Higher Order Graphon Theory

Fluctuations and Inference for Motifs and Eigenvalues

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Recent Advances in Random Networks: Theory and Applications, IMSI.

Bhaswar B. Bhattacharya

University of Pennsylvania

Soham Dan

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Jiaoyang Huang

University of Pennsylvania

Svante Janson

Uppsala University

Outline

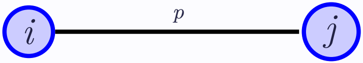
1. Fluctuation of Motif Counts in Graphon Models
2. Graphon Multiplier Bootstrap
3. Eigenvalues of W-random Graphs

Outline

1. Fluctuation of Motif Counts in Graphon Models
   - Network Models
   - Motif Density
   - Fluctuation of Motif Counts

Network Models

- Erdős-Rényi Random Graphs: $G(n, p)$.



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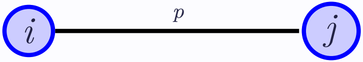
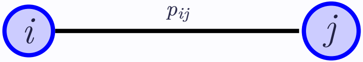


- Inhomogeneous Random Graphs: $G(n, \boldsymbol{P})$ where $\boldsymbol{P} = (p_{ij})_{1 \leq i \neq j \leq n}$ is a symmetric matrix.



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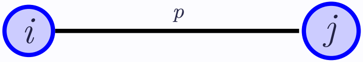

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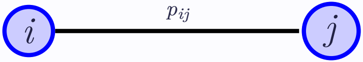

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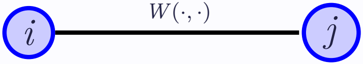

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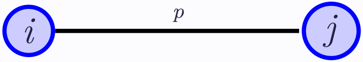

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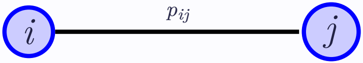

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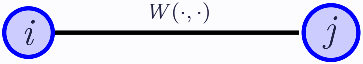

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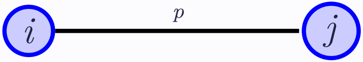

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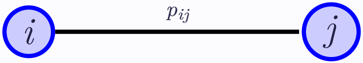

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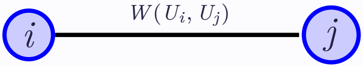

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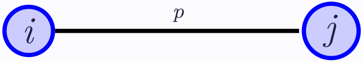

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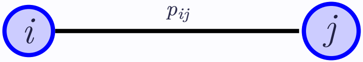

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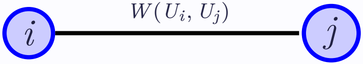

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  - Examples:
    - $W \equiv p \iff$ Erdős-Rényi random graph with edge probability p.
    - W is a K-block function $\iff$ Stochastic Block Model with K blocks.

Outline

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- Edge density in G_n:

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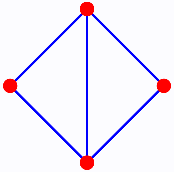

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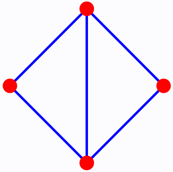

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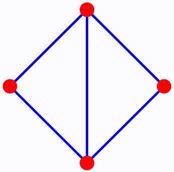

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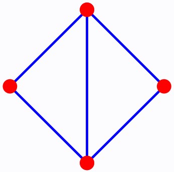

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$$X(H, G_n) = \#\text{ Copies of } H \text{ in } G_n.$$

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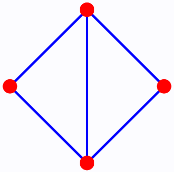

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$$\mathbb{E}\left[t(H, G_n)\right] = \int_{[0,1]^{|V(H)|}} \prod_{(i,j)\in E(H)} W(x_i, x_j) \prod_{k\in V(H)} \mathrm{d}x_k = t(H, W).$$

Motif Density: Applications

- Motifs encode structural information about networks like *clustering coefficient* $= \frac{t(K_3, G)}{t(K_{1,2}, G)}$ (Watts and Strogatz (1998)).

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- *Network Two-Sample Testing* (Ouadah et al. (2022), Maugis et al. (2017)):
  - $\boldsymbol{H}_0 : t(K_2, W_1) = t(K_2, W_2)$.
  - $\boldsymbol{H}_0 : (t(K_2, W_1), t(K_3, W_1)) = (t(K_2, W_2), t(K_3, W_2))$.

