Lecture 3: Random Graph Matching: Efficient Algorithms

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Joint work with
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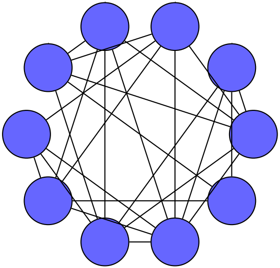
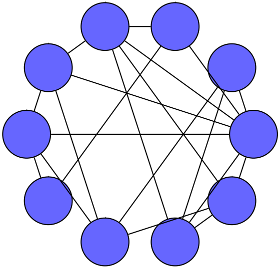
AI4OPT Tutorial Lectures

Graph matching (network alignment)





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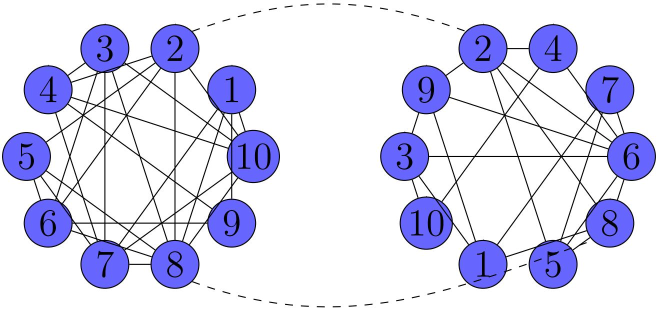

Goal: find a mapping between two node sets that maximally aligns the edges (i.e. minimizes # of adjacency disagreements)

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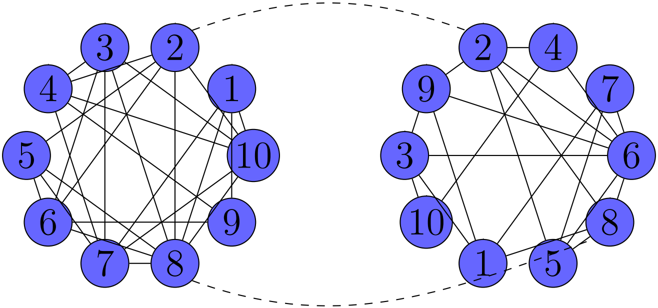

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Quadratic Assignment Problem (QAP) : $\max_{\Pi \in S_n} \langle A, \Pi B \Pi^\top \rangle$

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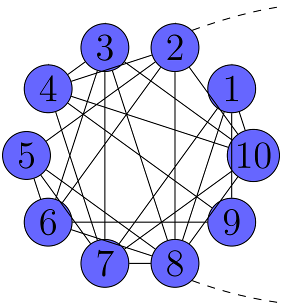

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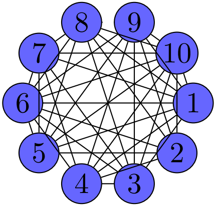
Noiseless case: reduce to graph isomorphism

Correlated Erdős-Rényi graphs model



$$G_0 \sim \mathcal{G}(n, p)$$

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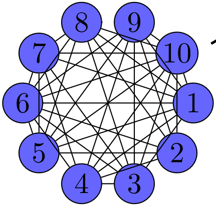

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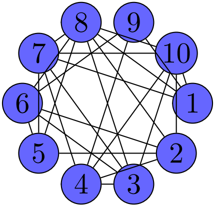

$G_1 \sim \mathcal{G}(n, q \triangleq ps)$

$G_0 \sim \mathcal{G}(n, p)$

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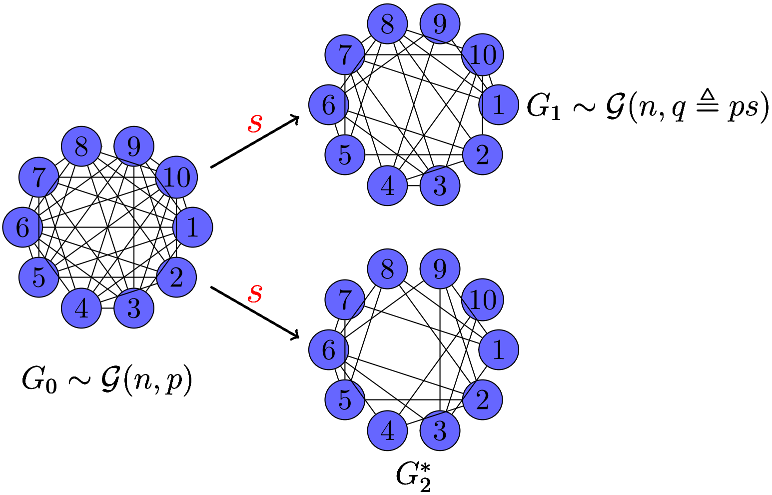

