Topic 4 Decoupling Inequalities for (Generalized) U-Statistics

Victor H. de la Peña

Professor of Statistics, Columbia University

Artificial Intelligence Institute for Advances in Optimization Georgia Institute of Technology 2024

Topics Preview

U-statistics

2 The Generalized U-statistics with Applications

3 Decoupling Inequalities for U-statistics

Topics Preview

U-statistics

2 The Generalized U-statistics with Applications

Opening Inequalities for U-statistics

U-Statistics

Let $X_1,...,X_n$ be a random sample (i.i.d. observations) from an unknown distribution F in \mathbb{R} . Given a known function $h:\mathbb{R}\to\mathbb{R}$, consider the estimation of the "parameter"

$$\theta = \theta(F) = \mathbb{E}[h(X_1, ..., X_m)],$$

Of course, you may interested in more complex spaces, which the random variables live in or h maps to, but now let us think about the simpler case.

A natural unbiased estimator of θ you propose is $h(X_1,...,X_m)$, and since n observations (with $n \geq m$) are available, this simple estimator can be improved. Now you decide to get the average of $h(X_{\alpha_1},...,X_{\alpha_m})$, where $(X_{\alpha_1},...,X_{\alpha_m}) \in \Pi$, the set of all permutations of m integers such that

$$1 \leq \alpha_i \leq n$$
, $\alpha_i \neq \alpha_j$ if $i \neq j$, $(i, j = 1, ...m)$.

Congratulations! You successfully construct a U-Statistic, which in this context is defined by

$$U_{n} = U(X_{1},...,X_{n}) = \frac{1}{n(n-1)...(n-m+1)} \sum_{(X_{\alpha_{1}},...,X_{\alpha_{m}}) \in \Pi} h(X_{\alpha_{1}},...,X_{\alpha_{m}}).$$
(1)

de la Peña Decoupling & U-statistics Al4OPT Atlanta 2024 5 / 29

If h is permutation invariant (for instance, when r=3: $h((x_1,x_2,x_3))=h((x_2,x_1,x_3))=h((x_3,x_1,x_2))=h((x_1,x_3,x_1))=h((x_2,x_3,x_1))=h((x_3,x_2,x_1))$), the definition (1) is equivalent to

$$U_n = \frac{1}{\binom{n}{m}} \sum_{1 \le \alpha_1 \le \dots \le \alpha_m \le n} h(X_{\alpha_1}, \dots, X_{\alpha_m})$$
 (2)

Although it may be the first time you hear U-Statistics, you have played with it for a long time. Look at equation (2), then set $h: \mathbb{R}^2 \to \mathbb{R}$ be such that $h(x_1, x_2) = \frac{1}{2}(x_1 - x_2)^2$, you can verify that U_n is exactly twice the sample variance, i.e.,

$$s_n^2 = \frac{\sum_{i=1}^n (X_i - \bar{X}_n)^2}{n-1} = \frac{\sum_{1 \le i < j \le n} \frac{1}{2} (X_i - X_j)^2}{\binom{n}{2}} = \frac{\sum_{1 \le i < j \le n} (X_i - X_j)^2}{n(n-1)}.$$

And by doing so, it is convenient to show that s_n^2 is an unbiasedness estimator. This is why we call such estimators U-statistics: the letter "U" stands for unbiased.

Examples

There are several examples of U-statistics. The sample mean is definitely a U-statistic. And when $X_1 \sim X \not\equiv 0$ is nonnegative a.s., the sample Gini mean difference (GMD), defined as

$$d = \frac{1}{n(n-1)} \sum_{i \neq j} |X_i - X_j| = \frac{2}{n(n-1)} \sum_{i < j} |X_i - X_j|,$$

is also a U-statistic. You can find several examples of U-statistics, together with many brilliant limiting theorems, in the giant paper by W. HOEFFDING (1948, [4]).



