

# Asymptotic behavior of $U$ -statistics on row-column exchangeable matrices

Application to bipartite network data analysis

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The Inria logo is written in a red, cursive script.The UGA logo consists of the letters 'UGA' in a bold, blue, sans-serif font. Below 'UGA' is the text 'Université Grenoble Alpes' in a smaller, blue, sans-serif font. A small orange triangle is positioned to the right of the 'A' in 'UGA'.

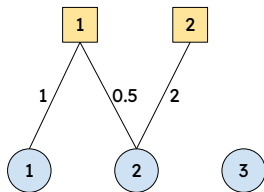
# Networks

## Network data

→ relational data (*links*) between entities (*nodes*)

## Bipartite networks

- two types of nodes
- links between nodes of different types
- represented by a *bipartite graph* or an *adjacency matrix*
- *binary* if only 0-1s, *weighted* otherwise



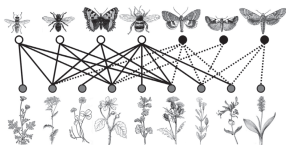
$$\begin{pmatrix} 1 & 0.5 & 0 \\ 0 & 2 & 0 \end{pmatrix}$$

# Matrix representation of a bipartite network

Examples of bipartite network data:

- recommender systems (users vs. items)
- scientific authorship (authors vs. articles)
- ecological networks (plant vs. animal species)

↪ Bipartite network = rectangular matrix  $Y$  of size  $m \times n$



Source: Macgregor et al. (2015)

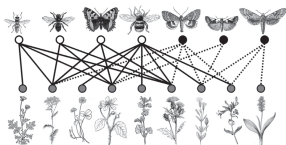
	1	2	3	4	5	6	7
A	■	■	■	■	■	■	■
B	■	■	■	■	■	■	■
C	■	■	■	■	■	■	■
D	■	■	■	■	■	■	■
E	■	■	■	■	■	■	■
F	■	■	■	■	■	■	■
G	■	■	■	■	■	■	■
H	■	■	■	■	■	■	■
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J	■	■	■	■	■	■	■

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I	■	■	■	■	■	■	■
J	■	■	■	■	■	■	■

Objective: characterize the network topology and perform statistical inference

# Outline

- 1 Introduction
  - (Network)  $U$ -statistics
  - Exchangeable network models
- 2 Asymptotic behavior of network  $U$ -statistics
  - Convergence in distribution
  - Hoeffding decomposition
  - Degenerate case
- 3 Conclusion

# Classic $U$ -statistics

$U$ -statistic on a vector of variables  $(X_1, \dots, X_n)$

$h : \mathbb{R}^k \rightarrow \mathbb{R}$  symmetric function,  $[n] := \{1, \dots, n\}$ ,

$$U_n = \binom{n}{k}^{-1} \sum_{I \in \mathcal{P}_k([n])} h(X_{i_1}, \dots, X_{i_k}).$$

# Network $U$ -statistics

Symmetric function  $h$  of a  $p \times q$  matrix

$$h(Y_{\{i_1, \dots, i_p; j_1, \dots, j_q\}}) = h \left( \begin{bmatrix} Y_{i_1 j_1} & Y_{i_1 j_2} & \dots & Y_{i_1 j_q} \\ Y_{i_2 j_1} & Y_{i_2 j_2} & \dots & Y_{i_2 j_q} \\ \dots & \dots & \dots & \dots \\ Y_{i_p j_1} & Y_{i_p j_2} & \dots & Y_{i_p j_q} \end{bmatrix} \right)$$

# Network $U$ -statistics

Symmetric function  $h$  of a  $p \times q$  matrix

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$U$ -statistic over a network of size  $m \times n$

$$U_{m,n} = \binom{m}{p}^{-1} \binom{n}{q}^{-1} \sum_{\substack{I \in \mathcal{P}_p([m]) \\ J \in \mathcal{P}_q([n])}} h(Y_{I,J})$$



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$U$ -statistic over a network of size  $m \times n$

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Example: subgraph density

$$\begin{aligned} h(Y_{\{1,2;1,2\}}) &= Y_{11} Y_{12} Y_{21} (1 - Y_{22}) + Y_{21} Y_{22} Y_{11} (1 - Y_{12}) \\ &\quad + Y_{12} Y_{11} Y_{22} (1 - Y_{21}) + Y_{22} Y_{21} Y_{12} (1 - Y_{11}) \end{aligned}$$



