

# 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

- 1 U-statistics
- 2 The Generalized U-statistics with Applications
- 3 Decoupling Inequalities for U-statistics

# Topics Preview

- 1 U-statistics
- 2 The Generalized U-statistics with Applications
- 3 Decoupling Inequalities for U-statistics

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

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

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

$$1 \leq \alpha_i \leq n, \quad \alpha_i \neq \alpha_j \text{ if } i \neq j, \quad (i, j = 1, \dots, m).$$

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

$$U_n = U(X_1, \dots, X_n) = \frac{1}{n(n-1)\dots(n-m+1)} \sum_{(X_{\alpha_1}, \dots, X_{\alpha_m}) \in \Pi} h(X_{\alpha_1}, \dots, X_{\alpha_m}). \quad (1)$$

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

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

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  $h : \mathbb{R}^2 \rightarrow \mathbb{R}$  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.,

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

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, [3]).



# Topics Preview

- 1 U-statistics
- 2 The Generalized U-statistics with Applications
- 3 Decoupling 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  $(S, \mathcal{S})$  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

$$U_n = \sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, X_j) \quad (3)$$

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  $X^T A X = \sum_{1 \leq i \neq j \leq n} a_{ij} X_i X_j$ , 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

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

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

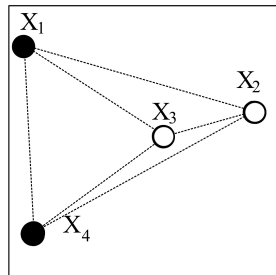
If we let  $X \sim \text{Ber}(p)$ , where the vertex  $X_i = 1$  (resp, 0) indicates that this vertex is black (resp, white), and  $f(x_1, x_2) = (1 - x_1)x_2$ , which is not symmetric, then

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

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

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

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



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

# Topics Preview

- 1 U-statistics
- 2 The Generalized U-statistics with Applications
- 3 Decoupling Inequalities for U-statistics

You may notice that, although  $X_1, \dots, X_n$  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  $\left\| \sum_{1 \leq i < j \leq n} f(X_i, X_j) \right\|$  and  $\Phi \left( \left\| \sum_{1 \leq i < j \leq n} f(X_i, X_j) \right\| \right)$  for some  $\Phi : \mathbb{R}_0^+ \rightarrow \mathbb{R}$  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  $(S, \mathcal{S})$  and let  $\{f_{ij}\}$  be a family of integrable functions such that  $f_{ij} : S \times S \mapsto D$  with  $(D, \|\cdot\|)$  a Banach space. Let  $\Phi : \mathbb{R}_0^+ \rightarrow \mathbb{R}$  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  $\mathcal{F}_i = \sigma(X_1, \dots, X_i)$ , and you can write

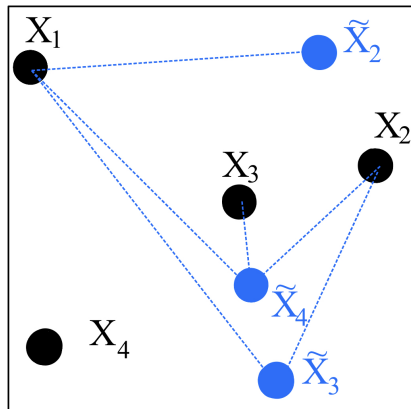
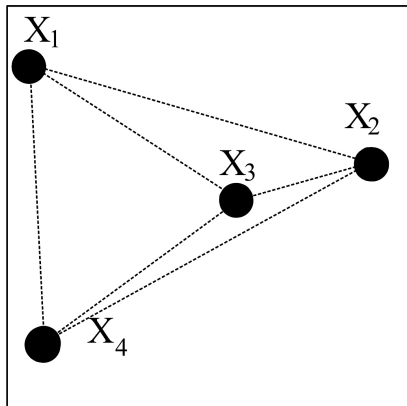
$$U_n = \sum_{1 \leq i < j \leq n} f_{ij}(X_i, X_j) = \sum_{j=2}^n \sum_{i=1}^{j-1} f_{ij}(X_i, X_j),$$

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  $\sigma(X_1, \dots, X_n)$ .





## Theorem (de la Peña [1])

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

$$\begin{aligned} M &:= \mathbb{E}\Phi\left(\left\|\sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, X_j)\right\|\right) \\ &\leq \mathbb{E}\Phi\left(8\left\|\sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, \tilde{X}_j)\right\|\right). \end{aligned} \tag{4}$$

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

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

then the reverse bound holds:

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

## 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,  $X^T A X$ , 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:*

