On Computing and the Complexity of Computing Higher-Order U-Statistics, Exactly

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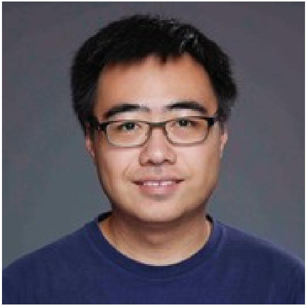
Coauthors



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Outline

U/V-Statistics

U-statistics are generally used to construct unbiased estimators of population parameters.

- Given a kernel $h(x_1, \dots, x_m) : \mathcal{X}^m \to \mathbb{R}$ and a sequence of samples $X_1, \dots, X_n$.
- The U-statistic takes the form

$$\mathbb{U}_{n,m}[h] = \cancel{\frac{n!}{(n-m)!}} \sum_{1 \leq i_1 \neq i_2 \neq \cdots \neq i_m \leq n} h(X_{i_1}, \dots, X_{i_m}).$$

- The V-statistic takes the form

$$\mathbb{V}_{n,m}[h] = \cancel{\frac{1}{n^m}} \sum_{1 \leq i_1, i_2, \cdots, i_m \leq n} h(X_{i_1}, \dots, X_{i_m}).$$

- There is a linear relationship between U-statistics and V-statistics

$$\mathbb{U} = \sum \mathbb{V}, \mathbb{V} = \sum \mathbb{U}.$$

Thus, if $\mathbb{V}$ can be computed efficiently, then so can $\mathbb{U}$, and vice versa.

The answer: V-statistics can be computed by `Einsum`

- `Einsum` can be used to compute the V-statistic efficiently.
  - The `Einsum` operation mainly performs **unconstrained summation** over selected indices of input tensors.
  - Can call `numpy.einsum` or `pytorch.einsum` in practice.
  - `pytorch` provides parallel computing on CPU and GPU.
- Examples:

```
Einsum('ij,jk->ik', A, B)
```

$$\sum_j A_{ij} B_{jk} = D_{ik}$$

```
Einsum('ijk->i', X)
```

$$\sum_{j,k} X_{ijk} = D_i$$

```
Einsum('ij,jk,kl->', A, B, C)
```

$$\sum_{i,j,k} A_{ij}\, B_{jk}\, C_{kl} = D$$

- Then what's the exact formula of the $\mathbb{U} = \sum \mathbb{V}$?

- The exact formula can be written as following:
- The proof will use the **Möbius inversion** technique.

Lemma 1 (C., Zhang, Liu, 25)

Let $\mathbb{X}$ be a non-empty set and $h : \mathbb{X}^m \to \mathbb{R}$ be a kernel function. Then for any $\boldsymbol{X} \in \mathbb{X}^n : n \geq m$,

$$\mathbb{U}[h] = \sum_{\pi \in \Pi_m} \mu_\pi \mathbb{V}[\pi](h),$$

where

$$\mu_\pi = (-1)^{(m-|\pi|)} \prod_{C \in \pi} (|C| - 1)!,$$

and Π_m denotes all partition of set $\{1, 2, \cdots, m\}$.

Decomposition of U-statistics to V-statistics

- The definition of $\mathbb{V}[\pi](h)$ is as following:

$$\pi = \{\{1\},\{2\},\{3\}\}, \quad \mathbb{V}[\pi](h) = \sum_{i_1,i_2,i_3} h(X_{i_1},X_{i_2},X_{i_3}), \quad \mu_\pi = +1,$$

$$\pi = \{\{1,2\},\{3\}\}, \quad \mathbb{V}[\pi](h) = \sum_{i_1=i_2,i_3} h(X_{i_1},X_{i_2},X_{i_3}), \quad \mu_\pi = -1,$$

$$\pi = \{\{1,3\},\{2\}\}, \quad \mathbb{V}[\pi](h) = \sum_{i_1=i_3,i_2} h(X_{i_1},X_{i_2},X_{i_3}), \quad \mu_\pi = -1,$$

$$\pi = \{\{2,3\},\{1\}\}, \quad \mathbb{V}[\pi](h) = \sum_{i_2=i_3,i_1} h(X_{i_1},X_{i_2},X_{i_3}), \quad \mu_\pi = -1,$$

$$\pi = \{\{1,2,3\}\}, \quad \mathbb{V}[\pi](h) = \sum_{i_1=i_2=i_3} h(X_{i_1},X_{i_2},X_{i_3}), \quad \mu_\pi = +2.$$