Topics Preview

U-statistics

2 The Generalized U-statistics with Applications

Opening Inequalities for U-statistics

Generalized U-statistics

We now extend this notion of U-statistics. Let $\{X_i\}$ be a sequence of independent random variables in a measurable space (S, S) and $\mathbf{f} = \{f_{ij}, \ 1 \leq i \neq j \leq n\}$, a family of functions of two variables taking $S \times S$ into $(D, \|\cdot\|)$. Then we define the generalized U-statistic U_n as

$$U_n = \sum_{1 \le i \ne j \le n} f_{ij}(X_i, X_j) \tag{3}$$

You can notice that the usual U-statistics can be obtained by letting $f_{ij}=f/\binom{n}{2}$. And such a generalized version may remind you more examples. For instance, the quadratic form $X^TAX=\sum\limits_{1\leq i\neq j\leq n}a_{ij}X_iX_j$,

where the diagonal elements of the symmetric matrix A are set to be zero.

Random Graph

We can also link the generalized U-Statistic to random colored graph theory. Let $\{X_i\}_{i=1}^n$ a independent sequence of i.i.d. random variables, i.e., $X_i \stackrel{\mathcal{D}}{=} X$ for some random variables X. Consider the complete graph G = (V, E), where |V| = n and X_i is the color of the vertex i. Now we let $f_{ij} = f$ for some f fixed, and if f is symmetric, then

$$S_n(f) = \sum_{1 \le i \ne j \le n} f(X_i, X_j)$$

is a U-statistic (not averaged) representing some color information of vertices.

If we let $X \sim Ber(p)$, where the vertex $X_i = 1$ (resp, 0) indicates that this vertex is black (resp, white), and $f(x_1, x_2) = (1 - x_1)x_2$, which is not symmetric, then

$$S'_n(f) = \sum_{1 \le i < j \le n} f(X_i, X_j)$$

counts patterns beginning with a white vertex and ending with a black vertex in this random sequence. And with $f(x_1, x_2) = \mathbb{I}_{\{x_1 \neq x_2\}}$, the statistic

$$S_n"(f) = \sum_{1 \le i < j \le n} f(X_i, X_j)$$

counts the edges with one black and one white end-point.

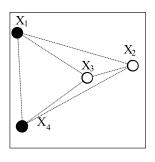


Figure: A example of a random graph, where $S'_n = 2$ and $S_n'' = 4$.

12/29

Topics Preview

U-statistics

The Generalized U-statistics with Applications

3 Decoupling Inequalities for U-statistics

You may notice that, although $X_1,...,X_n$ are mutually independent, the random variables $f_{ij}(X_i,X_j)$'s are dependent, if i or j is fixed. This cause a difficulty in evaluating the expectation of $\|\sum\limits_{1\leq i\leq j\leq n}f(X_i,X_j)\|$ and

 $\Phi\left(\|\sum\limits_{1\leq i< j\leq n}f(X_i,X_j)\|
ight)$ for some $\Phi:\mathbb{R}^+_0 o\mathbb{R}$ convex increasing.

Let us make the problem more complex, but give a formal statement: Let X_1, \dots, X_n be a sequence of independent random variables in a measurable space (S, S) and let $\{f_{ii}\}$ be a family of integrable functions such that $f_{ii}: S \times S \mapsto D$ with $(D, \|\cdot\|)$ a Banach space. Let $\Phi: \mathbb{R}_0^+ \to \mathbb{R}$ be convex such that

$$\max_{1\leq i\neq j\leq n}\mathbb{E}\Phi(\|f_{ij}(X_i,X_j)\|)<\infty.$$

Then how can we bound

$$\mathbb{E}\Phi(\|\sum_{1\leq i\neq j\leq n}f_{ij}(X_i,X_j)\|)?$$

Remember that in the last lecture, I briefly introduced tangent decoupling. Think about the filtration $\mathcal{F}_i = \sigma(X_1, ..., X_i)$, and you can write

$$U_n = \sum_{1 \le i \ne j \le n} f_{ij}(X_i, X_j) = \sum_{j=2}^n \sum_{i=1}^{j-1} f_{ij}(X_i, X_j),$$