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    - Cycles and Trees: Bickel, Chen and Levina (2011).
    - General Subgraphs: Féray, Meliot and Nikeghbali (2020).
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- σ^2 can equal 0: Hladký, Pelekis and Šileikis (2021) for cliques and, more generally, in Bhattacharya, C., Janson (2023).
- Example: $W = [a, b, b, a]$ and $H = K_2, K_3$.

Fluctuation of Edge Counts

- Hladký, Pelekis and Šileikis (2021) showed that,
  - For any W,

$$\sqrt{n}\frac{X(K_2, G_n) - \mathbb{E}X(K_2, G_n)}{n^2} \xrightarrow{d} \mathrm{N}\left(0, \sigma^2_{K_2,W}\right),$$

where

$$\sigma^2_{K_2,W} = \int_0^1 \left(d_W(x) - \int_0^1 d_W(y)\mathrm{d}y\right)^2 \mathrm{d}x$$

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  - If $d_W(x) = \text{constant} \iff W$ is degree regular,

$$n\frac{X(K_2, G_n) - \mathbb{E}X(K_2, G_n)}{n^2} \xrightarrow{d} \tau_{K_2,W} Z + \sum_{\lambda \in S(W,K_2)} \frac{\lambda}{2}(Z_\lambda^2 - 1)$$

    where,
    - $S(W, K_2)$ and $\tau_{K_2,W}$ are identified by W and K_2.
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- The results of Hladký, Pelekis and Šileikis (2021) hold for $H = K_r$ (the complete graph on r vertices).

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- This provides the marginal distribution of the motif density.
- *What about joint distributions?* For example, clustering coefficient, testing structure.

Joint Fluctuation of Motif Counts

- For a motif H, let $Z(H, G_n) = \frac{X(H,G_n)-\mathbb{E}X(H,G_n)}{n^{|V(H)|}}$.
- Joint distribution for $\boldsymbol{Z}(\mathcal{H}_r, G_n) = (Z(H_1, G_n), \cdots, Z(H_r, G_n))^\top$, where

$$\mathcal{H}_r := \{\overbrace{H_1, \ldots, H_q}^{W-\text{irregular}}, \quad \overbrace{H_{q+1}, \ldots, H_r}^{W-\text{regular}}\}.$$

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- *For* $1 \le i \le q$ *(irregular subgraphs),*

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- *For $q+1 \leq i \leq r$ (regular subgraphs),*

$$\begin{aligned} n Z(H_i, G_n) &\xrightarrow{d} \tau_{H_i, W} Z + \sum_{\lambda \in S(W, H_i)} \lambda (Z_\lambda^2 - 1) \\ &\equiv \zeta_i + \int_0^1 \int_0^1 f_{H_i, W}(x, y)\, \mathrm{d}B_x \mathrm{d}B_y \end{aligned}$$

where $(\zeta_{q+1}, \cdots, \zeta_r)^\top \sim \mathrm{N}_{r-q}(\mathbf{0}, \boldsymbol{\Sigma})$ are independent of the Brownian motion $\{B_t\}_{t \in [0,1]}$.

Outline

2. Graphon Multiplier Bootstrap
    - Regularity Testing
    - Confidence Sets for Motif Density

Testing for Regularity

- Consider the "pseudo" hypothesis,

$$\bar{\boldsymbol{H}}_0 : W \textit{ is H-regular vs } \bar{\boldsymbol{H}}_1 : W \textit{ is H-irregular.}$$

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- Therefore, rejecting $\bar{\boldsymbol{H}}_0$ when $\{\sqrt{n}\hat{\sigma}^2_{H,G_n} > 1\}$ gives a consistent test for regularity.

Outline

2. Graphon Multiplier Bootstrap
   - Regularity Testing
   - Confidence Sets for Motif Density

Confidence Interval for Edge Density

- If $\bar{\boldsymbol{H}}_0$ is rejected,

$$L_n := \left[t(K_2, G_n) - z_{\alpha/2} \frac{2\hat{\sigma}_{K_2, G_n}}{\sqrt{n}}, t(K_2, G_n) + z_{\alpha/2} \frac{2\hat{\sigma}_{K_2, G_n}}{\sqrt{n}} \right].$$

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- Let $\lambda_{n,1} \geq \lambda_{n,2} \geq \cdots \geq \lambda_{n,n}$ be the eigenvalues of $\boldsymbol{A}_n$ is the adjacency matrix of the observed graph G_n.

