 4 \sqrt{\ln (1/\delta)} \right) \sqrt{\frac{m}{M}} \right\} \leq \delta$$

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Proof. To prove these inequalities we show that $A$ and $B$ satisfy a self-bounding condition as in (6).

Fix a design $W$ and for each $j \in [M]$ choose $W'_j$ so as to minimize $A \left( S^j_{W'_j}W \right)$. Denote $S^j_{W'_j}W$ by $W^{(j)}$ in the following. Note that for any $k \in [n]$ and $j \in [M]$

$$
\sum_{i=1}^{M} Z^k_i(W) - \sum_{i=1}^{M} Z^k_i(W^{(j)}) = 1 \{ k \in W_j \} - 1 \{ k \in W'_{j} \},
$$

because the two designs differ only in the $j$-th element. Thus for $j \in [M]$

$$
\left( A(W) - A \left( W^{(j)} \right) \right)^2 = \frac{1}{M^2} \left( \sum_{k=1}^{n} \left( \sum_{i=1}^{M} Z^k_i(W) \right) - \left( \sum_{i=1}^{M} Z^k_i \left( W^{(j)} \right) \right) \right)^2
$$

$$
\leq \frac{1}{M^2} \sum_{k=1}^{n} \left( 1 \{ k \in W_j \} - 1 \{ k \in W'_{j} \} \right)^2 \left( \sum_{i=1}^{M} Z^k_i(W) \right) - \left( \sum_{i=1}^{M} Z^k_i \left( W^{(j)} \right) \right)^2
$$

$$
\leq \frac{4}{M^2} \sum_{k=1}^{n} \left( 1 \{ k \in W_j \} - 1 \{ k \in W'_{j} \} \right)^2 A(W)
$$

$$
\leq \frac{8m}{M^2} A(W).
$$

The first inequality is Cauchy-Schwarz. The second follows from $(b + c)^2 \leq 2b^2 + 2c^2$ and the minimality of $W^{(j)}$ and the last inequality follows from the cardinality constraint on the sets $W_j$ and $W'_j$. We conclude that

$$
D^2 A(W) = \sum_{j=1}^{M} \left( A(W) - A \left( W^{(j)} \right) \right)^2 \leq \frac{8m}{M} A(W),
$$

so using Corollary 4.8 with $a = 8m/M$ we get with probability at least $1 - \delta$

$$
\sqrt{A(W)} \leq \sqrt{E[A(W)]} + \sqrt{\frac{16m \ln(1/\delta)}{M}}
$$

$$
\leq \sqrt{\frac{m^2}{n} + \left( 1 + 4\sqrt{\ln(1/\delta)} \right) \frac{m}{M}},
$$

where we used Lemma 4.6.

The proof of the second assertion is similar. Choose $W'_j$ to minimize $B \left( S^j_{W'_j}W \right) = B \left( W^{(j)} \right)$. Then for fixed $j$ we get

$$
\left( B(W) - B \left( W^{(j)} \right) \right)^2 \leq \frac{1}{M^4} \sum_{k \neq l} \left( 1 \{ k, l \in W_j \} - 1 \{ k, l \in W'_j \} \right)^2 \left( \sum_{i=1}^{M} Z^{kl}_i(W) + \sum_{i=1}^{M} Z^{kl}_i \left( W^{(j)} \right) \right)^2
$$

$$
\leq \frac{4}{M^2} \sum_{k \neq l} \left( 1 \{ k, l \in W_j \} - 1 \{ k, l \in W'_j \} \right)^2 B(W)
$$

$$
\leq \frac{8m(m - 1)}{M^2} B(W).
$$
Analogous to the above we conclude with Lemma 4.6 that with probability at least 

\[ \sqrt{B(W)} \leq \sqrt{E[B(W)]} + \frac{\sqrt{16m(m-1)\ln(1/\delta)}}{M} \]

\[ \leq \frac{m^2}{n} + \left(1 + 4\sqrt{\ln(1/\delta)}\right)\frac{m}{\sqrt{M}} \]

\[ \leq m^2 + \frac{m^2}{n} + \sqrt{2m + 3} \ln(3/\delta) \]

\[ \leq m^2 + \sqrt{5m} \ln(3/\delta) \]

\[ \leq \alpha m + 9\sqrt{m} + 4 \sqrt{M} \ln(3/\delta) \]

Assembling the above pieces gives a proof of the bound for random design.

**Proof of Theorem 3.5** Fix \( \delta \in (0, 1) \). It follows from Lemma 4.5 that

\[ \Pr \left\{ C > \frac{m}{n} + \frac{\sqrt{2m} + 3}{\sqrt{M}} \ln(3/\delta) \right\} \leq \frac{\delta^2}{3}. \]

From Lemma 4.9 we have

\[ \Pr \left\{ \sqrt{A} > \frac{m^2}{n} + \frac{5\sqrt{m}}{\sqrt{M}} \ln(3/\delta) \right\} \leq \frac{\delta^2}{3} \text{ and} \]

\[ \Pr \left\{ \sqrt{B} > \frac{m^2}{n} + \frac{5m}{\sqrt{M}} \ln(3/\delta) \right\} \leq \frac{\delta^2}{3}. \]

From Theorem 3.3 we get

\[ \Pr \left\{ U_W(X) - \theta > \sqrt{A} \sqrt{2\sigma_1^2 \ln(1/\delta_1)} + \left(\alpha \sqrt{B} + \frac{4}{3} C\right) \ln(1/\delta_1) \right\} \leq \frac{\delta_1}{4}. \]