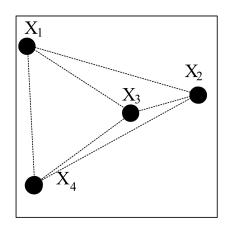
where $\sum_{i=1}^{j-1} f_{ij}(X_i, X_j)$ is adapted to \mathcal{F}_j . Suppose that we have $\{\tilde{X}_i\}_{i=1}^n$ an independent copy of $\{X_i\}_{i=1}^n$. Then

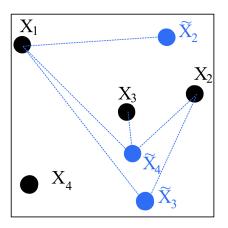
$$\sum_{j=2}^{n} \sum_{i=1}^{j-1} f_{ij}(X_i, \tilde{X}_j) = \sum_{j=2}^{n} T_j(\tilde{X}_j)$$

is a sum of conditionally independent variables given $\sigma(X_1,...,X_n)$.

16/29

de la Peña Decoupling & U-statistics Al4OPT Atlanta 2024





Theorem (de la Peña, 1992 [1])

With the aforementioned setting $(\Phi : \mathbb{R}_0^+ \to \mathbb{R} \text{ convex increasing})$,

$$M := \mathbb{E}\Phi(\|\sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, X_j)\|)$$

$$\leq \mathbb{E}\Phi(8\|\sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, \tilde{X}_j)\|).$$
(4)

And if $f_{ij} \in \Pi_{ij}$ satisfy the symmetry conditions

$$f_{ij} = f_{ji}$$
 and $f_{ij}(X_i, X_j) = f_{ij}(X_j, X_i)$,

then the reverse bound holds:

$$\mathbb{E}\Phi(\frac{1}{4}\|\sum_{1\leq i\neq i\leq n}f_{ij}(X_i,\tilde{X}_j)\|)\leq M. \tag{5}$$



Remark

The fact that the lower bound does not hold for general f_{ij} follows trivially by using

$$f_{ij}(X_i,X_j)=X_j-X_i$$

because then $\sum_{i\neq j} f_{ij}(X_i, X_j) = 0$. But one may still obtain a lower bound by using the symmetrized kernels $\hat{f}_{ij} = [f_{ij}(X_i, X_j) + f_{ij}(X_j, X_i)]/2$ for $i \neq j$ and letting $\hat{f}_{ji} = \hat{f}_{ij}$

Remark

Considering the situation of quadratic forms, X^TAX , where the diagonal entries of A are zero and $A = A^T$, we have inequalities (4) and (5) as follows when X_i 's are mean-zero:

$$\mathbb{E}\Phi(\frac{1}{4}|X^T A \tilde{X}|) \leq \mathbb{E}\Phi(|X^T A X|) \leq \mathbb{E}\Phi(4|X^T A \tilde{X}|).$$

I will explain the smaller constant 4 soon.

Warm-up Lemma

We demonstrate only the first equation (4) here, with a trivial lemma. But we first, for simplicity, denote by $\mathbb{E}_{\sigma}Y = \mathbb{E}[Y|\sigma]$, where Y is an r.v. and σ is a σ -field.

Let us first see the following warm-up lemma:

Lemma

For X_1, X_2 i.i.d., we have $\mathbb{E}(X_1|Z_1) = \frac{X_1 + X_2}{2}$, where $Z_1 = (X_1, X_2)$ w.p. 1/2 and $Z_1 = (X_2, X_1)$ w.p. 1/2.

