Lecture 2: Random Graph Matching: Information-theoretic Limits

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Joint work with
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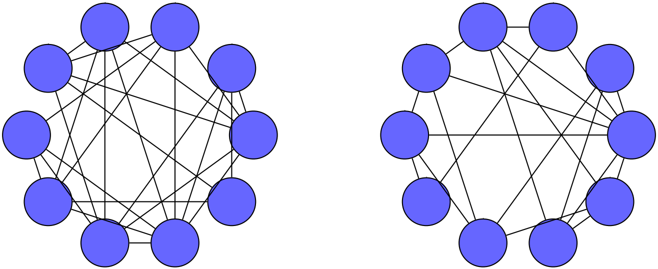
AI4OPT Tutorial Lectures

Graph matching (network alignment)



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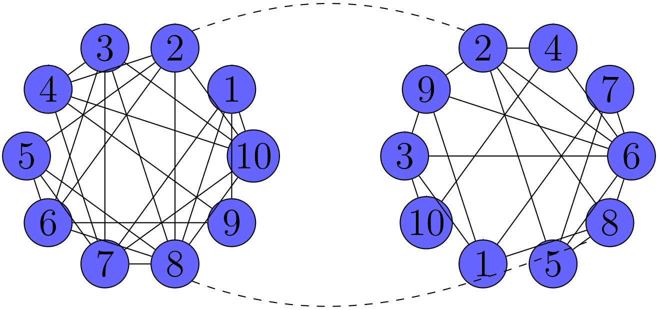

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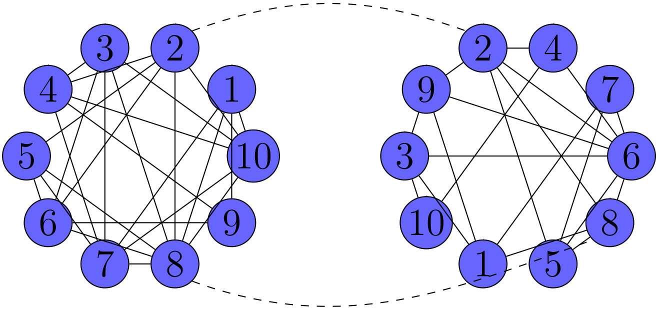

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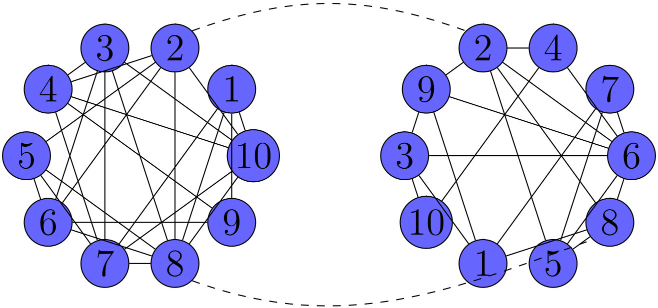

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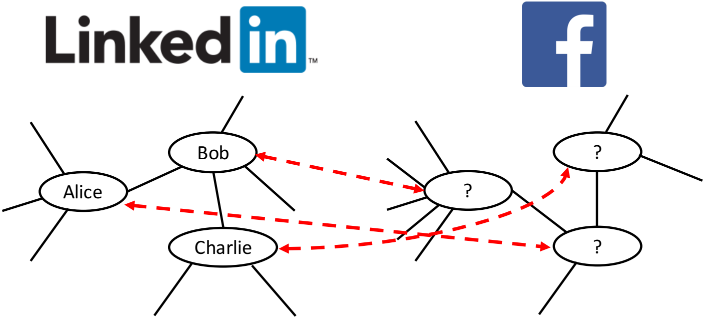
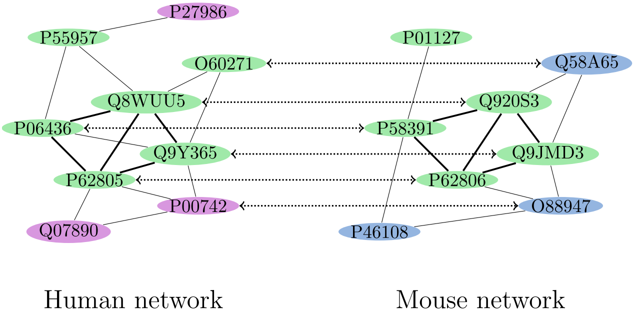
Noiseless case: reduce to graph isomorphism