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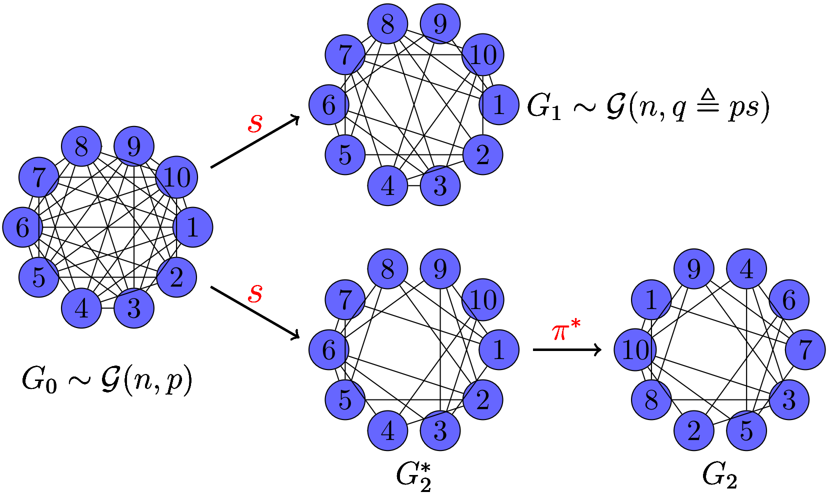

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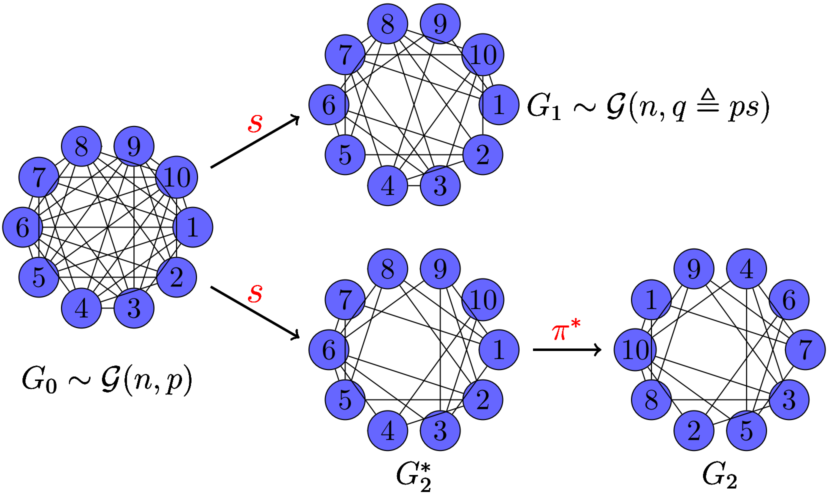

G_1 and G_2 differ by a fraction $\delta \triangleq 1 - s$ of edges, under the correct node mapping

Information-theoretic limits

p: edge probability $\delta = 1 - s$: fraction of errors (differed edges)

Theorem (Cullina-Kiyavash '18, Wu-X.-Yu' 21)

For $p = o(1)$, exact recovery of π^* is information-theoretically possible if and only if

$$nps^2 - \log n \to +\infty$$

Interpretation: Intersection graph $G_1 \wedge G_2^* \sim \mathcal{G}(n, ps^2)$ is connected

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Computationally:

- Noiseless $s = 1 (\delta = 0)$: optimal condition is attained in linear-time [Bollobás '82, Czajka-Pandurangan '08]
- Noisy case $s < 1 (\delta > 0)$: little is known for efficient algorithms until recently

Main result

p: edge probability $\qquad \delta = 1 - s$: fraction of errors (differed edges)

Theorem (Fan-Mao-Wu-X. '19)

Exact recovery is achieved efficiently by a new spectral method whp if

$$np \gtrsim (\log n)^C \quad \textit{and} \quad \delta \lesssim (\log n)^{-C}$$

for some absolute constant C.

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- holds for general correlated Wigner model

Outline

1. A new spectral algorithm
2. Analysis
3. Concluding remarks

Spectral methods and applications

Estimate hidden structure using leading eigenvectors of data matrix A

- Planted clique [Alon-Krivelevich-Sudakov '98]
- Planted partition/Stochastic block model [Mcsherry '98] [Massoulié '13] [Bordenave-Lelarge-Massoulié '15]
- Clustering [von-Luxburg-Bousquet-Belkin '05]
- Graphon estimation [Chatterjee '15]
- Matrix completion [Keshavan-Montanari-Oh '09]
- Ranking [Negahban-Oh-Shah '17]

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Underlying structure: A is approximately low-rank with large eigen-gap

Analyzing spectral methods: an example

Community detection: $A = \begin{bmatrix} p & & q \\ & p & \\ q & & p \end{bmatrix} + A - \mathbb{E}[A]$