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## 3 Conclusion

# RCE models

## Row-column exchangeability (RCE, Aldous, 1981)

For all permutations  $\sigma_1$  and  $\sigma_2$ ,

$$(Y_{\sigma_1(i)\sigma_2(j)})_{i,j \geq 1} \stackrel{D}{=} Y$$

# RCE models

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For all permutations  $\sigma_1$  and  $\sigma_2$ ,

$$(Y_{\sigma_1(i)\sigma_2(j)})_{i,j \geq 1} \stackrel{D}{=} Y$$

Meaning: Omission of the node labels

- No node labels, shuffling the rows or columns = same network.
- OK if interested in the general topology of the network.

# Dissociation

## Dissociated matrix (Silverman, 1976)

For all  $(m, n) \in \mathbb{N}^2$ ,  $(Y_{ij})_{i \leq m, j \leq n}$  and  $(Y_{ij})_{i > m, j > n}$  are independent.

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

*submatrices*

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*submatrices*

## Graphon form of RCE dissociated models (Diaconis and Janson, 2008)

$$\begin{aligned} \xi_i, \eta_j &\stackrel{iid}{\sim} \mathcal{U}[0, 1] \\ Y_{ij} \mid \xi_i, \eta_j &\sim \mathcal{L}(w(\xi_i, \eta_j)), \end{aligned}$$

where  $w : [0, 1]^2 \rightarrow \mathbb{R}$  (graphon,  $W$ -graph model).

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# Asymptotic normality

## Asymptotic framework

- $N := m_N + n_N$ ,  $U_N := U_{m_N, n_N}$ ,
- $m_N/N \xrightarrow{N \rightarrow \infty} \rho \in ]0, 1[$ ,  $n_N/N \xrightarrow{N \rightarrow \infty} 1 - \rho$ .



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## Asymptotic normality of $U$ -statistics of RCE matrices

If  $Y$  is row-column exchangeable and dissociated and  $\mathbb{E}[h(Y_{\{1, \dots, p; 1, \dots, q\}})^2] < \infty$ , then

$$\sqrt{N}(U_N - \theta) \xrightarrow[N \rightarrow \infty]{\mathcal{D}} \mathcal{N}(0, V)$$

with

$$\theta = \mathbb{E}[h(Y_{\{1, \dots, p; 1, \dots, q\}})] \quad \text{and} \quad V = \frac{p^2}{\rho} v^{1,0} + \frac{q^2}{1 - \rho} v^{0,1},$$

where  $v^{r,c} = \text{Cov}(h(Y_{I,J}), h(Y_{I',J'}))$ ,  $I$  and  $I'$  share  $r$  elements,  $J$  and  $J'$  share  $c$  elements.

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# A gentle introduction to the Hoeffding decomposition

Let  $h$  be a symmetric function and  $(X_1, X_2, \dots)$  i.i.d. random variables.

$$U_n = \binom{n}{k}^{-1} \sum_{I \in \mathcal{P}_k([n])} h(X_I),$$

where  $X_I = \{X_{i_1}, \dots, X_{i_k}\}$ .

Principle: An orthogonal decomposition of  $U_n$  based on spaces generated by observations.

## Hoeffding decomposition: the i.i.d. case

Let  $\langle X_1, X_2 \rangle = \mathbb{E}[X_1 X_2]$  and

$$L_2(\{X_1, \dots, X_k\}) = \{f(X_1, \dots, X_k) : \mathbb{E}[f(X_1, \dots, X_k)^2] < \infty\}.$$

Typically, we have

$$h(X_I) \in L_2(X_I).$$

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### Projection subspaces $L_2^*$

$$L_2^*(X_I) = L_2(X_I) \cap \left( \bigcup_{I' \subset I} L_2(X_{I'}) \right)^\perp.$$

# Hoeffding decomposition: the i.i.d. case

## Examples:

- $L_2^*(\emptyset) = L_2(\emptyset) = \mathbb{R}$ ,
- $L_2^*({X_1}) = L_2({X_1}) \cap L_2(\emptyset)^\perp$ ,
- $L_2^*({X_1, X_2}) = L_2({X_1, X_2}) \cap (L_2({X_1})^\perp \cup L_2({X_2})^\perp \cup L_2(\emptyset)^\perp)$ .