Application 1: Network de-anonymization



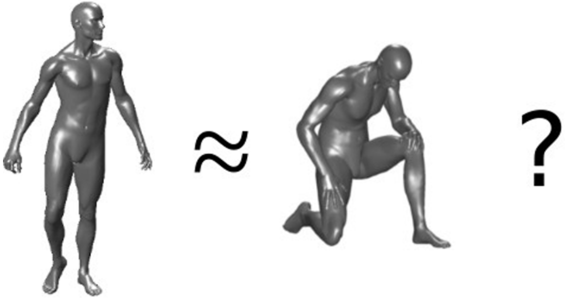
- Successfully de-anonymize Netflix dataset by matching it to IMDB [Narayanan-Shmatikov '08]
- Correctly identify 30.8% of shared users between Twitter and Flickr [Narayanan-Shmatikov '09]



[Kazemi-Hassani-Grossglauser-Modarres '16]

Graph matching for aligning PPI networks between different species, to identify conserved components and genes with common function [Singh-Xu-Berger '08]

A fundamental problem in computer vision: Detect and match similar objects that undergo different deformations



Shape REtrieval Contest (SHREC) dataset [Lähner et al '16]

Application 3: Computer vision

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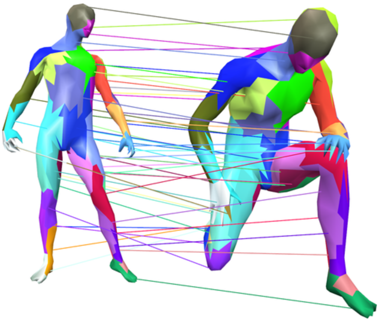
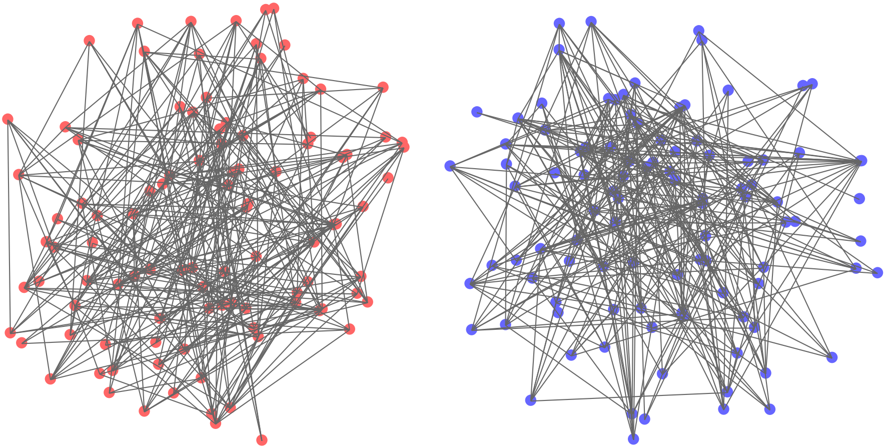


Shape REtrieval Contest (SHREC) dataset [Lähner et al '16]

3-D shapes $\to$ geometric graphs (features $\to$ nodes, distances $\to$ edges)

Two key challenges

- Statistical: two graphs may not be the same
- Computational: # of possible node mappings is $n!$ ($100! \approx 10^{158}$)



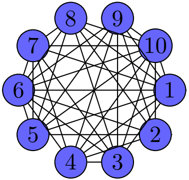
Beyond worst-case intractability

- NP-hard for matching two graphs in worst case
- However, real networks are not arbitrary and have latent structures