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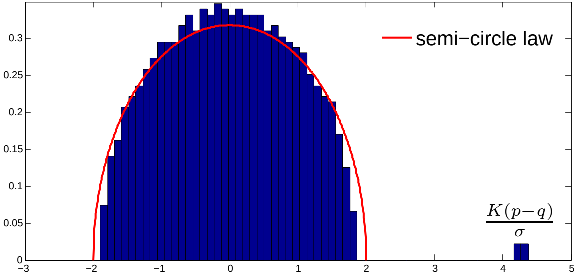

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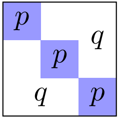
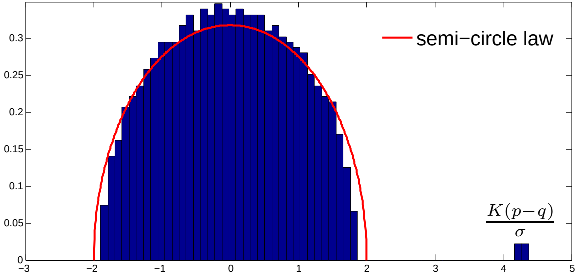
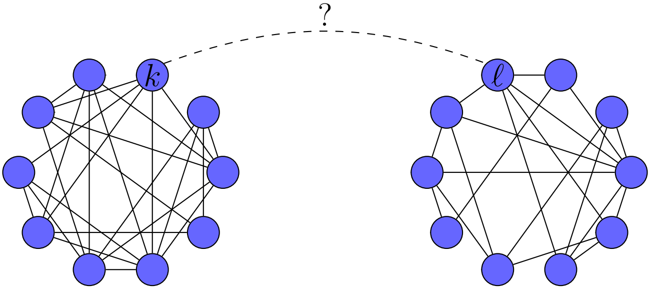
Community detection: $A \quad = $  $+ \; A - \mathbb{E}[A]$



- Davis-Kahan and variants: Top eigenvectors of $A \approx$ those of $\mathbb{E}[A]$, if eigen-gap $\gtrsim \|A - \mathbb{E}[A]\|_2$
- However, adjacency matrix of Erdős-Rényi graph has full rank and vanishing eigen-gaps

Spectral graph matching paradigm



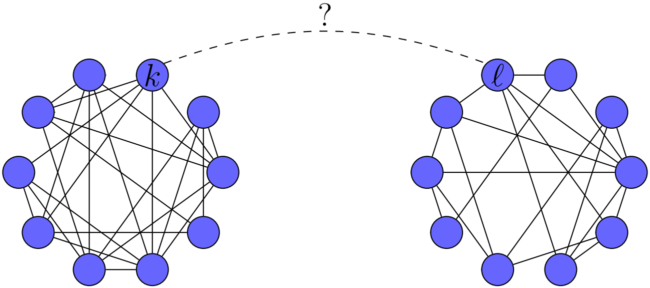
$$A = \sum_{i=1}^{n} \lambda_i u_i u_i^\top$$

$$\lambda_1 \geq \cdots \geq \lambda_n$$

$$B = \sum_{j=1}^{n} \mu_j v_j v_j^\top$$

$$\mu_1 \geq \cdots \geq \mu_n$$

Spectral graph matching paradigm



$$A = \sum_{i=1}^{n} \lambda_i u_i u_i^\top \qquad B = \sum_{j=1}^{n} \mu_j v_j v_j^\top$$

$$\lambda_1 \geq \cdots \geq \lambda_n \qquad \mu_1 \geq \cdots \geq \mu_n$$

1. Construct a similarity matrix X based on (λ_i, u_i) and (μ_j, v_j)
2. Project X to permutation by linear assignment: $\widehat{\Pi} \in \arg\max \langle X, \Pi \rangle$

Failure of previous spectral methods

- Low-rank methods: Aligning the leading eigenvectors

$$X = s_1 u_1 v_1^\top, \qquad s_1 \in \{\pm 1\}$$

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Similar ideas used in IsoRank [Singh-Xu-Berger '08] and EigenAlign [Feizi-Quon-Mendoza-Medard-Kellis-Jadbabaie '19]

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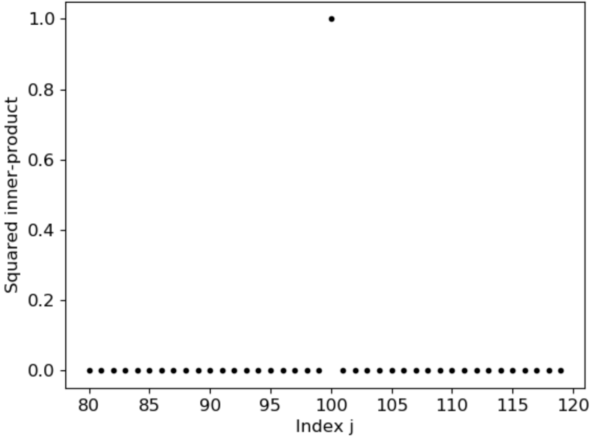
- Full-rank methods: [Umeyama '88]

$$X = \sum_{i=1}^{n} s_i u_i v_i^\top, \qquad s_i \in \{\pm 1\}$$

- All perform well with no noise, but are extremely fragile with noise
- A and B have full rank and vanishing eigen-gaps $\Rightarrow$ decorrelation of u_i and v_i when $\delta = n^{-c}$