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## Orthogonal decomposition of $L_2(X_I)$

$$L_2(X_I) = \bigoplus_{I' \subseteq I}^\perp L_2^*(X_{I'}).$$

# Hoeffding decomposition: the i.i.d. case

## Projections of $h(X_I) \in L_2(X_I)$ on the $L_2^*$ spaces

Defined by recursion:

- $\rho(\emptyset) = \mathbb{E}[h(X_I)] \in L_2^*(\emptyset)$ ,
- For  $I' \subseteq I$ ,

$$\rho(X_{I'}) = \mathbb{E}[h(X_I)|X_{I'}] - \sum_{I'' \subset I'} \rho(X_{I''}) \in L_2^*(X_{I'}).$$



# Hoeffding decomposition: the i.i.d. case

## Projections of $h(X_I) \in L_2(X_I)$ on the $L_2^*$ spaces

Defined by recursion:

- $p(\emptyset) = \mathbb{E}[h(X_I)] \in L_2^*(\emptyset)$ ,
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$$p(X_{I'}) = \mathbb{E}[h(X_I)|X_{I'}] - \sum_{I'' \subset I'} p(X_{I''}) \in L_2^*(X_{I'}).$$

## Decomposition of $h(X_I)$

$$h(X_I) = \sum_{I' \subseteq I} p(X_{I'}) = \sum_{0 \leq d \leq k} \sum_{I' \in \mathcal{P}_d(I)} p^{(d)}(X_{I'}).$$

# Application: CLT for $U$ -statistics

## Decomposition of $U_n$

$$U_n = \sum_{0 \leq d \leq k} \binom{k}{d} \binom{n}{d}^{-1} \sum_{I \in \mathcal{P}_d([n])} p^{(d)}(X_I).$$

# Application: CLT for $U$ -statistics

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$$U_n = \sum_{0 \leq d \leq k} \binom{k}{d} \binom{n}{d}^{-1} \sum_{I \in \mathcal{P}_d([n])} p^{(d)}(X_I).$$

## Asymptotic normality of $U_n$

$$U_n - \theta = \frac{k}{n} \sum_{1 \leq i \leq n} p^{(1)}(X_i) + o(n^{-1}).$$

↪ Central Limit Theorem.

## Case of network $U$ -statistics

$U$ -statistics on a RCE (row-column exchangeable) matrix:

$$U_{m,n} = \binom{m}{p}^{-1} \binom{n}{q}^{-1} \sum_{\substack{I \in \mathcal{P}_p([m]) \\ J \in \mathcal{P}_q([n])}} h(Y_{I,J}),$$

... but the entries of  $Y_{I,J}$  are not independent.

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... but the entries of  $Y_{I,J}$  are not independent.

### Aldous-Hoover-Kallenberg (AHK) representation (Kallenberg, 2005)

If  $Y$  is RCE dissociated, then there are

- $(\xi_i)_{1 \leq i < \infty}$ ,  $(\eta_j)_{1 \leq j < \infty}$  and  $(\zeta_{ij})_{1 \leq i < \infty, 1 \leq j < \infty}$  uniform i.i.d. random variables,
- a function  $\varphi$ ,

such that

$$Y_{ij} \stackrel{a.s.}{=} \varphi(\xi_i, \eta_j, \zeta_{ij}).$$

Remark: The AHK variables are unobserved!

# Graph sets of AHK variables

Representation of some AHK sets by **bipartite graphs** where:

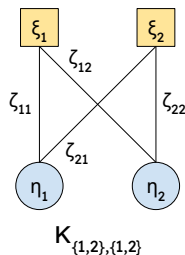
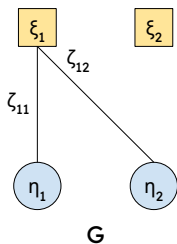
- sets of  $(\xi_i)_i$  and  $(\eta_j)_j =$  two types of vertices,
- set of  $(\zeta_{ij})_{(i,j)} =$  edges.

# Graph sets of AHK variables

Representation of some AHK sets by **bipartite graphs** where:

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Examples:

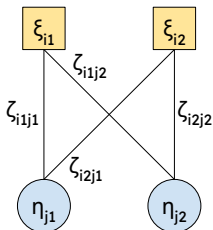


Notation:  $K_{I,J} =$  fully connected graph with sets of vertices  $I$  and  $J$ .