- For $m = 3$:

$$\begin{aligned}\mathbb{U}[h] &= \sum_{i_1\neq i_2\neq i_3} h(X_{i_1},X_{i_2},X_{i_3}) \\ &= \Big(\sum_{i_1,i_2,i_3} - \sum_{(i_1=i_2),i_3} - \sum_{(i_1=i_3),i_2} - \sum_{(i_2=i_3),i_1} +2 \sum_{i_1=i_2=i_3} \Big) h(X_{i_1},X_{i_2},X_{i_3}).\end{aligned}$$

Algorithm Framework

Basic Algorithm Framework

Input: Kernel function h, data samples $X_1, \ldots, X_n$, order m
Output: U-statistic $\mathbb{U}[h]$

1. Initialize $\mathbb{U}[h] \leftarrow 0$
2. For each partition $\pi \in \Pi_m$:
   2.1 Compute coefficient μ_π
   2.2 Compute V-statistic $\mathbb{V}[\pi](h)$ via `Einsum`
   2.3 $\mathbb{U}[h] \leftarrow \mathbb{U}[h] + \mu_\pi \cdot \mathbb{V}[\pi](h)$
3. Return $\mathbb{U}[h]$

Outline

On Computing U-Statistics

On Complexity of Computing U-Statistics

Applications

Limitations and Future Work

New Questions Arising in Computing U-Statistics

The following questions naturally arise:

Question 1

How to characterize the computational complexity theoretically?

- The naive nested-loop approach requires $O(n^m)$.
- Can the new algorithm compute U-statistics in substantially less than $O(n^m)$ time?

Question 2

The number of all set partitions $\pi \in \Pi_m$ is large, given by the **Bell number** B_m. Do we really need so many terms?

- B_m increases **super-exponentially** with m.
- For example:

$$B_6 = 203, \quad B_7 = 877, \quad B_8 = 4140,$$
$$B_9 = 21147, \quad B_{10} = 115975.$$

Both answers will strongly depend on the **structure of the kernel function** h.

Example 1: U-Statistics in Causal Inference: HOIFs

- Higher-order influence functions (HOIFs) (Robins et al., 2008, 2016) are rate-optimal estimators for many causal parameters.
- HOIFs are high order U-statistics, whose order can be up to $m \sim \sqrt{\log n}$.
- For example, HOIF of the treatment-specific mean is the combination of functions like

$$
\begin{aligned}
& h_m^{\mathsf{HOIF}}(X_1, \ldots, X_m) \\
& = [a_1 \phi(Z_1)^\top \phi(Z_2)][\phi(Z_2)^\top \phi(Z_3)] \cdots [\phi(Z_{m-1})^\top \phi(Z_m) b_m] \\
& = f_1(X_1, X_2) f_2(X_2, X_3) \cdots f_{m-1}(X_{m-1}, X_m)
\end{aligned}
$$

- For Question 1, given the $n \times n$ matrices $A_{ij}^{(k)} = f_k(X_i, X_j)$ for $k = 1, \cdots, m-1$:

$$
\mathrm{Complexity}(\mathbb{U}_{n,m}(h_m^{\mathsf{HOIF}})) = \begin{cases} O(n^2), & m \in \{2,3\}, \\ O(n^3), & m \in \{4,5,6,7\}, \\ O(n^4), & m \in \{8,9,10\}, \\ O(n^5), & m \in \{11,12\}. \end{cases}
$$

- For Question 2, some terms will be canceled.

Example 2: Dependence Measures

- High-order U-statistics are also used to estimate dependence measures, such as Distance Covariance (dCov^2) (Székely et al., 2007).
- dCov^2 can be represented as a 4-th order U-statistic (Yao et al., 2018):

$$\mathrm{dCov}^2(X, Y) = \frac{(n-4)!}{n!} \sum_{i \neq j \neq q \neq r} a_{ij} b_{qr} + a_{ij} b_{ij} - a_{ij} b_{iq} - a_{ij} b_{jr}$$

where $a_{ij} = \|X_i - X_j\|_2$ and $b_{ij} = \|Y_i - Y_j\|_2$.

- it can be decomposed to 3 kernel function:
- For Question 1, given the $n \times n$ matrices a_{ij}, b_{ij}:

$$\mathrm{Complexity}(\mathrm{dCov}^2(XY)) = O(n^2).$$

- For Question 2: Many terms will be canceled.