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

*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  $\sigma$  is a  $\sigma$ -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  $\mathcal{Z} = \sigma(Z_i, i = 1, \dots, n)$ , 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,

$$\begin{aligned}\mathbb{E}_{\mathcal{Z}} f_{ij}(X_i, X_j) &= \mathbb{E}_{\mathcal{Z}} f_{ij}(X_i, \tilde{X}_j) = \mathbb{E}_{\mathcal{Z}} f_{ij}(\tilde{X}_i, X_j) = \mathbb{E}_{\mathcal{Z}} f_{ij}(\tilde{X}_i, \tilde{X}_j) \\ &= \frac{1}{4} \mathbb{E}_{\mathcal{Z}} \left[ f_{ij}(X_i, X_j) + f_{ij}(X_i, \tilde{X}_j) + f_{ij}(\tilde{X}_i, X_j) + f_{ij}(\tilde{X}_i, \tilde{X}_j) \right] \\ &= \frac{1}{4} \left[ f_{ij}(X_i, X_j) + f_{ij}(X_i, \tilde{X}_j) + f_{ij}(\tilde{X}_i, X_j) + f_{ij}(\tilde{X}_i, \tilde{X}_j) \right]\end{aligned}\tag{6}$$

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  $\mathcal{Z}$ , and noticing that the sum of those four terms is measurable w.r.t.  $\mathcal{Z}$ .

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

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

# A Simpler Version

Recall the Lemma 6, that

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

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

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

$$\begin{aligned} \mathbb{E}\Phi(|\sum f(X_i, X_j)|) &= \mathbb{E}\Phi(|\sum f(X_i, X_j) + \mathbb{E}_{\mathcal{X}}[f(X_i, \tilde{X}_j) + f(\tilde{X}_i, X_j) + f(\tilde{X}_i, \tilde{X}_j)]|) \\ &\leq \mathbb{E}\Phi(|\sum (f(X_i, X_j) + f(X_i, \tilde{X}_j) + f(\tilde{X}_i, X_j) + f(\tilde{X}_i, \tilde{X}_j))|) \\ &= \mathbb{E}\Phi(|\sum 4\mathbb{E}_{\mathcal{X}} f(X_i, \tilde{X}_j)|) \\ &\leq \mathbb{E}\Phi(4|\sum f(X_i, \tilde{X}_j)|). \end{aligned}$$

From the preceding and the triangle inequality,

$$\begin{aligned}
 & \mathbb{E}\Phi\left(\left\|\sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, X_j)\right\|\right) \\
 & \leq \mathbb{E}\Phi\left(\left\|\sum_{1 \leq i \neq j \leq n} \mathbb{E}_{\mathcal{X}}[f_{ij}(X_i, X_j) + f_{ij}(X_i, \tilde{X}_j) + f_{ij}(\tilde{X}_i, X_j) + f_{ij}(\tilde{X}_i, \tilde{X}_j)]\right\|\right) \\
 & + \mathbb{E}\Phi\left(\left\|\sum_{1 \leq i \neq j \leq n} \mathbb{E}_{\mathcal{X}}[f_{ij}(X_i, \tilde{X}_j) + f_{ij}(\tilde{X}_i, X_j) + f_{ij}(\tilde{X}_i, \tilde{X}_j)]\right\|\right) \\
 & \leq \frac{1}{2} \mathbb{E}\Phi\left(2\left\|\sum_{1 \leq i \neq j \leq n} \mathbb{E}_{\mathcal{X}}[f_{ij}(X_i, X_j) + f_{ij}(X_i, \tilde{X}_j) + f_{ij}(\tilde{X}_i, X_j) + f_{ij}(\tilde{X}_i, \tilde{X}_j)]\right\|\right) \\
 & + \frac{1}{2} \mathbb{E}\Phi\left(2\left\|\sum_{1 \leq i \neq j \leq n} \mathbb{E}_{\mathcal{X}}[f_{ij}(X_i, \tilde{X}_j) + f_{ij}(\tilde{X}_i, X_j) + f_{ij}(\tilde{X}_i, \tilde{X}_j)]\right\|\right) \\
 & \quad [\text{by the convexity of } \Phi]
 \end{aligned}$$