# Decomposition of the probability space

$$Y_{\{i_1, i_2; j_1, j_2\}} = \begin{bmatrix} \varphi(\xi_{i_1}, \eta_{j_1}, \zeta_{i_1 j_1}) & \varphi(\xi_{i_1}, \eta_{j_2}, \zeta_{i_1 j_2}) \\ \varphi(\xi_{i_2}, \eta_{j_1}, \zeta_{i_2 j_1}) & \varphi(\xi_{i_2}, \eta_{j_2}, \zeta_{i_2 j_2}) \end{bmatrix}$$

$$\in L_2(K_{\{i_1, i_2\}, \{j_1, j_2\}})$$

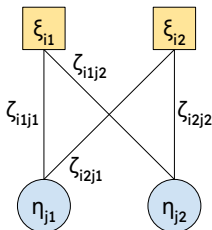




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$$\in L_2(K_{\{i_1, i_2\}, \{j_1, j_2\}})$$



## Decomposition of $L_2(G)$

Defined by recursion:

- $L_2^*(\emptyset) = \mathbb{R}$
- $L_2^*(G) = L_2(G) \cap (\cup_{G' \subsetneq G} L_2(G'))^\perp$

We have

$$L_2(G) = \bigoplus_{G' \subseteq G}^\perp L_2^*(G').$$

# Decomposition for network U-statistics

## Projections of $h(Y_{I,J})$

- $p(\emptyset) = \mathbb{E}[h(Y_{I,J})] = \theta \in L_2^*(\emptyset)$ ,
- For some graph  $G \subseteq K_{I,J}$ ,

$$p(G) = \mathbb{E}[h(Y_{I,J})|G] - \sum_{G' \subset G} p(G') \in L_2^*(G).$$

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## Hoeffding decomposition

Let  $\Gamma_{I,J}^{r,c}$  the set of subgraphs of  $K_{I,J}$  with  $r$  row vertices and  $c$  column vertices.

$$U_{m,n} = \sum_{\substack{0 \leq r \leq p \\ 0 \leq c \leq q}} \binom{p}{r} \binom{q}{c} \binom{m}{r}^{-1} \binom{n}{c}^{-1} \sum_{\substack{I \in \mathcal{P}_r([m] \\ J \in \mathcal{P}_c([n])}} \sum_{G \in \Gamma_{I,J}^{r,c}} p^{(r,c)}(G).$$

# CLT for network U-statistics

## Reminder: Asymptotic framework

- $N := m_N + n_N$ ,  $U_N := U_{m_N, n_N}$ ,
- $m_N/N \xrightarrow{N \rightarrow \infty} \rho \in ]0, 1[$ ,  $n_N/N \xrightarrow{N \rightarrow \infty} 1 - \rho$ .

$$U_N - \theta = \frac{p}{m_N} \sum_{i=1}^{m_N} \rho^{(1,0)}(\xi_i) + \frac{q}{n_N} \sum_{j=1}^{n_N} \rho^{(0,1)}(\eta_j) + o(N^{-1}).$$

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Central Limit Theorem:

$$\sqrt{N}(U_N - \theta) \xrightarrow[N \rightarrow \infty]{\mathcal{D}} \mathcal{N}(0, V)$$

with

$$V = \frac{p^2}{\rho} \mathbb{V}[p^{(1,0)}(\xi_1)] + \frac{q^2}{1 - \rho} \mathbb{V}[p^{(0,1)}(\eta_1)].$$

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# Principal support graphs

$$U_N = \sum_{\substack{0 \leq r \leq p \\ 0 \leq c \leq q}} \binom{p}{r} \binom{q}{c} \binom{m_N}{r}^{-1} \binom{n_N}{c}^{-1} \sum_{\substack{I \in \mathcal{P}_r([m_N]) \\ J \in \mathcal{P}_c([n_N])}} \sum_{G \in \Gamma_{I,J}^{r,c}} p^{(r,c)}(G).$$

## Principal support graphs (Janson and Nowicki, 1991)

- The **principal support graphs** of  $U_N$  are the graphs  $G$  such that  $p(G) \neq 0$  with the smallest number of nodes  $d = r + c$ ,
- $d$  is called the **principal degree** of  $U_N$ .