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Theorem (C., Dan, Bhattacharya (2024))

If W is degree-regular and $\{\eta_i : i \geq 1\} \sim \mathrm{N}(0,1)$, then,

$$E(K_2, G_n) := \sum_{i=1}^{n} \lambda_{i,n}(\eta_i^2 - 1) | G_n \overset{d}{\approx} Z(K_2, G_n).$$

Confidence Interval for Edge Density

- Recall the "pseudo" hypothesis,

$$\bar{\boldsymbol{H}}_0 : W \text{ is } K_2\text{-regular vs } \bar{\boldsymbol{H}}_1 : W \text{ is } K_2\text{-irregular.}$$

- If $\{\sqrt{n}\hat{\sigma}^2_{K_2,G_n} > 1\}$ reject $\bar{\boldsymbol{H}}_0$.
- If $\bar{\boldsymbol{H}}_0$ is rejected,

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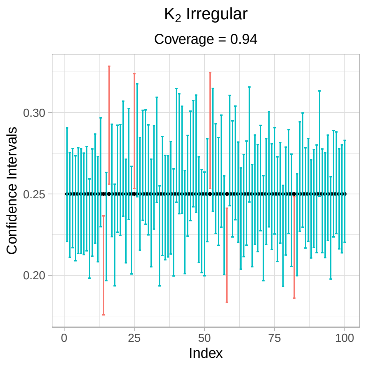
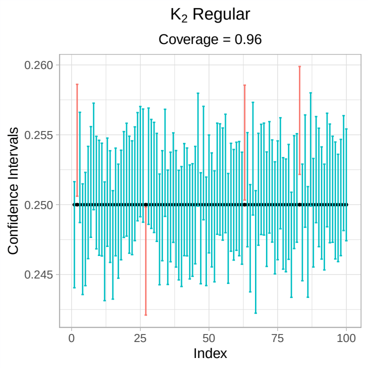
- If $\bar{\boldsymbol{H}}_0$ is accepted,

$$L_n := \left[t(K_2, G_n) - \hat{q}_{\alpha/2}\frac{2}{n}, t(K_2, G_n) + \hat{q}_{1-\alpha/2}\frac{2}{n} \right].$$

  where $\hat{q}_\alpha$ is the α-th quantile of $E(K_2, G_n)$.

CI for Edge Density





Joint Fluctuation of Motif Counts

- For a motif H, let $Z(H, G_n) = \frac{X(H,G_n) - \mathbb{E}X(H,G_n)}{n^{|V(H)|}}$.
- Joint distribution for

$$\boldsymbol{Z}(\mathcal{H}_r, G_n) = \left(Z(H_1, G_n), \cdots, Z(H_r, G_n)\right)^\top,$$

where

$$\mathcal{H}_r := \{\overbrace{H_1, \ldots, H_q}^{W-\text{irregular}}, \overbrace{H_{q+1}, \ldots, H_r}^{W-\text{regular}}\}.$$

Theorem (C., Dan, Bhattacharya (2024))

- *For* $1 \leq i \leq q$ *(irregular subgraphs)*,

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- *For* $q+1 \leq i \leq r$ *(regular subgraphs)*,

$$n Z(H_i, G_n) \xrightarrow{d} \zeta_i + \int_0^1 \int_0^1 f_{H_i,W}(x,y) \, \mathrm{d}B_x \mathrm{d}B_y$$

where $(\zeta_{q+1}, \cdots, \zeta_r)^\top \sim \mathrm{N}_{r-q}(\mathbf{0}, \boldsymbol{\Sigma})$ *is independent of the Brownian motion* $\{B_t\}_{t\in[0,1]}$.

Joint Confidence Set of Motif Densities

- Consider a collection $\mathcal{H}_r = \{H_1, , \ldots, H_r\}$.

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- Consider a collection $\mathcal{H}_r = \{H_1, , \ldots, H_r\}$.
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- Define $\boldsymbol{E}(\mathcal{H}, G_n) := \Big(E(H_1, G_n), \ldots, E(H_r, G_n)\Big)$ where,

$$E(H_i, G_n) := \begin{cases} \sum_{\ell=1}^{n} \frac{1}{\sqrt{n}} \boldsymbol{w}_{H_i, G_n}(\ell)\ \eta_\ell & \text{if } \bar{\boldsymbol{H}}_0^{(i)} \text{ is rejected.} \\ \sum_{\ell, j=1}^{n} \frac{1}{n} \boldsymbol{w}_{H_i, G_n}(\ell, j)\ (\eta_\ell \eta_j - \delta_{\ell j}) & \text{if } \bar{\boldsymbol{H}}_0^{(i)} \text{ is accepted.} \end{cases}$$

with $\{\eta_i, 1 \le i \le n\} \sim \mathrm{N}(0, 1)$.