Eigenvector correlation decay

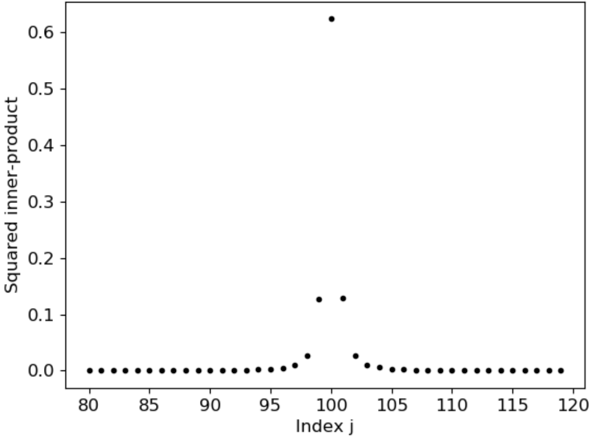
Isomorphic Erdős-Rényi graphs: 500 vertices, edge probability $\frac{1}{2}$



$\langle u_{100}, v_j \rangle^2$ for $j \in \{80, \ldots, 120\}$, averaged across 1000 simulations

Eigenvector correlation decay

Erdős-Rényi graphs with $\delta = 0.1\%$ differed edges



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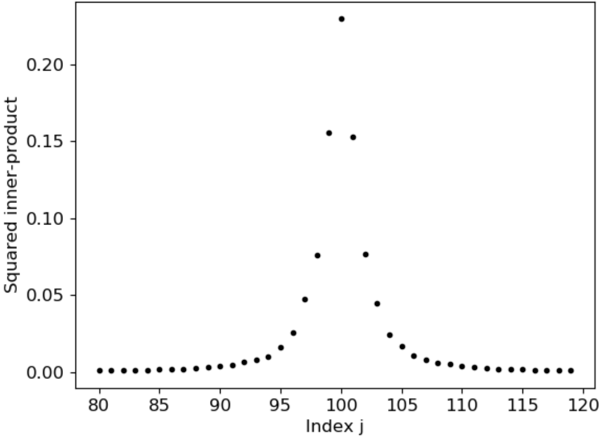
Erdős-Rényi graphs with $\delta = 0.5\%$ differed edges



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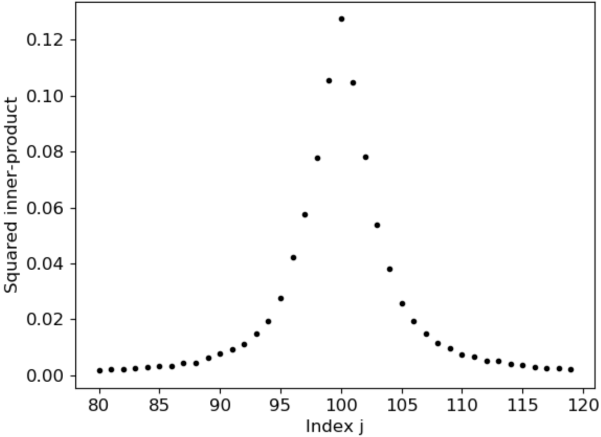
Eigenvector correlation decay

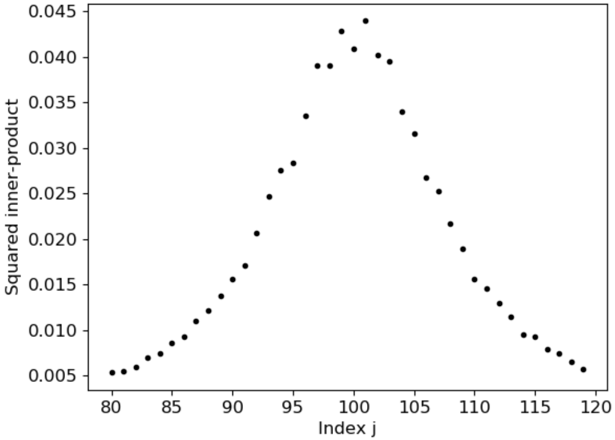
Erdős-Rényi graphs with $\delta = 1\%$ differed edges



$\langle u_{100}, v_j \rangle^2$ for $j \in \{80, \ldots, 120\}$, averaged across 1000 simulations