Beyond worst-case intractability

- NP-hard for matching two graphs in worst case
- However, real networks are not arbitrary and have latent structures
- Recent surge of interests on the average-case analysis of matching two correlated random graphs [Feizi at el.'16, Lyzinski at el'16, Cullina-Kiyavash'16,17, Ding-Ma-Wu-Xu'18, Barak-Chou-Lei-Schramm-Sheng'19, Fan-Mao-Wu-Xu'19a,19b, Ganassali-Massoulié'20, Hall-Massoulié'20, ...]
- Focus on correlated Erdős-Rényi graphs model [Pedarsani-Grossglauser '11]

Correlated Erdős-Rényi graphs model $\mathcal{G}(n, p, s)$



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

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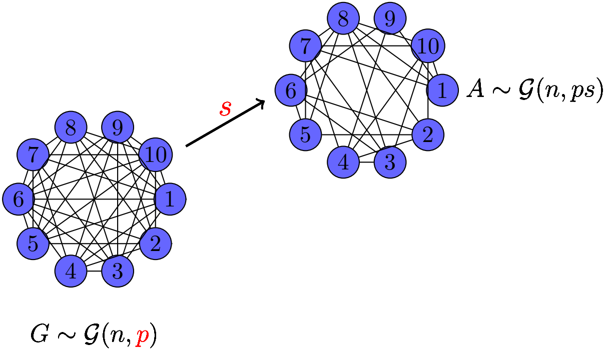

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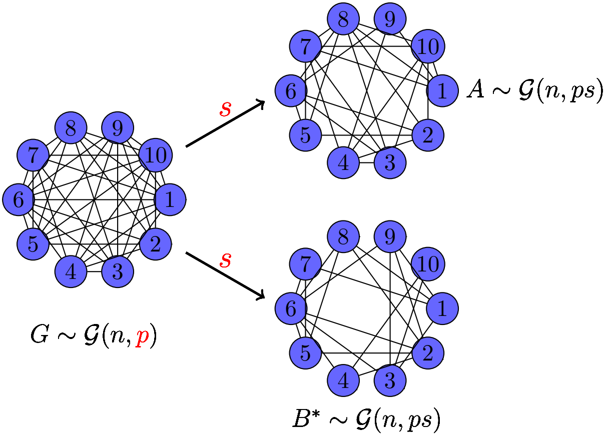

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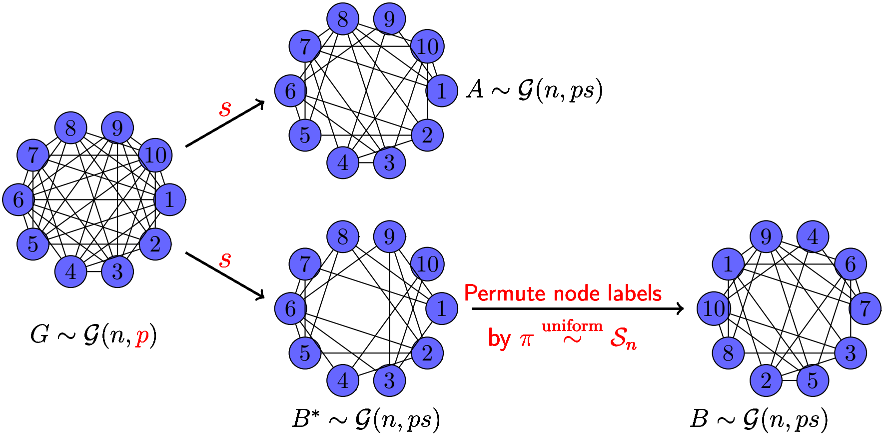

