A SURVEY OF CONCENTRATION INEQUALITIES FOR U-STATISTICS

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Abstract. The aim of this paper is to discuss various concentration inequalities for U-statistics and most recent results. A special focus will be on providing short proofs for bounds on the U-statistics using classical concentration inequalities, which, although well known, are not easy to locate in the literature.

1. Introduction

U-statistics appear in statistics when producing minimum variance unbiased estimators. Naturally, they’re especially present in clustering, ranking, and learning on graphs. In other words, any time we deal with exchangeable sequences, U-statistics are likely to come up. First, we begin with a definition of a U-statistic due to Joly and Lugosi (2015). Hoeffding (1948) was the first to introduce U-statistics in his paper "A class of statistics with asymptotically normal distributions."

Definition 1.1. Let $X$ be a random variable taking values in a measurable space $\mathcal{X}$ and let $h : \mathcal{X}^m \to \mathbb{R}$ be a measurable function of $m \geq 2$ variables. Let $P$ be the probability measure of $X$ and suppose we can access $n \geq m$ i.i.d. random variables $X_1, \ldots, X_n \sim X$. Then the U-statistics of order $m$ and kernel $h$ based on $\{X_i\}$ are defined as

$$U_n(h) = \frac{(n-m)!}{n!} \sum_{(i_1, \ldots, i_m) \in I_m^n} h(X_{i_1}, \ldots, X_{i_m}),$$

where

$$I_m^n = \{(i_1, \ldots, i_m) : 1 \leq i_j \leq n, i_j \neq i_k \text{ if } j \neq k\}$$

is the set of all $m$-tuples of different integers between 1 and $n$.

Alternatively, if we restrict $I_m^n$ to be the set of increasing $m$-tuples of integers between 1 and $n$, i.e. $i_j < i_k$ for $j < k$, then we have

$$U_n(h) = \frac{1}{\binom{n}{m}} \sum_{(i_1, \ldots, i_m) \in I_m^n} h(X_{i_1}, \ldots, X_{i_m}).$$

U-statistics are unbiased estimators of the mean $m_h = Eh(X_1, \ldots, X_m)$ and have minimal variance among all unbiased estimators. A few examples of U-statistics include the sample variance $s_n^2$, which is a U-statistic of order 2 with kernel given by $h(x, y) = (1/2)(x - y)^2$, and the third $k$-statistic, $\frac{n}{(n-1)(n-2)} \sum_{i=1}^n (X_i - \bar{X}_n)^3$, which estimates the third cumulant.

It is of interest to understand the concentration of a U-statistic around its expected value. We will discuss classical concentration bounds from decades ago and also put current results into context.
2. Classical Bounds

First, we start by taking a look at some classical bounds that do not involve special conditions on the kernel. An inequality of Hoeffding (1963) established that

\[
P \left\{ \left| U_n(h) - m_h \right| > \|h\|_\infty \sqrt{\frac{\log(\frac{2}{\delta})}{2 \left\lfloor n/m \right\rfloor}} \right\} \leq \delta
\]

for \( h \) bounded, for all \( \delta > 0 \) and one can also derive

\[
P \left\{ \left| U_n(h) - m_h \right| > \sqrt{\frac{2\sigma^2 \log(\frac{2}{\delta})}{\left\lfloor n/m \right\rfloor}} \vee \frac{2\|h\|_\infty \log(\frac{2}{\delta})}{3 \left\lfloor n/m \right\rfloor} \right\} \leq \delta,
\]

where \( \sigma^2 \) is the variance of \( h(\{X_i\}) \). These bounds follow from applications of two classic inequalities.

For our purposes, I will state the aforementioned inequalities in detail. The proofs can be seen in the book Concentration Inequalities by Lugosi, Massart, and Bousquet.