Example 3: Motif Counts

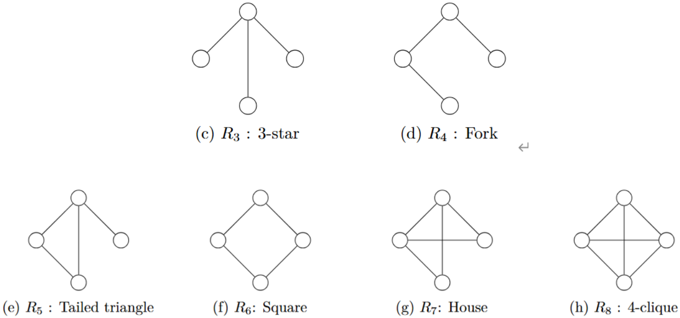
- Motif counts refer to the number of occurrences of small subgraphs (motifs) in a random graph.
- They can be used to test certain properties of the underlying random graphon (Chatterjee et al., 2024).
- The motif counts can also be written as a form similar to U-statistics.
- 3-node motifs,

(a) R_1: V-shape (b) R_2: Triangle

3-node motifs in a random graph

Example 3: Motif Counts

- 4-node motifs,



4-node motifs in a random graph

Example 3: Motif Counts

- For example :

  - V-shape

$$C(R_1) = \frac{1}{2} \sum_{i_1 \neq i_2 \neq i_3} A_{i_1 i_2} A_{i_2 i_3} B_{i_3 i_1}$$

  - Triangle:

$$C(R_2) = \frac{1}{6} \sum_{i_1 \neq i_2 \neq i_3} A_{i_1 i_2} A_{i_2 i_3} A_{i_3 i_1}$$

  - A is the adjacency matrix of the graph and $B = 1 - A$.

- For Question 1, given adjacency matrix A, the complexity is still $O(n^m)$ for m-motif.
- For Question 2, only 1 term is needed.

(a) R_1: V-shape (b) R_2: Triangle

Key Assumption: Multiplicative-Decomposable

The key of answering the above questions is the **multiplicative-decomposition** of kernels.

- We observed that many kernels of U-statistics is product of some functions with less arguments.
- Let's give a notation to capture this structure, it mimics the `Einsum` notation "ij,jk -> ".
- For $h_3^{\mathrm{HOIF}}(\boldsymbol{X}) = f_1(X_1, X_2) f_2(X_2, X_3)$:

$$\mathcal{A}_3^{\mathrm{HOIF}} = ((1,2),(2,3)),\ T_{ij}^{(k)} = f_k(X_1, X_2), k = 1, 2.$$

- For a part of $\mathrm{dCov}^2(X, Y)$: $\frac{(n-4)!}{n!} \sum_{i \neq j \neq q \neq r} a_{ij} b_{qr}$

$$\mathcal{A}^{\mathrm{dCov},1} = ((1,2),(3,4)),\ T^{(1)} = a,\ T^{(2)} = b.$$

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- For $C(R_1) = \frac{1}{2} \sum_{i_1 \neq i_2 \neq i_3} A_{i_1 i_2} A_{i_2 i_3} B_{i_3 i_1}$

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- For $C(R_1) = \frac{1}{2} \sum_{i_1 \neq i_2 \neq i_3} A_{i_1 i_2} A_{i_2 i_3} B_{i_3 i_1}$

$$\mathcal{A}_3^{\text{Motif}} = ((1,2),(2,3),(3,1)),\ T^{(1)} = T^{(2)} = A,\ T^{(3)} = B.$$

The Answer to Question 2 : Sparsification

For **Question 2 (Sparsification trick)**:

- For $h_3^{\text{HOIF}}(\boldsymbol{X}) = f_1(X_1, X_2) f_2(X_2, X_3)$, let

$$T_{ij}^{(k)} = f_1(X_i, X_j), \quad k = 1, 2.$$

$$\tilde{T}_{ij}^{(k)} = \begin{cases} T_{ij}^{(1)} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}, \quad k = 1, 2.$$