We extend this result to the bi-variate case in the following lemma:

Lemma

Let $\mathscr{Z}=\sigma(Z_i,i=1,...,n)$, where $\{Z_i\}$ is a sequence of independent random vectors with $Z_i=(X_i,\tilde{X}_i)$ w.p. $\frac{1}{2}$ and $Z_i=(\tilde{X}_i,X_i)$ w.p. $\frac{1}{2}$. Then,

$$\mathbb{E}_{\mathscr{Z}}f_{ij}(X_i, X_j) = \mathbb{E}_{\mathscr{Z}}f_{ij}(X_i, \tilde{X}_j)$$

$$= \frac{1}{4}[f_{ij}(X_i, X_j) + f_{ij}(X_i, \tilde{X}_j) + f_{ij}(\tilde{X}_i, X_j) + f_{ij}(\tilde{X}_i, \tilde{X}_j)]$$
(6)

It is not hard to verify this lemma, by applying the same conditional law of $f_{ij}(X_i, \tilde{X}_j)$ and $f_{ij}(\tilde{X}_i, X_j)$ given \mathscr{Z} , and noticing that the sum of those four terms is measurable w.r.t. \mathscr{Z} .

Setting $\mathscr{X} = \sigma(X_1, ..., X_n)$, we use the following identity (remember we denote by $\mathbb{E}_{\sigma}Y = \mathbb{E}[Y|\sigma]$):

$$\begin{split} \sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, X_j) &= \sum_{1 \leq i \neq j \leq n} [\mathbb{E}_{\mathscr{X}} f_{ij}(X_i, X_j) + \mathbb{E}_{\mathscr{X}} f_{ij}(X_i, \tilde{X}_j) \\ &+ \mathbb{E}_{\mathscr{X}} f_{ij}(\tilde{X}_i, X_j) + \mathbb{E}_{\mathscr{X}} f_{ij}(\tilde{X}_i, \tilde{X}_j)] \\ &- \sum_{1 \leq i \neq j \leq n} [\mathbb{E}_{\mathscr{X}} f_{ij}(X_i, \tilde{X}_j) + \mathbb{E}_{\mathscr{X}} f_{ij}(\tilde{X}_i, X_j) \\ &+ \mathbb{E}_{\mathscr{X}} f_{ij}(\tilde{X}_i, \tilde{X}_j)]. \end{split}$$

A Simpler Version

Recall the Lemma 6, that

$$\mathbb{E}_{\mathscr{Z}}f(X_i,X_j)=\frac{1}{4}[f(X_i,X_j)+f(X_i,\tilde{X}_j)+f(\tilde{X}_i,X_j)+f(\tilde{X}_i,\tilde{X}_j)].$$

We **assume** that $\mathbb{E}_{\mathscr{X}} f(X_i, \tilde{X}_j) = \mathbb{E}_{\mathscr{X}} f(\tilde{X}_i, X_j) = \mathbb{E}_{\mathscr{X}} f(\tilde{X}_i, \tilde{X}_j) = 0$ (e.g., $f(x_1, x_2) = ax_1x_2$ for some constant a).

For the U-statistic $\sum_{1 \le i \ne j \le n} f(X_i, X_j)$ with symmetric kernel f, we have

$$\mathbb{E}\Phi(|\sum f(X_i, X_j)|) = \mathbb{E}\Phi(|\sum f(X_i, X_j) + \mathbb{E}_{\mathscr{Z}}[f(X_i, \tilde{X}_j) + f(\tilde{X}_i, X_j) + f(\tilde{X}_i, \tilde{X}_j)]|)$$

$$\leq \mathbb{E}\Phi(|\sum (f(X_i, X_j) + f(X_i, \tilde{X}_j) + f(\tilde{X}_i, X_j) + f(\tilde{X}_i, \tilde{X}_j))|)$$