## Principal support graphs

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$$U_N = \binom{N}{d}^{-1} \sum_{r+c=d} \frac{p!}{(p-r)! \rho^r} \frac{q!}{(q-c)! (1-\rho)^c} \sum_{\substack{I \in \mathcal{P}_r([m_N]) \\ J \in \mathcal{P}_c([n_N])}} \sum_{G \in \Gamma_{I,J}^{r,c}} p^{(r,c)}(G) + o(N^{-d}).$$



# Convergence of degenerate $U$ -statistics

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$$N^{d/2}(U_N - \theta) \xrightarrow[N \rightarrow \infty]{\mathcal{D}} W,$$

where  $W$  is a random variable with finite variance  $V^{(d)}$ , only depending on the principal support graphs.

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where  $W$  is a random variable with finite variance  $V^{(d)}$ , only depending on the principal support graphs.

## Gaussian case

If all the principal support graphs are connected, then

$$N^{d/2}(U_N - \theta) \xrightarrow[N \rightarrow \infty]{\mathcal{D}} \mathcal{N}(0, V^{(d)}).$$

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# Summary

A **Hoeffding decomposition for  $U$ -statistics on RCE matrices** can be defined using **graph sets of Aldous-Hoover-Kallenberg variables**.

The **asymptotic behavior of these  $U$ -statistics** is characterized by the **topology of the principal support graphs**.

**These results** can be used to perform **statistical inference on bipartite network data** with symmetry assumptions (exchangeable nodes = graphon models).

Preprint:

Le Minh, T. (2024). Characterization of the asymptotic behavior of  $U$ -statistics on row-column exchangeable matrices. *arXiv:2401.07876*.

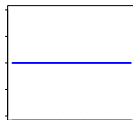
# Outline

## 4 Applications

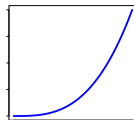
## Poisson product graphon

$$\begin{aligned} \xi_i, \eta_j &\stackrel{iid}{\sim} \mathcal{U}[0, 1] \\ Y_{ij} \mid \xi_i, \eta_j &\sim \mathcal{P}(\lambda f(\xi_i)g(\eta_j)) \end{aligned}$$

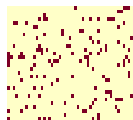
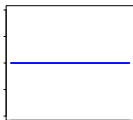
$g(v) =$



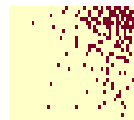
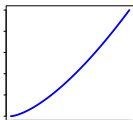
$g(v) =$



$f(u) =$



$f(u) =$



$$\int f = 1, F_2 := \int f^2$$

# Example 1: Test of $\mathcal{H}_0 : F_2 = 1$

## Estimators

- $h_1(Y_{\{1,2;1,2\}}) = Y_{11} Y_{12}$ ,  $\mathbb{E}h_1 = \lambda^2 F_2$
- $h_2(Y_{\{1,2;1,2\}}) = Y_{11} Y_{22}$ ,  $\mathbb{E}h_2 = \lambda^2$
- $h = h_1 - h_2$ ,  $U_N^h := U_N^{h_1} - U_N^{h_2}$ ,  $\mathbb{E}[U_N^h] = \lambda^2(F_2 - 1)$ .

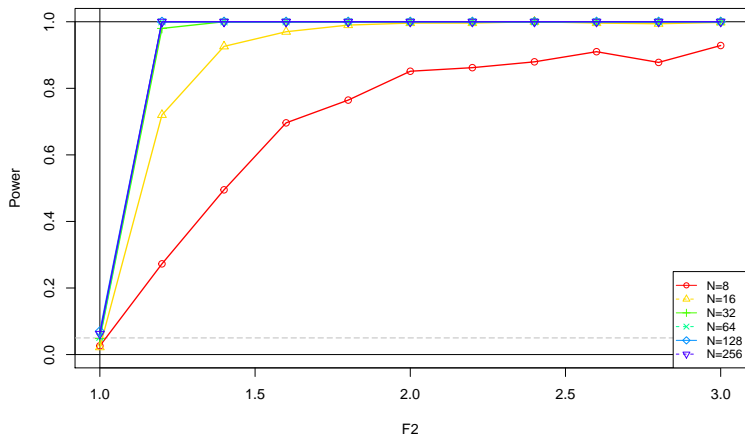
## Limit distribution

If  $F_2 = 1$ , then  $U_N^h$  is degenerate, with principal degree = 3,

$$\frac{N^{3/2}}{\sqrt{V}} U_N^h \xrightarrow[N \rightarrow \infty]{\mathcal{D}} \mathcal{N}(0, 1)$$

where  $V = \frac{2\lambda^2}{\rho(1-\rho)^2}$ .