- Then we have

$$\begin{aligned}
&\mathbb{U}[h_3^{\text{HOIF}}] \\
&= \sum_{i_1 \neq i_2 \neq i_3} T_{i_1 i_2}^{(1)} T_{i_2 i_3}^{(2)} \\
&= \sum_{i_1 \neq i_2 \neq i_3} \tilde{T}_{i_1 i_2}^{(1)} \tilde{T}_{i_2 i_3}^{(2)} \\
&= \Bigg(\sum_{i_1, i_2, i_3} - \sum_{(i_1 = i_2), i_3} - \sum_{(i_1 = i_3), i_2} - \sum_{(i_2 = i_3), i_1} + 2 \sum_{i_1 = i_2 = i_3} \Bigg) \tilde{T}_{i_1 i_2}^{(1)} \tilde{T}_{i_2 i_3}^{(2)} \\
&= \Bigg(\sum_{i_1, i_2, i_3} - \cancel{\sum_{(i_1 = i_2), i_3}} - \sum_{(i_1 = i_3), i_2} - \cancel{\sum_{(i_2 = i_3), i_1}} + 2 \cancel{\sum_{i_1 = i_2 = i_3}} \Bigg) \tilde{T}_{i_1 i_2}^{(1)} \tilde{T}_{i_2 i_3}^{(2)}
\end{aligned}$$

The Answer to Question 2 : Sparsification

For **Question 2 (Sparsification trick)**:

- In general,let

$$\Pi_m^{\mathcal{A}} = \{\pi \in \Pi_m \mid \forall Q \in \pi, \forall A \in \mathcal{A}, |Q \cap \mathrm{set}[A]| < 2\}.$$

- We just need to sum over $\pi \in \Pi_m^{\mathcal{A}}$.

Order (m)	**V-stat terms (Bell number)**	**V-stat terms (Sparsification)**	**Ratio**
3	5	2	0.4
4	15	5	0.333
5	52	15	0.288
6	203	52	0.256
7	877	203	0.231
8	4140	877	0.212
9	21147	4140	0.196
10	115975	21147	0.182
11	678570	115975	0.171
12	4213597	678570	0.161

Table: The Sparsification trick on HOIF

Updated Algorithm Framework

Input: decomposition signature $\mathcal{A}$, corresponding **diagonal-excluded** tensors $\tilde{T}^{(1)}, \tilde{T}^{(2)}, \cdots$
Output: U-statistic $\mathbb{U}[h]$

1. Initialize $\mathbb{U}[h] \leftarrow 0$
2. Get m from $\mathcal{A}$
3. For each partition $\pi \in \Pi_m^{\mathcal{A}}$:
   3.1 Compute coefficient μ_π
   3.2 Compute V-statistic $\mathbb{V}[\pi](h)$ via `Einsum` with $\tilde{T}^{(1)}, \tilde{T}^{(2)}, \cdots$
   3.3 $\mathbb{U}[h] \leftarrow \mathbb{U}[h] + \mu_\pi \cdot \mathbb{V}[\pi](h)$
4. Return $\mathbb{U}[h]$

Our new package `u-stats` for computing U-statistics is available on `PyPI`:

https://pypi.org/project/u-stats/

Install via:

```
pip install u-stats
```

For **Question 1 (Complexity)**:

- For $h_3^{\text{HOIF}}(\boldsymbol{X}) = f_1(X_1, X_2) f_2(X_2, X_3)$, recall

$$\mathbb{U}[h_3^{\text{HOIF}}] = \sum_{i_1, i_2, i_3} \tilde{T}^{(1)}_{i_1 i_2} \tilde{T}^{(2)}_{i_2 i_3} - \sum_{i_1, i_2} \tilde{T}^{(1)}_{i_1 i_2} \tilde{T}^{(2)}_{i_2 i_1}$$

- Consider the first part, with $\mathcal{A}_{\pi_1} = ((1,2),(2,3))$.

Order $(1 \to 2 \to 3)$:

$$\sum_{i_1, i_2, i_3} \tilde{T}^{(1)}_{i_1 i_2} \tilde{T}^{(2)}_{i_2 i_3} \xrightarrow[\text{sum over } i_1]{O(n^2)} \sum_{i_2, i_3} \tilde{T}^{(3)}_{i_2} \tilde{T}^{(2)}_{i_2 i_3} \xrightarrow[\text{sum over } i_2]{O(n^2)} \sum_{i_3} \tilde{T}^{(4)}_{i_3} \xrightarrow[\text{sum over } i_3]{O(n)} \text{Final Result}$$