Combining the last four inequalities in a union bound, using \( \sigma_1^2 \leq 1 \) and simplifying, gives with probability at least \( 1 - \delta \) that

\[ U_W(X) - \theta \leq \sqrt{2m^2\sigma_1^2 \ln(1/\delta_1)} + \frac{\alpha m^2 + (4/3) m}{n} \ln(1/\delta_1) + \frac{5\alpha m + 9\sqrt{m} + 4}{\sqrt{M}} \ln^2(3/\delta_2). \]

4.3 Proof of the sub-Gaussian lower bound

**Proof of Theorem 3.6** The proof is based on the lower-tail bound of Corollary 4.8. For each \( k \) choose \( x_k \) so as to minimize \( U_W(x_{(k)}) \). This means that

\[ 0 \leq \sum_{i=1}^{M} K(x_{W^i}) - K(x_{W^i}) = \sum_{i,k \in W_i} K(x_{W^i}) - K(x_{W^i}). \]

Consequently

\[ \sum_{i,k \in W_i} K(x_{W^i}) \leq \sum_{i,k \in W_i} K(x_{W^i}). \] (7)
Now
\[
\sum_{k=1}^{n} \left( U_W(x) - U_W(x_{(k)}) \right)^2
\]
\[
= \frac{1}{M^2} \sum_{k=1}^{n} \left( \sum_{i: k \in W_i} \left( K(x_i) - K(x_{(k)}) \right) \right)^2
\]
\[
= \frac{1}{M^2} \sum_{k=1}^{n} \left( \sum_{i: k \in W_i} \left( \sqrt{K}(x_i) - \sqrt{K}(x_{(k)}) \right) \left( \sqrt{K}(x_i) + \sqrt{K}(x_{(k)}) \right) \right)^2
\]
\[
\leq \frac{1}{M^2} \sum_{k=1}^{n} \sum_{i: k \in W_i} \left( \sqrt{K}(x_i) - \sqrt{K}(x_{(k)}) \right)^2 \sum_{i: k \in W_i} \left( \sqrt{K}(x_i) + \sqrt{K}(x_{(k)}) \right)^2
\]
\[
\leq \frac{1}{M} \max_k \left| \sum_{i: k \in W_i} \left( \sqrt{K}(x_i) - \sqrt{K}(x_{(k)}) \right)^2 \right| \frac{1}{M} \sum_{k=1}^{n} \sum_{i: k \in W_i} \left( \sqrt{K}(x_i) + \sqrt{K}(x_{(k)}) \right)^2
\]
We bound the second factor, using \((a - b)^2 \leq 2a^2 + 2b^2\) and \(7\)
\[
= \frac{1}{M} \sum_{k=1}^{n} \sum_{i: k \in W_i} \left( \sqrt{K}(x_i) + \sqrt{K}(x_{(k)}) \right)^2
\]
\[
\leq \frac{2}{M} \sum_{k=1}^{n} \left( \sum_{i: k \in W_i} K(x_i) + \sum_{i: k \in W_i} K(x_{(k)}) \right)
\]
\[
\leq \frac{4}{M} \sum_{k=1}^{n} \sum_{i: k \in W_i} K(x_i) = \frac{4}{M} \sum_{k} \sum_{i: k \in W_i} K(x_i)
\]
Thus if \(\sqrt{K} \in [0, 1]\)
\[
\sum_{k=1}^{n} \left( U_W(x) - U_W(x_{(k)}) \right)^2 \leq \frac{4m}{M} \max_k \left| \sum_{i: k \in W_i} \left( \sqrt{K}(x_i) - \sqrt{K}(x_{(k)}) \right)^2 \right| U_W(x)
\]
\[
\leq \frac{4m}{M} \max_k R_k U_W(x) = 4mC(W)U_W(x).
\]
So we can use \(a = 4mC(W)\) in Corollary 4.8 We also have
\[
\frac{1}{M} \sum_{i=1}^{M} K(x_i) - K(x_{(k)}) \leq 1 \frac{1}{M} \sum_{i: k \in W_i} K(x_i) - K(x_{(k)}) \leq C(W),
\]
So with \(b = C(W)\) and \(\max \{a, b\} = 4mC(W)\) Corollary 4.8 gives
\[
\Pr \{ E[U_W] - U_W(X) > t \} \leq \exp \left( -\frac{t^2}{8mC E[U_W]} \right).
\]
\[
\square
\]
Lemma 4.10. If \(K: x \in X^m \to [-1, 1]\) then \(\beta(K) \leq \gamma(K) \leq 8\).

Proof. The first inequality is obvious. We have
\[
\beta(K) \leq \gamma(K) = \mathbb{E} \left[ \left( D_{g,y}^1 D_{X_2,X_2}^2 K(x_1, x_2, x_3, \ldots, x_m) \right)^2 \right]
\]
\[
\leq 4 \sup_{x \in X^m} \mathbb{E} \left[ \left( D_{X_1,X_1}^2 K(x_1, x_2, x_3, \ldots, x_m) \right)^2 \right]
\]
\[
\leq 8 \sup_{x \in X^m} \text{Var} \left[ K(X_1, \ldots, X_m) | X_2 = x_2, \ldots, X_m = x_m \right]
\]
\[
\leq 8.
\]
\[
\square
\]
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