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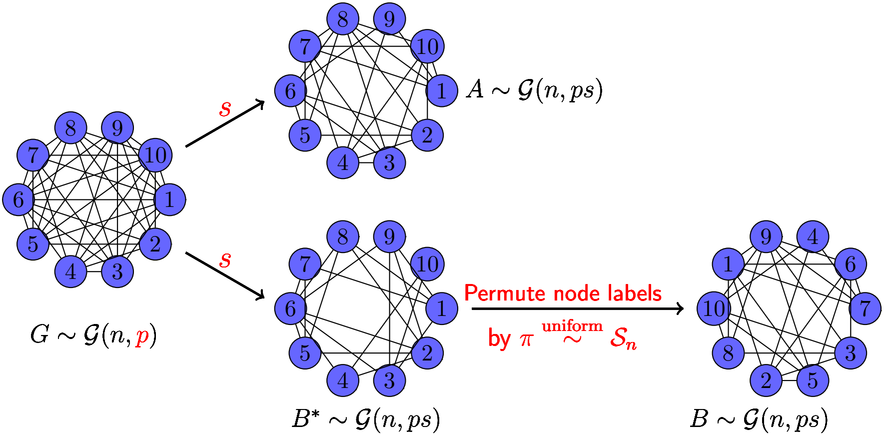

- $(A_{\pi(i)\pi(j)}, B_{ij})$ are $i.i.d.$ pairs of correlated $\mathrm{Bern}(ps)$
- Key parameter nps^2: average degree of intersection graph $A \wedge B^*$;

Correlated Gaussian model

$$B = \rho A^{\pi} + \sqrt{1-\rho^2} Z \,,$$

where

- A and Z are independent Gaussian Wigner matrices with $i.i.d.$ standard normal entries;
- $A^{\pi} = (A_{\pi(i)\pi(j)})$ denote the relabeled version of A
- Conditional on π, for any $1 \le i < j \le n$,

$$(A_{\pi(i)\pi(j)}, B_{ij}) \overset{\text{i.i.d.}}{\sim} \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right).$$

Two statistical tasks: detection and estimation

- Detection:
  - $\mathcal{H}_0$: A and B are two independent Erdős-Rényi graphs $\mathcal{G}(n, ps)$
  - $\mathcal{H}_1$: A and B are two correlated Erdős-Rényi graphs $\mathcal{G}(n, p, s)$
  - Test between $\mathcal{H}_0$ and $\mathcal{H}_1$ based on observation of (A, B)
- Estimation:
  - Observe two correlated Erdős-Rényi graphs $A, B \sim \mathcal{G}(n, p, s)$
  - Recover the underlying true vertex correspondence π

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Focus of this lecture

What are the information-theoretic limits of detection and estimation?

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10+ years of development:

[Pedarsani-Grossglauser '11], [Cullina-Kiyavash '16,17], [Hall-Massoulié '20], [Ganassali '20], [Wu-X.-Yu '20,21], [Ganassali-Lelarge-Massoulié '21], [Ding-Du '21 22]

Maximum likelihood estimation as quadratic assignment

Maximum likelihood estimation reduces to quadratic assignment (QAP):

$$\widehat{\pi}_{\mathsf{ML}} \in \arg\max_{\pi} \sum_{i<j} A_{ij} B_{\pi(i)\pi(j)} \,.$$

- QAP is NP-hard in worst case
- How much does $\widehat{\pi}_{\mathrm{ML}}$ have in common with π^*?

$$\mathrm{overlap}(\pi, \widehat{\pi}) \triangleq \frac{1}{n} \Big| \{ i \in [n] : \widehat{\pi}(i) = \pi(i) \} \Big|$$

Sharp threshold for detection: Gaussian

Theorem (Wu-X.-Yu '20)

$$n\rho^2 \geq (4+\epsilon)\log n \implies \mathrm{TV}\left(\mathcal{P},\mathcal{Q}\right) = 1 - o(1)\,(\textit{test error}{=}o(1))$$