Eigenvector correlation decay

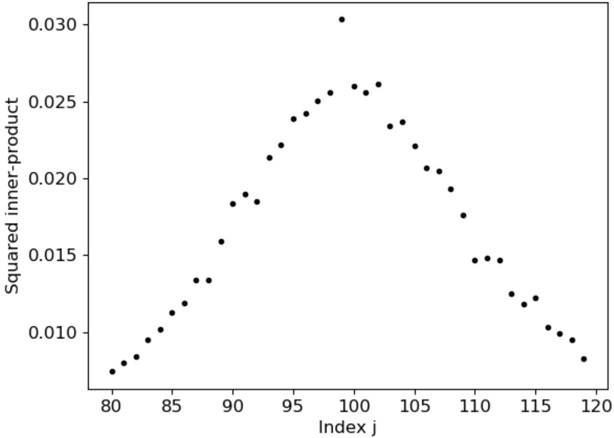
Erdős-Rényi graphs with $\delta = 3\%$ differed edges



$\langle u_{100}, v_j \rangle^2$ for $j \in \{80, \ldots, 120\}$, averaged across 1000 simulations

Eigenvector correlation decay

Erdős-Rényi graphs with $\delta = 5\%$ differed edges



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A new spectral method: GRAMPA

GRAph Matching by Pairwise eigen-Alignments:

$$X = \sum_{i,j=1}^{n} \underbrace{K\left(\frac{\lambda_i - \mu_j}{\eta}\right)}_{\text{spectral weights}} \times \underbrace{u_i^\top \mathbf{J} v_j \cdot u_i v_j^\top}_{\text{"Alignment" between } u_i \text{ and } v_j}$$

where η = bandwidth parameter, $\mathbf{J}$ = all-one matrix

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- All pairs matter:
  - Spectral weight penalizes pairs whose eigenvalues are far apart
  - Cauchy weight kernel is inspired by the eigenvector correlation decay [Bourgade-Yau '17], [Benigni '17]:

$$n \cdot \mathbb{E}\left[\langle u_i, v_j \rangle^2\right] \approx \frac{\delta}{(\lambda_i - \mu_j)^2 + C\delta^2}$$

- GRAMPA is invariant to the choices of signs for u_i and v_j

GRAMPA as regularized QP relaxation

- Graph matching as a quadratic assignment problem (QAP):

$$\arg\max_{\Pi \in S_n} \langle A, \Pi B \Pi^\top \rangle = \arg\min_{\Pi \in S_n} \|A - \Pi B \Pi^\top\|_F^2$$

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- A popular quadratic programming relaxation [Zaslavskiy-Bach-Vert '09], [Aflalo-Bronstein-Kimmel '15], [Lyzinski-Fishkind-Fiori-Vogelstein-Priebe-Sapiro '15]

$$\arg\min_{X \geq 0:\ X\mathbf{1}=\mathbf{1},\ X^\top \mathbf{1}=\mathbf{1}} \|AX - XB\|_F^2 \qquad \text{(QP-DS)}$$

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- The GRAMPA similarity matrix X is (a multiple of)

$$\arg\min_{X:\ \mathbf{1}^\top X \mathbf{1}=n} \|AX - XB\|_F^2 + \eta^2 \|X\|_F^2$$

This further relaxes the DS constraint and adds a ridge regularizer

Analysis of GRAMPA

Diagonal dominance in population version

Question: Is X "close" to true permutation matrix Π^*?

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Assume $\Pi^* = \mathbf{I}$ and $A \leftarrow \frac{A - \mathbb{E}[A]}{\sqrt{nq(1-q)}}$ and $B \leftarrow \frac{B - \mathbb{E}[B]}{\sqrt{nq(1-q)}}$:

$$X_{\text{pop}} = \epsilon \mathbf{I} + (1-\epsilon)\frac{\mathbf{J}}{n}, \qquad \epsilon \approx \frac{2(1-\delta)}{n(2\delta + \eta^2)}$$

- X_{pop} is close to $\frac{\mathbf{J}}{n}$ (center of the Birkhoff polytope)

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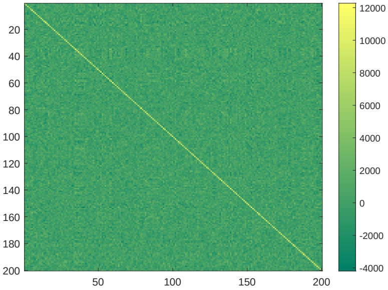
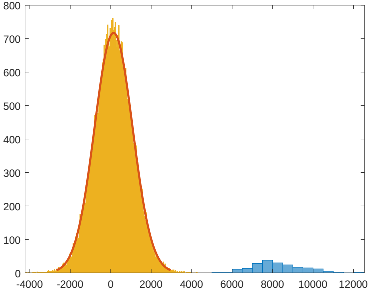
- X_{pop} is close to $\frac{\mathbf{J}}{n}$ (center of the Birkhoff polytope)
- Same analysis holds for tighter QP-DS
- X_{pop} is diagonally dominant: diagonals are $\approx \frac{2}{2\delta + \eta^2}$ times off-diagonals