# Example 1: Test on $F_2 = 1$



Null hypothesis  $\mathcal{H}_0 : F_2 = 1$



## Example 2: Estimation of $F_2$ , network comparison

### Estimators

- $h_1(Y_{\{1,2;1,2\}}) = Y_{11} Y_{12}$ ,  $\mathbb{E}h_1 = \lambda^2 F_2$
- $h_2(Y_{\{1,2;1,2\}}) = Y_{11} Y_{22}$ ,  $\mathbb{E}h_2 = \lambda^2$
- $\hat{\theta}_N := U_N^{h_1} / U_N^{h_2}$

### Limit distribution

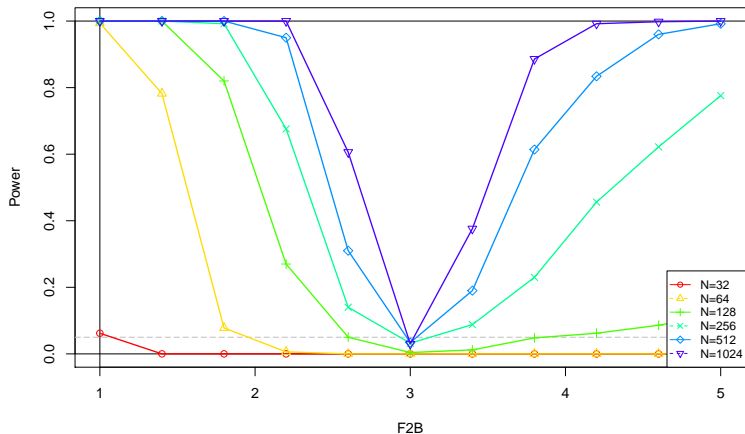
$$\sqrt{\frac{N}{V^\delta}} \left( \hat{\theta}_N - F_2 \right) \xrightarrow[N \rightarrow \infty]{\mathcal{D}} \mathcal{N}(0, 1)$$

where  $V^\delta = \frac{1}{\lambda^4} V^{h_1} - \frac{2F_2}{\lambda^4} C^{h_1, h_2} + \frac{F_2^2}{\lambda^4} V^{h_2}$  (delta-method).

Compare the value of  $F_2$  for 2 independent networks  $Y^A$  and  $Y^B$ :

$$Z_N = \hat{\theta}_{N_A}(Y^A) - \hat{\theta}_{N_B}(Y^B).$$

## Example 2: Estimation of $F_2$ , network comparison



Null hypothesis  $\mathcal{H}_0 : F_2^A = F_2^B$ , simulations with fixed  $F_2^A = 3$

# Example 1: Motif counts

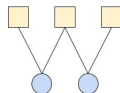
## Exchangeable binary network model

$$\begin{aligned}
 U_i, V_j &\stackrel{iid}{\sim} \mathcal{U}[0, 1] \\
 Y_{ij} \mid U_i, V_j &\sim \mathcal{B}(w(U_i, V_j))
 \end{aligned}$$