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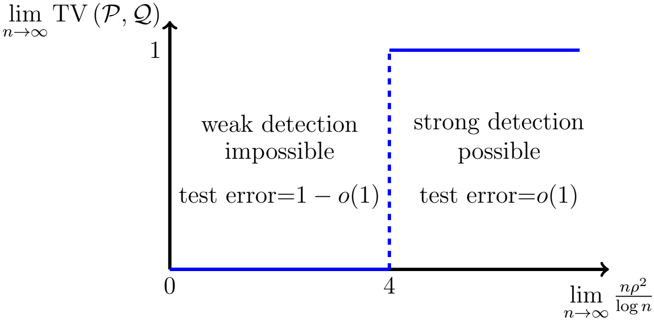

Sharp threshold for recovery: Gaussian model

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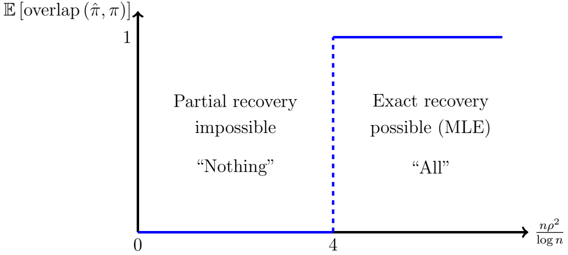

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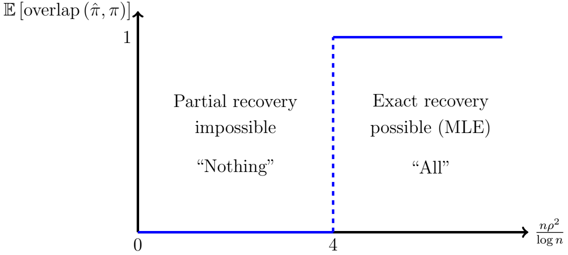

- Exact recovery threshold is derived in [Ganassali '20]
- Exhibits a stronger form of "all or nothing" phenomenon

Sharp detection threshold: dense Erdős-Rényi graphs

Theorem (Wu-X.-Yu '20)

Suppose $n^{-o(1)} \leq p \leq 1 - \Omega(1)$. *Then,*

$$nps^2 \geq \frac{(2+\epsilon)\log n}{\log \frac{1}{p} - 1 + p} \implies \mathrm{TV}\left(\mathcal{P}, \mathcal{Q}\right) = 1 - o\left(1\right) \ (\textit{test error}{=}o(1))$$

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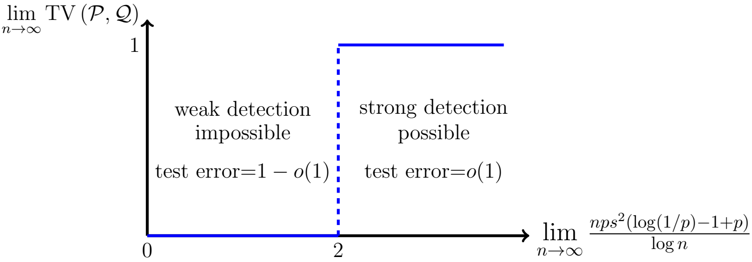

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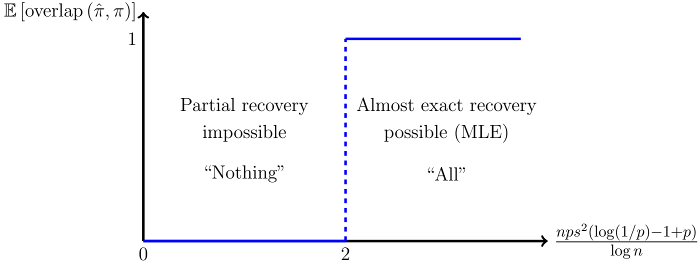

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Interpretation of threshold:

- $I(\pi; A, B) \approx \binom{n}{2} \times \underbrace{ps^2\left(\log\frac{1}{p} - 1 + p\right)}_{\text{mutual info btw two correlated edges}}$
- $H(\pi) \approx n \log n$
- Threshold is at $I(\pi; A, B) \approx H(\pi)$