**Lemma 2.1. Hoeffding’s Lemma:** Let \( X \in [a, b] \) with probability 1 and \( EX = \mu \). Then

\[
E[e^{s(X-\mu)}] \leq e^{s^2(b-a)^2/8}.
\]

**Theorem 2.2. Hoeffding’s Inequality:** Let \( X_1, \ldots, X_n \) be independent observations such that \( E(X_i) = \mu \) and \( X_i \in [a, b] \). Then, for any \( \epsilon > 0 \),

\[
P(\left| \bar{X}_n - \mu \right| \geq \epsilon) \leq 2e^{-2n\epsilon^2/(b-a)^2}.
\]

**Corollary 2.3.** If \( X_1, \ldots, X_n \) have the same properties as previously (independent, bounded in \( [a, b] \), common mean \( \mu \)), then, with probability at least \( 1 - \delta \),

\[
\left| \bar{X}_n - \mu \right| \leq \sqrt{\frac{(b-a)^2}{2n} \log \left( \frac{2}{\delta} \right)}.
\]

**Theorem 2.4. Bernstein’s Inequality:** Let \( X_1, \ldots, X_n \) be independent real-valued random variables with zero mean such that \( |X_i| < c \) almost surely. Let \( \sigma_i^2 = \text{Var}(X_i) \) and \( \sigma^2 = \frac{1}{n} \sum_{i=1}^n \sigma_i^2 \). Then,

\[
P(\bar{X} \geq \epsilon) \leq \exp \left( -\frac{ne^2}{2(\sigma^2 + c\epsilon/3)} \right).
\]

**Lemma 2.5. Bernstein’s Lemma:** Let \( X \) be a random variable such that \( EX = \mu \), \( \text{Var}(X) = \sigma^2 \), and \( |X - \mu| < c \) almost surely. Then

\[
E[e^{s(X-\mu)}] \leq \exp \left( \frac{\sigma^2}{c^2}(e^{sc} - 1 - sc) \right).
\]

3. Proof of Hoeffding and Bernstein bounds for U-statistics

We cannot immediately apply the above concentration inequalities to our U-statistics because there may be dependence between terms. Thus, in order to get concentration bounds on the U-statistics using these inequalities, we observe that, due to symmetry, we can rewrite U-statistics as sums of independent random variables. Let \( k = \left\lfloor n/m \right\rfloor \) and

\[
V(X_1, \ldots, X_n) = \frac{1}{k} \left\{ h(X_1, \ldots, X_m) + \cdots + h(X_{km-m+1}, \ldots, X_{km}) \right\}.
\]
One can see that
\[ U_n(h) = \frac{\sum_{\sigma \in S_n} V(X_{\sigma_1}, \ldots, X_{\sigma_n})}{n!} \]
and each term on the right-hand side is a sum of \( k \) independent random variables. Each of these can be bounded individually and then one may use the following lemma:

**Lemma 3.1.** Suppose \( T \) is a random variable that can be written as
\[ T = \sum_{i=1}^{N} p_i T_i, \quad \text{where} \quad \sum p_i = 1, p_i \geq 0 \quad \forall i \]
Then \( P(T \geq t) \leq \sum_{i=1}^{N} p_i E[e^{s(T_i - t)}] \).

**Proof.** Let \( h > 0 \). The lemma follows from Markov’s inequality
\[ P(T \geq t) \leq e^{-st} E[e^{sT}] = E[e^{s(T-t)}] \]
and Jensen’s inequality.
\[ \exp(sT) = \exp \left( s \sum p_i T_i \right) \leq \sum p_i \exp(sT_i) \]
Combining these two, we get \( P(T \geq t) \leq e^{-st} E[e^{sT}] \leq \sum p_i E[e^{s(T_i-t)}] \)

Now we’ll finish the proof of the Hoeffding bound for U-statistics. In the following steps, \( V \) is shorthand for \( V(\{X_\sigma(i)\}_{i=1}^{n}) \).