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Theorem (C., Dan, Bhattacharya (2024))

$$\boldsymbol{E}(\mathcal{H}_r, G_n) | G_n \overset{d}{\approx} \boldsymbol{Z}(\mathcal{H}_r, G_n) \text{ as } n \to \infty.$$

- For each $1 \leq i \leq r$ define,

$$\widehat{Z}(H_i, G_n) = \begin{cases} \sqrt{n} Z(H_i, G_n) & \text{if } \bar{\boldsymbol{H}}_0^{(i)} \text{ is rejected.} \\ n Z(H_i, G_n) & \text{if } \bar{\boldsymbol{H}}_0^{(i)} \text{ is accepted.} \end{cases}$$

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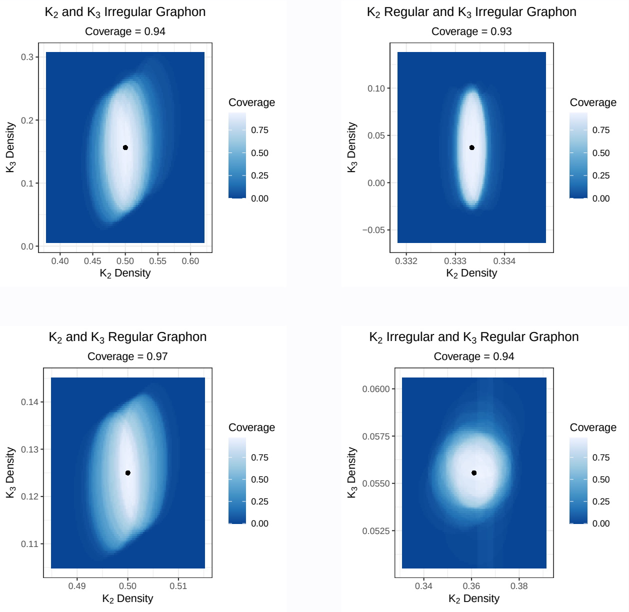
For $\widehat{\boldsymbol{Z}}(\mathcal{H}_r, G_n) = \left(\widehat{Z}(H_1, G_n), \ldots, \widehat{Z}(H_r, G_n)\right)^\top$,

$$\|\widehat{\boldsymbol{Z}}(\mathcal{H}_r, G_n)\|_2 \leq \widehat{q}_{1-\alpha}(G_n),$$

where $\widehat{q}_{1-\alpha}(G_n)$ *is* α^{th} *quantile of* $\|\boldsymbol{E}(\mathcal{H}_r, G_n)\|_2 | G_n$ *is asymptotically valid confidence set.*

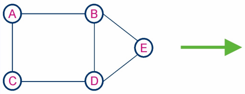
Confidence Sets for Edge and Triangle Density



Outline

3. Eigenvalues of W-random Graphs
   - Spectra of Networks
   - Asymptotic distribution of $\lambda_1(\boldsymbol{W}_n)$
   - Asymptotic distribution of $\lambda_1(\boldsymbol{A}_n)$

Spectra of Networks



	A	B	C	D	E
A	0	1	1	0	0
B	1	0	0	1	1
C	1	0	0	1	0
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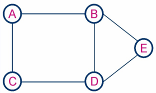
- Eigenvalues of the adjacency matrix $\boldsymbol{A}_n$,

$$\lambda_1\left(\boldsymbol{A}_n\right) \geq \ldots, \geq \lambda_n\left(\boldsymbol{A}_n\right).$$



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$$\frac{\lambda_1 (\boldsymbol{A}_n)}{n} \xrightarrow{d} \text{Gaussian.}$$

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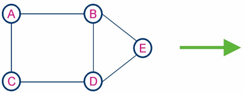

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- Eigenvalue encode structural properties of networks:
  - Expansion properties - Hoory, Linial and Wigderson (2006), Malliaros and Megalooikonomou (2011).
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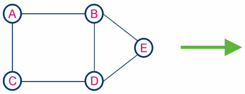
Spectra of Networks



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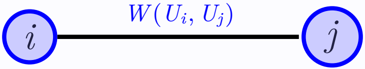
- Fluctuations for $\boldsymbol{A}_n \sim$ Random-Graphon Model!

Spectra of Random Graphon Model



- $\boldsymbol{A}_n = (A_{ij})$ is the adjacency matrix and $A_{ij} = A_{ji} \sim \mathrm{Ber}\,(W(U_i, U_j))$.