# Proof

$$\begin{aligned}
&\leq \frac{1}{2} \mathbb{E} \Phi(2 \left\| \sum_{1 \leq i \neq j \leq n} [f_{ij}(X_i, X_j) + f_{ij}(X_i, \tilde{X}_j) + f_{ij}(\tilde{X}_i, X_j) + f_{ij}(\tilde{X}_i, \tilde{X}_j)] \right\|) \\
&+ \frac{1}{2} \mathbb{E} \Phi(2 \left\| \sum_{1 \leq i \neq j \leq n} \mathbb{E}_{\mathcal{X}} [f_{ij}(X_i, \tilde{X}_j) + f_{ij}(\tilde{X}_i, X_j) + f_{ij}(\tilde{X}_i, \tilde{X}_j)] \right\|) \quad [\text{conditional JENSEN inequality}] \\
&\leq \frac{1}{2} \mathbb{E} \Phi(8 \left\| \sum_{1 \leq i \neq j \leq n} \mathbb{E}_{\mathcal{X}} f_{ij}(X_i, \tilde{X}_j) \right\|) + \frac{1}{6} [\mathbb{E} \Phi(6 \left\| \sum_{1 \leq i \neq j \leq n} \mathbb{E}_{\mathcal{X}} f_{ij}(X_i, \tilde{X}_j) \right\|) \\
&+ \mathbb{E} \Phi(6 \left\| \sum_{1 \leq i \neq j \leq n} \mathbb{E}_{\mathcal{X}} f_{ij}(\tilde{X}_i, X_j) \right\|) + \mathbb{E} \Phi(6 \left\| \sum_{1 \leq i \neq j \leq n} \mathbb{E}_{\mathcal{X}} f_{ij}(\tilde{X}_i, \tilde{X}_j) \right\|)] [\text{by (6) and } \Phi \text{ convex}] \\
&\leq \frac{1}{2} \mathbb{E} \Phi(8 \left\| \sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, \tilde{X}_j) \right\|) + \frac{2}{6} \mathbb{E} \Phi(6 \left\| \sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, \tilde{X}_j) \right\|) \\
&+ \frac{1}{6} \mathbb{E} \Phi(6 \left\| \sum_{1 \leq i \neq j \leq n} f_{ij}(\tilde{X}_i, \tilde{X}_j) \right\|) \quad [\text{by conditional JENSEN, and } \mathbb{E} f_{ij}(\tilde{X}_i, \tilde{X}_j) = \mathbb{E} f_{ij}(X_i, \tilde{X}_j)] \\
&\leq \frac{1}{2} \mathbb{E} \Phi(8 \left\| \sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, \tilde{X}_j) \right\|) + \frac{1}{2} \mathbb{E} \Phi(6 \left\| \sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, \tilde{X}_j) \right\|) \quad [\text{by JENSEN inequality}] \\
&\leq \mathbb{E} \Phi(8 \left\| \sum_{1 \leq i \neq j \leq n} f_{ij}(X_i, \tilde{X}_j) \right\|) \quad [\text{by } \Phi \text{ increasing}]
\end{aligned}$$

# Decoupling Inequalities for General Kernels $h$

While this lecture primarily emphasizes the (generalized) U-statistics cases with kernels of the form  $h : S^2 \rightarrow D$ , it's worth noting that we have also established decoupling inequalities for the more general  $h : S^k \rightarrow D$ . Consequently, we arrive at a frequently employed concentration inequality (See de la Peña and Montgomery-Smith [4] in the Bulletin of the American Mathematical Society, or [2]).

Let  $X_1, \dots, X_n$  be a sequence of independent random variables on a measurable space  $(S, \mathcal{S})$  and let  $\{X_i^{(j)}\}$ ,  $j = 1, \dots, k$  be  $k$  independent copies of  $\{X_i\}$ . Let  $f_{i_1, \dots, i_k}$  be family of functions of  $k$  variables taking  $S^k$  into a Banach space  $(D, \|\cdot\|)$ . Assume that each  $f_{i_1, \dots, i_k}$  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  $(i_1, \dots, i_k) \in \{1, \dots, n\}^k$ )

$$\begin{aligned} & \mathbb{P} \left( \left\| \sum_{(i_1, \dots, i_k) \in P_{n,k}} f_{i_1, \dots, i_k}(X_{i_1}, \dots, X_{i_k}) \right\| \geq t \right) \\ & \leq C_k \mathbb{P} \left( C_k \left\| \sum_{(i_1, i_2, \dots, i_k) \in P_{n,k}} f_{i_1, \dots, i_k}(X_{i_1}^{(1)}, \dots, X_{i_k}^{(k)}) \right\| \geq t \right). \end{aligned}$$

In addition,

$$\begin{aligned} & \tilde{C}_k \mathbb{P} \left( \tilde{C}_k \left\| \sum_{(i_1, i_2, \dots, i_k) \in P_{n,k}} f_{i_1, \dots, i_k}(X_{i_1}, \dots, X_{i_k}) \right\| \geq t \right) \\ & \geq \mathbb{P} \left( \left\| \sum_{(i_1, i_2, \dots, i_k) \in P_{n,k}} f_{i_1, \dots, i_k}(X_{i_1}^{(1)}, \dots, X_{i_k}^{(k)}) \right\| \geq t \right). \end{aligned}$$

# References I

- [1] V. H. de la Peña. “Decoupling and Khintchine’s inequalities for U-statistics”. In: *Ann. Proba.* (1992), pp. 1877–1892.
- [2] 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.
- [3] Wassily Hoeffding. “A class of statistics with asymptotically normal distribution”. In: *Breakthroughs in Statistics: Foundations and Basic Theory* (1992), pp. 308–334.
- [4] Victor H de la Peña and SJ Montgomery-Smith. “Bounds on the tail probability of U-statistics and quadratic forms”. In: *the Bulletin of the American Mathematical Society* 31.2 (1994), pp. 223–227.