**Proof.** Denote \( h_i \) to represent \( h(X_{im-m+1}, \ldots, X_{im}) \) in the sum for \( V(X_1, \ldots, X_n) \) for \( i = 1 \) to \( k \). Note that, in our case, \( p_i = 1/n! \) and \( N = n! \), and using Hoeffding’s lemma, we have
\[ E[e^{s(V-m_h-t)}] = E \left[ \exp \left( s \sum_{i=1}^{k} \frac{h_i}{k} - \frac{m_h}{k} - \frac{t}{k^2} \right) \right] \]
\[ = E \left[ \exp \left( s \left( \sum_{i=1}^{k} \frac{h_i}{k} - \frac{m_h}{k} \right) \right) \right] e^{-st} \leq [\exp \left( s^2((2\|h\|_\infty/k)^2/8) \right)]^k e^{-st} \]
and since this is independent of the permutation of \( X_i \)'s, we see that
\[ P(U_n - m_h \geq t) \leq (1/n!) \sum_{\sigma \in S_n} E[e^{s(V-m_h-t)}] = \exp \left\{ \frac{s^2\|h\|_\infty^2}{2k} - st \right\} \]
and minimizing the right-hand side over \( s \), we see that it’s minimized when \( s = kt/\|h\|_\infty \), and evaluating at this choice of \( s \), we see that
\[ P(U_n - m_h \geq t) \leq \exp \left\{ -\frac{kt^2}{2\|h\|_\infty^2} \right\} \]
and thus
\[ P(|U_n - m_h| \geq t) \leq 2 \exp \left\{ -\frac{t^2 |n/m|}{2\|h\|_\infty^2} \right\} \]
by union-bound. This completes the proof of the Hoeffding bound for U-statistics.

We can use a similar approach to develop a bound involving the variance of \( h(X_1, \ldots, X_m) \).
Proof. For the Bernstein bound, we can repeat the same steps except now
\[
\mathbb{E}\left[ \exp\left\{ s\left( \sum_{i=1}^{k} \frac{h_i}{k} - m_h\right) \right\} \right] \leq \exp\left\{ \frac{\sigma^2}{\|h\|_\infty^2} \left( e^{s\|h\|_\infty} - 1 - \frac{s\|h\|_\infty}{k} \right) \right\}^k
\]
by letting \(c = \|h\|_\infty / k\) and \(\text{Var}(\frac{h}{k} - m_h) = \text{Var}(h_i/k) = \frac{\sigma^2}{k^2}\) in the Bernstein lemma.

Then we once again find \(s > 0\) to minimize
\[
k\sigma^2 \left( e^{s\|h\|_\infty} - 1 - \frac{s\|h\|_\infty}{k} \right) - st
\]
Setting \(s = \frac{k\sigma^2}{\|h\|_\infty} \log(1 + \frac{\|h\|_\infty}{\sigma^2})\), we see that
\[
P(U_n - m_h \geq t) \leq \exp\left( \frac{-kt^2}{2(\sigma^2 + \frac{\|h\|_\infty t}{3})} \right)
\]
and thus
\[
P(|U_n - m_h| \geq t) \leq 2 \exp\left( \frac{-kt^2}{2(\sigma^2 + \frac{\|h\|_\infty t}{3})} \right)
\]

So far, all these results are general and don’t involve any assumptions about the kernel \(h\) besides measurability.

4. Discussion of Recent Work

Under certain conditions, these concentration bounds can be tightened. Arcones and Giné required that the kernel was symmetric (invariant under permutation of the \(X_i\)’s) as well as bounded. In the presence of this and a degeneracy assumption, they were able to establish tighter bounds.

**Definition 4.1.** A symmetric kernel \(h\) is \(P\)-degenerate of order \(q - 1\), \(1 < q \leq m\), if for all \(x_1, \ldots, x_{q-1} \in \mathcal{X}\),
\[
\int h(x_1, \ldots, x_m)dP^{m-q+1}(x_q, \ldots, x_m) = \int h(x_1, \ldots, x_m)dP^m(x_1, \ldots, x_m)
\]
and \((x_1, \ldots, x_q) \mapsto \int f(x_1, \ldots, x_m)dP^{m-q}(x_{q+1}, \ldots, x_m)\) is not a constant function (Lugosi and Joly, 2015).

When the kernel is \(P\)-degenerate with order \(m-1\) and \(m_h = E[h(X_1, \ldots, X_m)] = 0\), then \(h\) is considered to be \(P\)-canonical.

The method used by Arcones and Giné to improve concentration guarantees in this scenario relied on decoupling arguments, where they replaced quadratic forms of random variables by bilinear forms. For example, a decoupling argument would be something along the lines of the following, taken from a monograph by Vershynin:
Example 4.2. Let $A$ be an $n \times n$ matrix with zero diagonal and $X = (X_1, \ldots, X_n)$ is a random vector with independent mean 0 coefficients. If $F$ is convex, then

$$EF(\langle AX, X \rangle) \leq EF(4\langle AX, X' \rangle)$$

where $X'$ is an independent copy of $X$.