Sharp detection threshold: sparse Erdős-Rényi

Theorem (Ding-Du '22a)

Suppose $p = n^{-\alpha}$ *for* $\alpha \in (0,1)$ *and* $\lambda^* = \gamma^{-1}(1/\alpha)$.

$$nps^2 \geq \lambda^* + \epsilon \implies \mathrm{TV}\left(\mathcal{P}, \mathcal{Q}\right) = 1 - o(1) \, (\textit{test error}{=}o(1))$$
$$nps^2 \leq \lambda^* - \epsilon \implies \mathrm{TV}\left(\mathcal{P}, \mathcal{Q}\right) = o(1) \, (\textit{test error}{=}1 - o(1))$$

- Sharpened our threshold at $nps^2 = \Theta(1)$ [Wu-X.-Yu '20]
- $\gamma : [1, \infty) \to [1, \infty)$ is given by the densest subgraph problem in Erdős-Rényi $\mathcal{G}(n, \frac{\lambda}{n})$ [Hajek '90, Anantharam-Salez' 16]

$$\max_{\emptyset \neq U \subset [n]} \frac{|\mathcal{E}(U)|}{|U|} \to \gamma(\lambda)$$

- When $np = \Theta(1)$, there is no zero-one phase transition.

Sharp recovery threshold: sparse Erdős-Rényi

Theorem (Ding-Hu '22b)

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- The negative result of $\alpha = 1$ is proved in [Ganassali-Lelarge-Massoulié '21]
- Sharpen our partial recovery threshold at $nps^2 = \Theta(1)$ [Wu-X.-Yu '21]
- "All-or-nothing" phenomenon does not exist, as almost exact recovery (overlap $= 1 - o(1)$) requires $nps^2 \to \infty$ [Cullina-Kiyavash-Mittal-Poor '19]

Exact recovery threshold

Theorem (Wu-X.-Yu '21)

Suppose $p \leq 1 - \Omega(1)$. *Then*

$$nps^2 \geq \frac{(1+\epsilon)\log n}{\left(1-\sqrt{p}\right)^2} \implies \mathrm{overlap}\left(\widehat{\pi}_{\mathrm{ML}}, \pi\right) = 1 \textit{ w.h.p.}$$

$$nps^2 \leq \frac{(1-\epsilon)\log n}{\left(1-\sqrt{p}\right)^2} \implies \mathrm{overlap}\left(\widehat{\pi}, \pi\right) \neq 1 \textit{ w.h.p. } \forall\, \widehat{\pi}\,.$$

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- $p = o(1)$: reduces to the connectivity threshold of the intersection graph $A \wedge B^* \sim \mathcal{G}(n, ps^2)$ [Cullina-Kiyavash'16,17]

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- $p = o(1)$: reduces to the connectivity threshold of the intersection graph $A \wedge B^* \sim \mathcal{G}(n, ps^2)$ [Cullina-Kiyavash'16,17]
- $p = \Omega(1)$: strictly higher than the connectivity threshold

Analysis

- Proof of detection thresholds
- Proof of partial recovery thresholds
- Proof of exact recovery thresholds

Proof of detection thresholds: Positive results

- Gaussian or dense Erdős-Rényi: analyzing QAP statistic

$$\max_{\pi \in \mathcal{S}_n} \sum_{i<j} A_{ij} B_{\pi(i)\pi(j)} \quad (\text{\# of common edges})$$

- Sparse Erdős-Rényi: analyzing densest subgraph statistic

$$\max_{\pi \in \mathcal{S}_n} \max_{U \subset [n]: |U| \geq n/\log n} \frac{\mathcal{E}_\pi(U)}{|U|},$$

  where $\mathcal{E}_\pi(U)$ is the set of edges induced by vertices in U in intersection graph $A^\pi \wedge B$