Diagonal dominance of the similarity matrix



Heatmap of X



Histogram of off-diagonal (orange) and diagonal (blue) entries

When $\Pi^* = \mathbf{I}$, prove **diagonal dominance**

$$\min_k X_{kk} > \max_{k \neq \ell} X_{k\ell}$$

Heuristic argument: noiseless Gaussian case

$$X = \sum_{i,j=1}^{n} \frac{\eta}{(\lambda_i - \lambda_j)^2 + \eta^2} \langle u_i, \mathbf{1} \rangle \langle u_j, \mathbf{1} \rangle u_i u_j^\top$$

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For Gaussian matrices

- eigenvectors are uniform:

$$u_i \sim \text{Uniform}(n\text{-sphere}) \approx \frac{1}{\sqrt{n}} \mathcal{N}(0, I_n)$$

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$$u_i \sim \text{Uniform}(n\text{-sphere}) \approx \frac{1}{\sqrt{n}} \mathcal{N}(0, I_n)$$

  - Sum: $\langle u_i, \mathbf{1} \rangle \approx 1$

Heuristic argument: noiseless Gaussian case

$$X = \sum_{i,j=1}^{n} \frac{\eta}{(\lambda_i - \lambda_j)^2 + \eta^2} \langle u_i, \mathbf{1} \rangle \langle u_j, \mathbf{1} \rangle u_i u_j^\top$$

For Gaussian matrices

- eigenvectors are uniform:

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- eigenvalues and eigenvectors are independent

Heuristic argument: noiseless Gaussian case

$$X = \sum_{i,j=1}^{n} \frac{\eta}{(\lambda_i - \lambda_j)^2 + \eta^2} \langle u_i, \mathbf{1} \rangle \langle u_j, \mathbf{1} \rangle u_i u_j^\top$$

Heuristic argument: noiseless Gaussian case

$$X = \sum_{i=1}^{n} \frac{1}{\eta} \langle u_i, \mathbf{1} \rangle^2 u_i u_i^\top + \sum_{i \neq j} \frac{\eta}{(\lambda_i - \lambda_j)^2 + \eta^2} \langle u_i, \mathbf{1} \rangle \langle u_j, \mathbf{1} \rangle u_i u_j^\top$$

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- First term is diagonally dominant:

$$\sum_{i=1}^{n} \frac{1}{\eta} \underbrace{\langle u_i, \mathbf{1} \rangle^2}_{\approx 1} \underbrace{(u_i)_k}_{\mathcal{N}(0, \frac{1}{n})} \underbrace{(u_i)_\ell}_{\mathcal{N}(0, \frac{1}{n})} \approx \begin{cases} \frac{1}{\eta} & \text{if } k = \ell \\ \frac{1}{\eta \sqrt{n}} & \text{if } k \neq \ell \end{cases}$$

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- Second term is perturbation:

$$\sum_{i \neq j} \frac{\eta}{(\lambda_i - \lambda_j)^2 + \eta^2} \langle u_i, \mathbf{1} \rangle \langle u_j, \mathbf{1} \rangle (u_i)_k (u_j)_\ell \approx \sqrt{\frac{1}{n^2} \sum_{i \neq j} \left(\frac{\eta}{(\lambda_i - \lambda_j)^2 + \eta^2} \right)^2}$$

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Heuristic argument: noiseless Gaussian case

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$$\approx \frac{1}{\sqrt{\eta}} \quad \text{(using semicircle law)}$$

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$$\approx \frac{1}{\sqrt{\eta}} \text{ (using semicircle law)}$$

- Made rigorous when A, B are Gaussian since eigenvalues and eigenvectors are independent, but hard to extend to Erdős-Rényi graphs

Universality: Correlated Wigner model

Standardized weighted adjacency matrices A, B where (A_{ij}, B_{ij}) are independent pairs satisfying

$$\mathbb{E}[A_{ij}] = \mathbb{E}[B_{ij}] = 0, \quad \mathbb{E}[A_{ij}^2] = \mathbb{E}[B_{ij}^2] = \frac{1}{n}, \quad \mathbb{E}[A_{ij}B_{ij}] = \frac{1-\delta}{n}$$

Key proof technique: Resolvent and local laws

$$R_A(z) \triangleq (A - z\mathbf{I})^{-1} = \sum_i \frac{1}{\lambda_i - z} u_i u_i^\top, \qquad z \in \mathbb{C} \backslash \mathbb{R}$$