$$= \mathbb{E}\Phi(|\sum 4\mathbb{E}_{\mathscr{Z}}f(X_i, \tilde{X}_j)|)$$

$$\leq \mathbb{E}\Phi(4|\sum f(X_i, \tilde{X}_i)|).$$

Proof

From the preceding and the triangle inequality,

$$\begin{split} &\mathbb{E}\Phi(\|\sum_{1\leq i\neq j\leq n}f_{ij}(X_{i},X_{j})\|)\\ &\leq \mathbb{E}\Phi(\|\sum_{1\leq i\neq j\leq n}\mathbb{E}_{\mathscr{X}}[f_{ij}(X_{i},X_{j})+f_{ij}(X_{i},\tilde{X}_{j})+f_{ij}(\tilde{X}_{i},X_{j})+f_{ij}(\tilde{X}_{i},\tilde{X}_{j})]\|\\ &+\|\mathbb{E}_{\mathscr{X}}[f_{ij}(X_{i},\tilde{X}_{j})+f_{ij}(\tilde{X}_{i},X_{j})+f_{ij}(\tilde{X}_{i},\tilde{X}_{j})]\|)\\ &\leq \frac{1}{2}\mathbb{E}\Phi(2\|\sum_{1\leq i\neq j\leq n}\mathbb{E}_{\mathscr{X}}[f_{ij}(X_{i},X_{j})+f_{ij}(X_{i},\tilde{X}_{j})+f_{ij}(\tilde{X}_{i},X_{j})+f_{ij}(\tilde{X}_{i},\tilde{X}_{j})]\|)\\ &+\frac{1}{2}\mathbb{E}\Phi(2\|\sum_{1\leq i\neq j\leq n}\mathbb{E}_{\mathscr{X}}[f_{ij}(X_{i},\tilde{X}_{j})+f_{ij}(\tilde{X}_{i},X_{j})+f_{ij}(\tilde{X}_{i},\tilde{X}_{j})]\|)\\ &[\text{by the convexity of }\Phi] \end{split}$$

Proof

$$\leq \frac{1}{2}\mathbb{E}\Phi(2\|\sum_{1\leq i\neq j\leq n}[f_{ij}(X_{i},X_{j})+f_{ij}(X_{i},\tilde{X}_{j})+f_{ij}(\tilde{X}_{i},X_{j})+f_{ij}(\tilde{X}_{i},\tilde{X}_{j})]\|)$$

$$+\frac{1}{2}\mathbb{E}\Phi(2\|\sum_{1\leq i\neq j\leq n}\mathbb{E}_{\mathscr{Z}}[f_{ij}(X_{i},\tilde{X}_{j})+f_{ij}(\tilde{X}_{i},X_{j})+f_{ij}(\tilde{X}_{i},\tilde{X}_{j})\|) \text{ [conditional Jensen inequality]}$$

$$\leq \frac{1}{2}\mathbb{E}\Phi(8\|\sum_{1\leq i\neq j\leq n}\mathbb{E}_{\mathscr{Z}}f_{ij}(X_{i},\tilde{X}_{j})\|)+\frac{1}{6}[\mathbb{E}\Phi(6\|\sum_{1\leq i\neq j\leq n}\mathbb{E}_{\mathscr{X}}f_{ij}(X_{i},\tilde{X}_{j})\|)] \text{[by (6) and }\Phi \text{ convex]}$$

$$+\mathbb{E}\Phi(6\|\sum_{1\leq i\neq j\leq n}\mathbb{E}_{\mathscr{Z}}f_{ij}(\tilde{X}_{i},X_{j})\|)+\mathbb{E}\Phi(6\|\sum_{1\leq i\neq j\leq n}\mathbb{E}f_{ij}(\tilde{X}_{i},\tilde{X}_{j})\|)] \text{[by (6) and }\Phi \text{ convex]}$$

$$\leq \frac{1}{2}\mathbb{E}\Phi(8\|\sum_{1\leq i\neq j\leq n}\mathbb{E}_{\mathscr{Z}}f_{ij}(X_{i},\tilde{X}_{j})\|) \text{ [by conditional Jensen and that }\mathbb{E}f_{ij}(\tilde{X}_{i},\tilde{X}_{j})=\mathbb{E}f_{ij}(X_{i},\tilde{X}_{j})]$$