$$h_6(Y_{\{1,2;1,2\}}) = Y_{11} Y_{12} Y_{21} Y_{22}$$

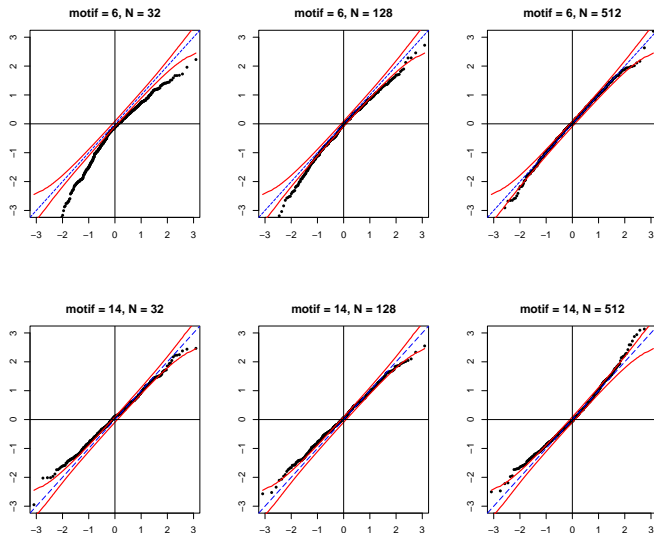


$$h_{14}(Y_{\{1,2,3;1,2\}}) = Y_{11} Y_{21} Y_{22} Y_{32} (1 - Y_{12})(1 - Y_{31})$$



The respective  $U_N^h$  are the densities of these motifs in the observed network.

# Example 1: Motif counts



## Example 2: Form of a graphon

### Graphon model

$$\begin{aligned} U_i, V_j &\stackrel{iid}{\sim} \mathcal{U}[0, 1] \\ Y_{ij} \mid U_i, V_j &\sim \mathcal{P}(\lambda \tilde{w}(U_i, V_j)) \end{aligned}$$

where

- $\lambda = \mathbb{E}[Y_{ij}]$
- $\tilde{w} : [0, 1]^2 \rightarrow [0, \frac{1}{\lambda}]$ ,  $\iint \tilde{w} = 1$ .

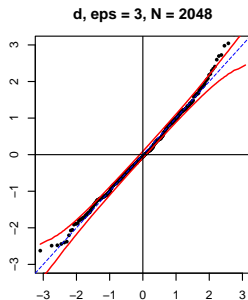
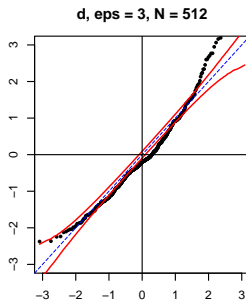
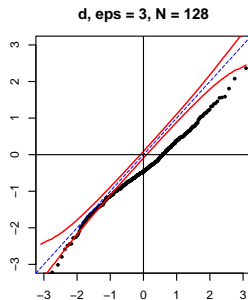
Link with the  $f$  and  $g$  functions of the BEDD model:

$$f(u) = \int \tilde{w}(u, v) dv \qquad g(v) = \int \tilde{w}(u, v) du$$

Dissimilarity measure to the BEDD model:

$$d(w) = \|\tilde{w} - fg\|_2^2 = \int \int (\tilde{w}(u, v) - f(u)g(v))^2 du dv$$

## Example 2: Form of a graphon



## Example 3: Assessing overdispersion

### Overdispersed Poisson-BEDD model

$$\begin{array}{rcl}
 U_i, V_j & \stackrel{iid}{\sim} & \mathcal{U}[0, 1] \\
 W_{ij} & \stackrel{iid}{\sim} & \mathcal{Q} \\
 Y_{ij} \mid U_i, V_j & \sim & \mathcal{P}(\lambda f(U_i)g(V_j)W_{ij})
 \end{array}$$

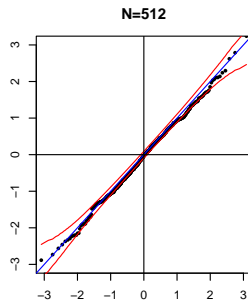
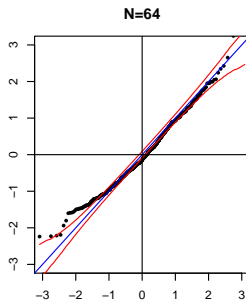
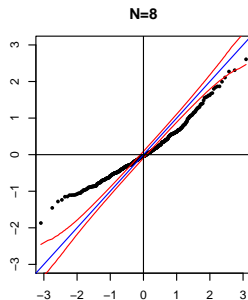
where

- $\lambda = \mathbb{E}[Y_{ij}]$ ,
- $\int f = \int g = 1$ ,  $\int f^k = F_k$ ,  $\int g^k = G_k$ ,
- $\mathbb{E}[W_{ij}] = 1$ .

The model becomes a simple Poisson-BEDD if  $W_{ij} = 1$ , i.e.  $W_2 := \mathbb{E}[W_{ij}^2] = 1$ .

$W_2$  is a property of the model, not a parameter of the BEDD model.

# Example 4: Test on $F_2 = 1$





# References

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