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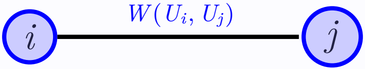
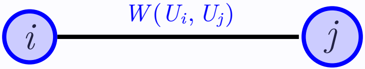


- $\boldsymbol{A}_n = (A_{ij})$ is the adjacency matrix and $A_{ij} = A_{ji} \sim \mathrm{Ber}\left(W(U_i, U_j)\right)$.
- $\boldsymbol{W}_n = \left(W(U_i, U_j)\right)$ is the edge-probability matrix.

$$\lambda_1\left(\boldsymbol{W}_n\right) \geq \lambda_2\left(\boldsymbol{W}_n\right) \geq \ldots \geq \lambda_n\left(\boldsymbol{W}_n\right).$$

Spectra of Random Graphon Model



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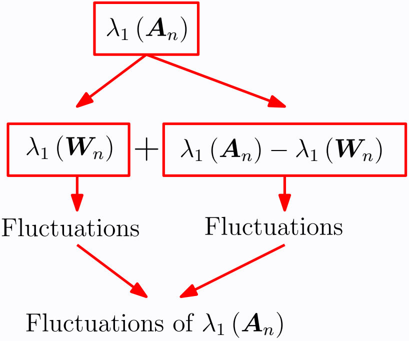

Outline

3. Eigenvalues of W-random Graphs
   - Spectra of Networks
   - Asymptotic distribution of $\lambda_1(\boldsymbol{W}_n)$
   - Asymptotic distribution of $\lambda_1(\boldsymbol{A}_n)$

Asymptotic distribution of $\lambda_1(\boldsymbol{W}_n)$

$$\int W(x,y)\phi(y)\mathrm{d}y = \lambda\phi(x)$$

- λ - eigenvalue and ϕ - corresponding eigenfunction.

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Theorem (C., Huang (2025))

Suppose W is Lipschitz continuous and $\lambda_1(W)$ is unique. Then,

- *for any graphon W satisfying above assumptions,*

$$\sqrt{n}\left(\frac{\lambda_1(\boldsymbol{W}_n)}{n} - \lambda_1(W)\right) \xrightarrow{d} \mathrm{N}\left(0, \sigma_W^2\right),$$

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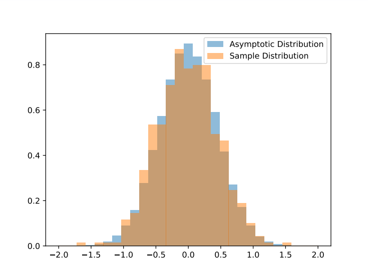
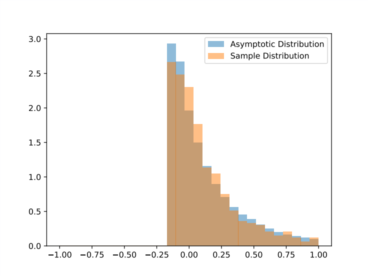
- *and if $\sigma_W = 0$ then,*

$$\lambda_1(\boldsymbol{W}_n) - (n-1)\lambda_1(W) \xrightarrow{d} \sum_{\lambda \in S(W)} w_\lambda \left(Z_\lambda^2 - 1\right) + \sum_{\lambda \in S(W)} c_\lambda$$

Asymptotic distribution of $\lambda_1(\boldsymbol{W}_n)$



Non-degenerate



Degenerate

Outline

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Proposition (C., Huang (2025))

Suppose W is Lipschitz continuous and $\lambda_1(W)$ is unique. Consider $\boldsymbol{U}_n = \{U_1, \ldots, U_n\}$. Then,

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Asymptotic distribution of $\lambda_1(\boldsymbol{A}_n)$

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Proposition (C., Huang (2025))

Suppose W is Lipschitz continuous and $\lambda_1(W)$ is unique. Consider $\boldsymbol{U}_n = \{U_1, \ldots, U_n\}$. Then,

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Suppose W is Lipschitz continuous and $\lambda_1(W)$ is unique. Then,

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- Lunde and Sarkar (2023) - Gaussian regime for finite rank W.