$$+\frac{1}{6}\mathbb{E}\Phi(8\|\sum_{1\leq i\neq j\leq n}\mathbb{E}_{\mathscr{Z}}f_{ij}(X_{i},\tilde{X}_{j})\|)+\frac{1}{2}\mathbb{E}\Phi(6\|\sum_{1\leq i\neq j\leq n}\mathbb{E}f_{ij}(X_{i},\tilde{X}_{j})\|) \text{ [by Jensen inequality]}$$

$$\leq \frac{1}{2}\mathbb{E}\Phi(8\|\sum_{1\leq i\neq j\leq n}\mathbb{E}_{\mathscr{Z}}f_{ij}(X_{i},\tilde{X}_{j})\|) \text{ [by Φ increasing]}$$

Decoupling Inequalities for General Kernels h

While this lecture primarily emphasizes the (generalized) U-statistics cases with kernels of the form $h: S^2 \to D$, it's worth noting that we have also established decoupling inequalities for the more general $h: S^k \to D$ Consequently, we arrive at a frequently employed concentration inequality (See de la Peña and Montgomery-Smith [2] in Bulletin of the American Mathematical Society, or [3]).

Let $X_1,...,X_n$ be a sequence of independent random variables on a measurable space (S,S) and let $\{X_i^{(j)}\}$, j=1,...,k be k independent copies of $\{X_i\}$. Let $f_{i_1,...,i_k}$ be family of functions of k variables taking S^k into a Banach space $(D,\|\cdot\|)$. Assume that each $f_{i_1,...,i_k}$ is permutation invariant. Then for all $n\geq k\geq 2$, t>0, there exist numerical constants C_k, \tilde{C}_k depending on k only such that (with $P_{n,k}$ the set of all permutations $(i_1,...,i_k)\in\{1,...,n\}^k$)

$$\mathbb{P}\left(\|\sum_{(i_{1},...,i_{k})\in P_{n,k}}f_{i_{1},...,i_{k}}(X_{i_{1}},...,X_{i_{k}})\|\geq t\right)$$

$$\leq C_{k}\mathbb{P}\left(C_{k}\|\sum_{(i_{1},i_{2},...,i_{k})\in P_{n,k}}f_{i_{1},...,i_{k}}(X_{i_{1}}^{(1)},...,X_{i_{k}}^{(k)})\|\geq t\right).$$

In addition,

$$egin{aligned} ilde{\mathcal{C}}_k \mathbb{P} \left(ilde{\mathcal{C}}_k \| \sum_{(i_1,i_2,...,i_k) \in P_{n,k}} f_{i_1,...,i_k}(X_{i_1},...,X_{i_k}) \| \geq t
ight) \ & \geq \mathbb{P} \left(\| \sum_{(i_1,i_2,...,i_k) \in P_{n,k}} f_{i_1,...,i_k}(X_{i_1}^{(1)},...,X_{i_k}^{(k)}) \| \geq t
ight). \end{aligned}$$

References I

- [1] V. H. de la Peña. "Decoupling and Khintchine's inequalities for U-statistics". In: *Ann. Proba.* (1992), pp. 1877–1892.
- [2] V. H. de la Peña and S.J. Montgomery-Smith. "Bounds on the tail probability of U-statistics and quadratic forms". In: AMERICAN MATHEMATICAL SOCIETY 31.2 (1994), pp. 223–227.
- [3] Victor H de la Peña and Stephen J Montgomery-Smith. "Decoupling inequalities for the tail probabilities of multivariate U-statistics". In: *The Annals of Probability* (1995), pp. 806–816.
- [4] Wassily Hoeffding. "A class of statistics with asymptotically normal distribution". In: *Breakthroughs in Statistics: Foundations and Basic Theory* (1992), pp. 308–334.