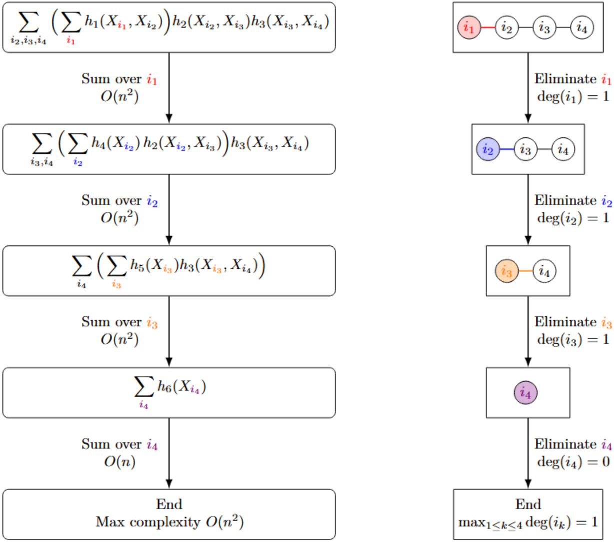
$$\Rightarrow \max \text{ complexity } = O(n^2)$$

Order $(2 \to 1 \to 3)$:

$$\sum_{i_1, i_2, i_3} \tilde{T}^{(1)}_{i_1 i_2} \tilde{T}^{(2)}_{i_2 i_3} \xrightarrow[\text{sum over } i_2]{O(n^3)} \sum_{i_1, i_3} \tilde{T}^{(5)}_{i_1 i_3} \xrightarrow[\text{sum over } i_1]{O(n^2)} \sum_{i_3} \tilde{T}^{(6)}_{i_3} \xrightarrow[\text{sum over } i_3]{O(n)} \text{Final Result}$$

$$\Rightarrow \max \text{ complexity } = O(n^3)$$

The Answer to Question 1: Complexity



Procedure of Computing a 4-th order V-statistic with $\mathcal{A} = ((1,2),(2,3),(3,4))$

The Answer to Question 1: Complexity

- In general, the computational complexity of a V-statistics depends on the summation ordering.
  - The optimal ordering corresponding to the **treewidth** of the corresponding graph G. precisely $O(n^{\mathrm{tw}(G)+1})$.
  - Finding the optimal ordering is known to be NP-hard.
  - In practice, heuristic algorithm such as greedy algorithm is used.
  - In the low-order case, the proof can be derived manually.
- For U-statistics, the computational complexity is determined by the maximum treewidth across all graphical representations induced by the corresponding V-statistics.

Outline

Application 1: Higher-Order Influence Functions

- HOIFs involve computing a class of U-statistics like

$$h_m^{\text{HOIF}}(X_1, \ldots, X_m) = f_1(X_1, X_2) f_2(X_2, X_3) \cdots f_{m-1}(X_{m-1}, X_m)$$

- We test `u-stats` on computing HOIFs on platforms both in CPU and GPU (with `pytorch`).
- For CPU

Table: Average runtime (in seconds) using CPU parallel computation. Experiments were conducted on Intel Xeon ICX Platinum 8358 CPUs (2.6GHz, 64 total cores) with 512 GB of memory, evaluated across varying sample sizes and orders of HOIF-type U-statistics.

$m \backslash n$	**1000**	**2000**	**4000**	**8000**	**10000**
2	0.64	0.00141	0.01298	0.03174	0.04746
3	0.00396	0.01518	0.07392	0.26849	0.45976
4	0.02321	0.07313	0.32765	2.09545	2.36766
5	0.09853	0.36239	1.71419	9.11349	14.21350
6	0.38878	1.47719	7.44444	40.22143	58.85063
7	1.91677	6.75947	34.08805	195.31414	290.54295

Application 1: Higher-Order Influence Functions

- For GPU

Table: Average runtime (in seconds) using a single GPU (NVIDIA RTX 4090, 24GB) with parallel computation, across varying sample sizes and orders of HOIF-type U-statistics.