Arcones and Giné were able to show under the assumption that $h$ was canonical of $m$ variables, then there exist positive constants $c_1$ and $c_2$ depending only on $m$ such that for all $\delta \in (0, 1)$,

$$P\left\{ |U_n(h) - mh| \geq c_1 \|h\|_\infty \left( \frac{\log(\frac{c_2}{\delta})}{n} \right)^{m/2} \right\} \leq \delta,$$

and

$$P\left\{ |U_n(h) - mh| \geq \left( \frac{\sigma^2 \log(\frac{c_2}{\delta})}{c_2 n} \right)^{m/2} \vee \frac{\|h\|_\infty \left( \frac{\log(\frac{c_2}{\delta})}{c_2} \right)^{(m+1)/2}}{\sqrt{n}} \right\} \leq \delta.$$

If $m \geq 2$, then the first of the two proposed inequalities by Arcones and Giné provides a rate of convergence of $O_p(n^{-1})$, which is much faster than the $O_p(n^{-1/2})$ rate implied by the classical Hoeffding bound. In the case where the kernel had a unbounded but light-tailed distribution (subgaussian as an example), the above inequalities could be extended as done in a work by Giné et al. (2000). However, these results do not hold anymore if the kernel were heavy-tailed.

To get around this roadblock, Nemirovsky and Yudin (1983) introduce a more robust median-of-means estimator that outperforms $U$-statistics for estimating the mean of the kernel function. What they did was take a confidence level $\delta \in (0, 1)$ and divide the data into $V \approx \log \frac{1}{\delta} - 1$ blocks. Then they computed the empirical mean for each block and took the median of these empirical means, call this $\bar{\mu}$. In their paper, they show that

$$\|\bar{\mu} - mh\| \leq c \sqrt{\text{Var}(X)} \sqrt{\frac{\log(1/\delta)}{n}}$$

with probability at least $1 - \delta$ for a constant $c$. This is an improvement in that these guarantees would still hold even if $X$ were heavy-tailed.

Joly and Lugosi use a median-of-means style estimator as well, except instead of taking the mean on each block, they calculated the empirical means over $m$-tuples of different blocks to compute (decoupled) U-statistics. Then they computed the medians over all these values. Notably, when the kernel was degenerate of order $m - 1$, the rate of convergence of their estimator was $(\log(1/\delta)/n)^{m/2}$, which is similar to that of the U-statistics except without any assumption of boundedness. However, the tradeoff is degeneracy is required.

5. Concluding Remarks

This is a relatively complete discussion and the first, to my knowledge, that explicitly provides derivations for standard concentration bounds on the U-statistics involving Hoeffding’s and Bernstein’s inequalities. These are well known to the statistics and machine learning communities, but it is difficult to find a proof that explains how to "create independence where there is not" before applying moment bounds – in our case we needed to use a representation of the U-statistics involving symmetric sums. Then we gave a summary of the tradeoffs in approaches of current work finding
moment bounds of U-statistics, with emphasis on the techniques of decoupling and median-of-means estimators.

REFERENCES

[1] Arcones, M. A. and E. Giné (1993), Limit theorems for U-processes. The Annals of Probability 21, 1494-1542
[2] Stéphane Boucheron and Gábor Lugosi and Olivier Bousquet (2004), Concentration inequalities. Springer-Verlag.
[3] V. de la Pena, E. Gine (1999), Decoupling. From dependence to independence. Randomly stopped processes. U-statistics and processes. Martingales and beyond. Probability and its Applications (New York). Springer-Verlag, New York.
[4] W. Hoeffding (1963), On Sequences of Sums of Independent Random Vectors Journal of the American Statistical Association 58, 13-30
[5] W. Hoeffding (1948), A Class of statistics with asymptotically normal distribution The Annals of Mathematical Statistics, 293-325
[6] Joly, E. and Lugosi, G. (2015) Robust estimation of U-statistics Stochastic Processes and their Applications Volume 126, Issue 12, December 2016, Pages 3760-3773
[7] Nemirovsky, A. and D. Yudin (1983), Problem complexity and method efficiency in optimization
[8] Vershynin, Roman (2011) A Simple Decoupling Inequality in Probability Theory

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