Key proof technique: Resolvent and local laws

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Denote Wigner's semicircle density and its Stieltjes transform by

$$\rho(x) = \frac{1}{2\pi}\sqrt{4 - x^2} \cdot \mathbf{1}_{\{|x| \le 2\}} \quad \text{and} \quad m(z) = \int \frac{1}{x - z} \rho(x) dx$$

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- Empirical eigenvalue distribution converges to ρ

$$\frac{1}{n} \operatorname{Tr} R_A(z) \to m(z)$$

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- $R_A(z) \approx m(z)\mathbf{I}$ entrywise [Erdos-Knowles-Yau-Yin '13]:

$$(R_A(z))_{ij} \approx m(z) \cdot \mathbf{1}_{\{i=j\}}$$

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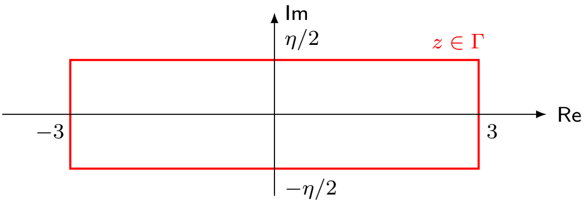
- Similarly, row-sum and total-sum satisfy:

$$\sum_j (R_A(z))_{ij} \lesssim \text{polylog}(n) \qquad \sum_{i,j} (R_A(z))_{ij} \approx n \cdot m(z)$$

Universality proof step 1: Resolvent representation

Lemma (Fan-Mao-Wu-X. '19)

$$X \triangleq \sum_{i,j=1}^{n} \frac{\eta}{(\lambda_i - \mu_j)^2 + \eta^2} \langle u_i, \mathbf{1} \rangle \langle v_j, \mathbf{1} \rangle u_i v_j^\top$$
$$= \frac{1}{2\pi} \operatorname{Re} \oint_\Gamma R_A(z) \mathbf{1}\mathbf{1}^\top R_B(z + \mathbf{i}\eta) dz$$



Γ encloses $\lambda_1, \ldots, \lambda_n$ but not $\mu_1 - \mathbf{i}\eta, \ldots, \mu_n - \mathbf{i}\eta$

Step 2: Leave-one-out relation

$$X_{11} = \frac{1}{2\pi} \mathrm{Re} \oint_{\Gamma} \underbrace{\left[e_1^\top R_A(z)\mathbf{1}\right] \left[\mathbf{1}^\top R_B(z + \mathbf{i}\eta)e_1\right]}_{\text{correlated 1st row sums}} dz$$

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-
$$A = \begin{pmatrix} a_{11} & a_1^\top \\ a_1 & A^{(1)} \end{pmatrix} \qquad R_A(z) = \begin{pmatrix} R_{A,11} & R_{A,1*} \\ R_{A,*1} & R_{A,**} \end{pmatrix}$$

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- By the Schur-complement formula

$$\begin{aligned} R_{A,1*}(z) &= -R_{A,11}(z) \cdot a_1^\top (A^{(1)} - z\mathbf{I})^{-1} \\ &= -R_{A,11}(z) \cdot a_1^\top R_{A^{(1)}}(z) \end{aligned}$$

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$$\approx -m(z) \cdot a_1^\top R_{A^{(1)}}(z)$$
- Writing a similar expression for B, we get
$$X_{11} \approx \frac{1}{2\pi} \mathrm{Re} \oint_\Gamma m(z)m(z+\mathbf{i}\eta) \left[a_1^\top R_{A^{(1)}}(z)\mathbf{1}\mathbf{1}^\top R_{B^{(1)}}(z+\mathbf{i}\eta)b_1\right] dz$$

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- Writing a similar expression for B, we get
$$X_{11} \approx \frac{1}{2\pi} \mathrm{Re} \oint_\Gamma m(z)m(z+\mathbf{i}\eta) \left[a_1^\top R_{A^{(1)}}(z)\mathbf{1}\mathbf{1}^\top R_{B^{(1)}}(z+\mathbf{i}\eta)b_1\right] dz$$
- The vectors (a_1, b_1) are correlated, and independent of $(A^{(1)}, B^{(1)})$

Step 3: Separating signal from noise

Diagonal entries: Apply concentration of the bilinear form

$$X_{11} \approx \frac{1}{2\pi} \mathrm{Re}\; a_1^\top \left[\oint_\Gamma m(z)m(z+\mathbf{i}\eta)R_{A^{(1)}}(z)\mathbf{1}\mathbf{1}^\top R_{B^{(1)}}(z+\mathbf{i}\eta)dz \right] b_1$$

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Off-diagonal entries:

$$X_{12} \approx \frac{1}{2\pi} \operatorname{Re} a_1^\top \left[\oint_\Gamma m(z)m(z+\mathbf{i}\eta) R_{A^{(12)}}(z) \mathbf{1}\mathbf{1}^\top R_{B^{(12)}}(z+\mathbf{i}\eta) dz \right] b_2$$