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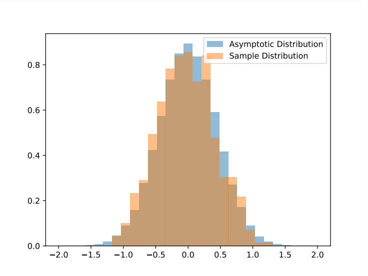
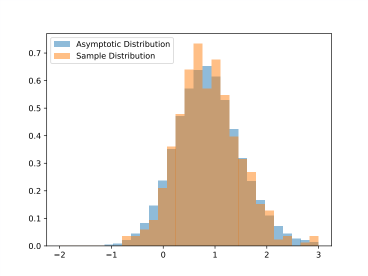


Non-degenerate



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Thank You

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Non-Degeneracy of Limiting Distribution

- For a motif H let $Z(H, G_n) = \frac{X(H,G_n) - \mathbb{E}X(H,G_n)}{n^{|V(H)|}}$.
- If W is H-regular,

$$nZ(H, G_n) \xrightarrow{d} \tau_{H,W} Z + \sum_{\lambda \in S(W,H)} \lambda(Z_\lambda^2 - 1)$$

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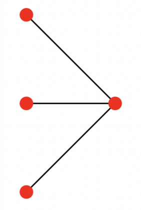
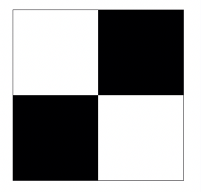
- What about other H?

Degeneracy of the limit: An Example



$K_{1,3}$



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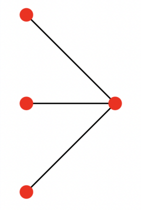

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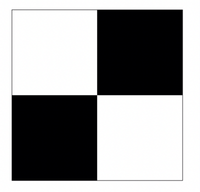

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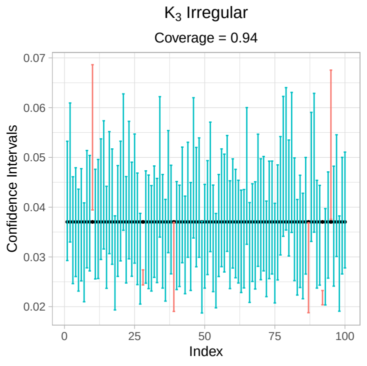
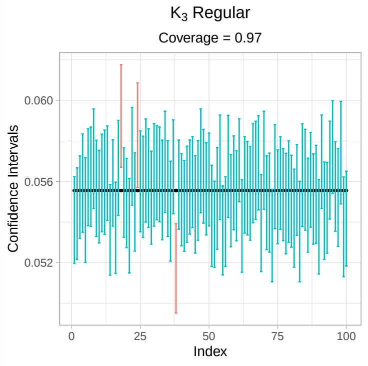
- Let h_4 be the fourth Hermite polynomial. Then,

$$n^2 Z\left(K_{1,3}, G_n\right) \xrightarrow{d} -\frac{1}{48} h_4(Z) = -\frac{1}{48}\left(Z^4 - 6Z^2 + 3\right).$$

CI for Triangle Density





Regularity Testing for Cliques

- Recall the "pseudo" hypothesis,

$$\bar{\boldsymbol{H}}_0 : W \textit{ is } K_r\textit{-regular vs } \bar{\boldsymbol{H}}_1 : W \textit{ is } K_r\textit{-irregular.}$$

and W is K_r-regular $\iff \sigma_{K_r,W} = 0$.

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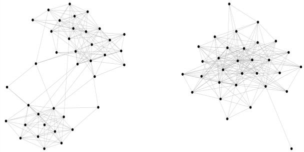
- We can construct $\hat{R}(K_r, G_n) \mid G_n \xrightarrow{d} R(K_r, W)$.
- Therefore, rejecting $\bar{\boldsymbol{H}}_0$ when $\{n\hat{\sigma}^2_{K_r,G_n} > \hat{q}_{\alpha,K_r,G_n}\}$ gives a valid test for regularity.

Broader Scope: Structure Testing



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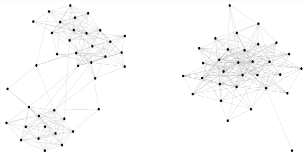

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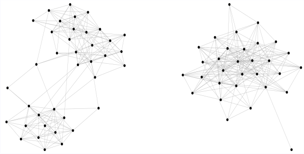

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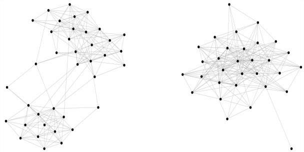

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- Reject $\boldsymbol{H}_0$ if,

$$\frac{n^{3/2}}{\hat{\sigma}_n}\left|t(C_4, G_n) - t(K_2, G_n)^4\right| > z_{\alpha/2}$$