$m \backslash n$	**1000**	**2000**	**4000**	**8000**	**10000**
2	0.00184	0.00151	0.00155	0.00238	0.00339
3	0.00172	0.00147	0.00193	0.00577	0.00745
4	0.00305	0.00353	0.00707	0.03612	0.06245
5	0.00835	0.01089	0.03456	0.19807	0.36160
6	0.02608	0.03906	0.16981	1.12072	2.13328
7	0.12031	0.19132	0.91884	6.45225	12.21350

Application 2: Distance Covariance

- We also test our algorithm on computing dCov^2

$$\text{dCov}^2(X, Y) = \frac{(n-4)!}{n!} \sum_{i \neq j \neq q \neq r} a_{ij}b_{qr} + a_{ij}b_{ij} - a_{ij}b_{iq} - a_{ij}b_{jr}$$

- We compare the performance with Shao et al. (2025), $n = 138$.
  - They use a randomized incomplete algorithm to compute dCov^2.
  - α is a tuning parameter to control the degree of completeness.
  - Randomized algorithm of α takes $O(n^\alpha)$ time.

Table: Runtime (in seconds) comparison of various methods for computing dCov^2. Experiments were run on Intel Xeon ICX Platinum 8358 CPUs (2.6GHz, 64 total cores) with memory of 512 GB.

`u-stats`		Shao et al. (2025)'s `MATLAB` code			
No Parallel	**Parallel**	**Randomized** $\alpha = 1.5$	**Randomized** $\alpha = 2.0$	**Randomized** $\alpha = 2.5$	**Complete**
4.0928	0.1847	0.4211	4.5744	53.0265	3395.4001

Application 3: Motif Counts

- We compare the performance of our `u-stats` with `igraph`.
- On Erdős-Rényi graphs $G(n, p)$:
  - n is the number of vertices.
  - p is the probability of edge existence.
  - CPU parallel with 64 cores via `pytorch` for `u-stats`.
  - Count all types of 3-node or 4-node motifs.

Application 3: Motif Counts

- For the 3-node motifs,

Table: Runtime comparison of exact all 3-node motif counts using `u-stats` and `igraph` on Erdős-Rényi graphs $G(n, p)$ with $n = 5623$. Experiments were run on Intel Xeon ICX Platinum 8358 CPUs (2.6GHz, 64 total cores) with 512 GB of memory. "Speedup ratio" compares `igraph` to our parallel method; "single core speedup" assumes single-core execution.

Edge Prob. p	`u-stats` Time (s)	`igraph` Time (s)	Speedup Ratio	Single-Core Speedup
0.001	0.617	0.025	0.040	0.001
0.005	0.649	0.353	0.544	0.008
0.010	0.692	1.795	2.595	0.041
0.020	0.783	10.594	13.529	0.211
0.050	1.038	136.272	131.288	2.051
0.080	1.298	514.702	396.415	6.194
0.100	1.453	960.299	660.690	10.323
0.150	1.864	3003.490	1611.389	25.178
0.200	2.275	6725.515	2955.656	46.182

Application 3: Motif Counts

- For the 4-node motifs,

Table: Runtime comparison of exact all 4-node motif counts using `u-stats` and `igraph` on Erdős-Rényi graphs $G(n, p)$ with $n = 2000$. Experiments were run on Intel Xeon ICX Platinum 8358 CPUs (2.6GHz, 64 total cores) with 512 GB of memory. "Speedup ratio" compares `igraph` to our parallel method; "single core speedup" assumes single-core execution.

Edge Prob. p	`u-stats` **Time (s)**	`igraph` **Time (s)**	**Speedup Ratio**	**Single-Core Speedup**
0.001	70.959	0.004	0.	0.
0.005	71.947	0.168	0.002	0.
0.010	68.463	1.453	0.021	0.
0.020	65.634	15.573	0.237	0.004
0.050	65.786	394.532	5.997	0.094
0.080	66.866	2371.373	35.465	0.554
0.100	68.219	5396.057	79.099	1.236
0.150	65.969	23003.041	348.692	5.448
0.200	65.259	61796.760	946.940	14.796

Outline

Limitations and Future Work

- Limitations:
  - Memory usage is high: for HOIFs, it's not available for sample size larger than 2000 and order larger than 8 – Hybrid between for-loop & Einsum (or we can wait for better GPUs)?
  - How to combine our techniques with randomized incomplete U-statistics (Chen and Kato, 2019; Shao et al., 2025)?
- Future work:
  - Interface for `R`.
  - Non-scalar-valued U-statistics.

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Thank You!

For more details:

- Paper draft (arXiv):
  https://arxiv.org/abs/2508.12627
- Software (GitHub):
  github.com/Amedar-Asterisk/U-Statistics-python
- Personal website:
  cxy0714.github.io