Here (a_1, b_2) are independent, so the conditional mean is 0

Step 3: Separating signal from noise

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Here (a_1, b_2) are independent, so the conditional mean is 0

Step 4: Proof of diagonal dominance

- Diagonal entries:

$$
\begin{aligned}
X_{11} &\approx \frac{1-\delta}{2\pi} \mathrm{Re} \frac{1}{n} \mathrm{Tr} \left[\oint_\Gamma m(z) m(z+\mathbf{i}\eta) R_{A^{(1)}}(z) \mathbf{J} R_{B^{(1)}}(z+\mathbf{i}\eta) dz \right] \\
&\approx \frac{1-\delta}{2\pi} \mathrm{Re} \frac{1}{\mathbf{i}\eta} \oint_\Gamma m(z) m(z+\mathbf{i}\eta) \left(m(z+\mathbf{i}\eta) - m(z) \right) dz + \frac{\sqrt{\delta}}{\eta^2} \\
&\approx \frac{1-\delta}{\eta} + \frac{\sqrt{\delta}}{\eta^2}
\end{aligned}
$$

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$$\approx \frac{1-\delta}{2\pi} \operatorname{Re} \frac{1}{\mathbf{i}\eta} \oint_\Gamma m(z) m(z+\mathbf{i}\eta) \left(m(z+\mathbf{i}\eta) - m(z) \right) dz + \frac{\sqrt{\delta}}{\eta^2}$$

$$\approx \frac{1-\delta}{\eta} + \frac{\sqrt{\delta}}{\eta^2}$$

- Off-diagonal entries

$$X_{12} \lesssim \frac{(\log n)^{2+\varepsilon}}{n} \left\| \oint_\Gamma m(z) m(z+\mathbf{i}\eta) R_{A^{(12)}}(z) \mathbf{J} R_{B^{(12)}}(z+\mathbf{i}\eta) dz \right\|_F$$

$$\lesssim \frac{(\log n)^{2+\varepsilon}}{\sqrt{\eta}}$$

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$$\approx \frac{1-\delta}{\eta} + \frac{\sqrt{\delta}}{\eta^2}$$

- Off-diagonal entries

$$X_{12} \lesssim \frac{(\log n)^{2+\varepsilon}}{n} \left\| \oint_\Gamma m(z) m(z+\mathbf{i}\eta) R_{A^{(12)}}(z) \mathbf{J} R_{B^{(12)}}(z+\mathbf{i}\eta) dz \right\|_F$$

$$\lesssim \frac{(\log n)^{2+\varepsilon}}{\sqrt{\eta}}$$

- Applying this and a union bound for every $X_{k\ell}$ shows that X is diagonally dominant when

$$\sqrt{\delta} \lesssim \eta \lesssim (\log n)^{-(4+2\varepsilon)}$$

Extensions

- Dense graphs $q = \Theta(1)$: improvement to $\delta \lesssim (\log n)^{-(4+\epsilon)}$
- Gaussian weighted graphs: improvement to $\delta \lesssim (\log n)^{-2}$ by direct analysis
- Similar result for a tighter QP relaxation (this is not automatic!)

$$\arg \max_{X:\, X\mathbf{1}=\mathbf{1}} \|AX - XB\|_F^2 + \eta^2 \|X\|_F^2$$

- Similar results for matching bipartite graphs

Outline

1. Degree profile matching algorithm
2. Spectral graph matching algorithm
3. Concluding remarks

Concluding remarks

- New spectral graph matching algorithm: "full-rank" spectral method

$$X = \sum_{i,j=1}^{n} \frac{\eta}{(\lambda_i - \mu_j)^2 + \eta^2} u_i u_i^\top \mathbf{J} v_j v_j^\top$$

- Efficiently matches two graphs with average degree $\geq \mathrm{polylog}(n)$ and fraction of differed edges $\leq 1/\mathrm{polylog}(n)$

Open problems

- Theoretical guarantees for QP-DS

$$\min_{X \text{ doubly stochastic}} \|AX - XB\|_F^2$$

Open problems

- Theoretical guarantees for QP-DS

$$\min_{X \text{ doubly stochastic}} \|AX - XB\|_F^2$$

- Other random graphs ensembles, e.g., geometric graphs

References

- J. Ding, Z. Ma, Y. Wu, J. Xu. *Efficient random graph matching via degree profiles*. Probability Theory & Related Fields, arXiv:1811.07821.
- Z. Fan, C. Mao, Y. Wu, J. Xu. *Spectral graph matching and regularized quadratic relaxations I: Algorithm and Gaussian analysis*, Foundations of Computational Mathematics, arxiv:1907.08880.
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