- Standard first-moment computation

Proof of detection thresholds: Negative results

Second-moment method

$$\mathbb{E}_{\mathcal{Q}}\left[\left(\frac{\mathcal{P}(A,B)}{\mathcal{Q}(A,B)}\right)^2\right] = O(1) \qquad \Longrightarrow \mathrm{TV}(\mathcal{P},\mathcal{Q}) \le 1 - \Omega(1)$$

Strong detection is impossible

$$\mathbb{E}_{\mathcal{Q}}\left[\left(\frac{\mathcal{P}(A,B)}{\mathcal{Q}(A,B)}\right)^2\right] = 1 + o(1) \qquad \Longrightarrow \mathrm{TV}(\mathcal{P},\mathcal{Q}) = o(1)$$

Weak detection is impossible

Cycle (orbit) decomposition

- **Node permutation** σ acts on $[n]$
- **Edge permutation** σ^{E} acts on $\binom{[n]}{2}$: $\sigma^{\mathsf{E}}((i,j)) \triangleq (\sigma(i), \sigma(j))$

Cycle (orbit) decomposition

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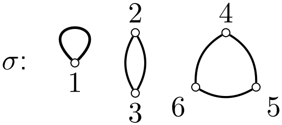
Example: $n = 6$ and $\sigma = (1)(23)(456)$:



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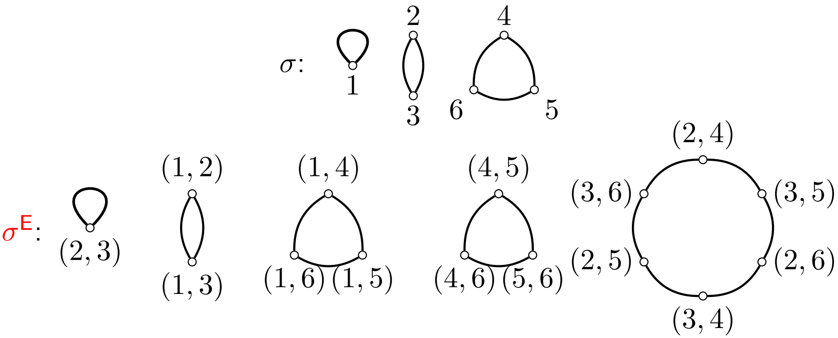

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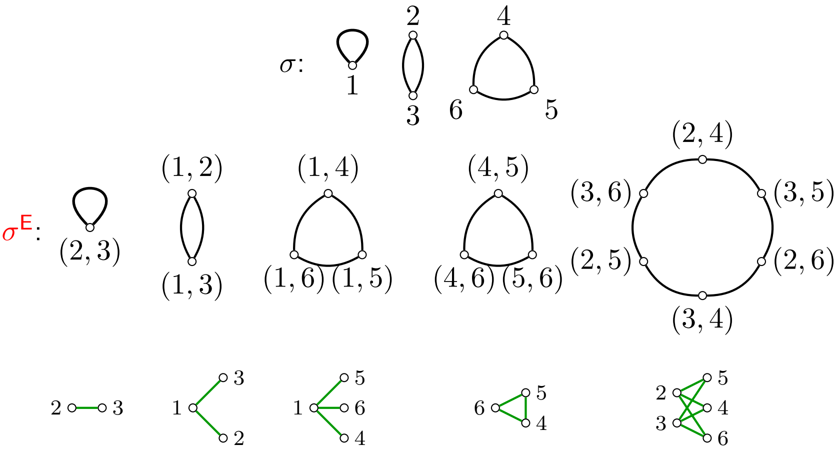

Second-moment calculation via orbit decomposition

$$\left(\frac{\mathcal{P}(A,B)}{\mathcal{Q}(A,B)}\right)^2 = \left(\mathbb{E}_\pi\left[\frac{\mathcal{P}(A,B|\pi)}{\mathcal{Q}(A,B)}\right]\right)^2$$

$$= \mathbb{E}_{\widetilde{\pi} \perp\!\!\!\perp \pi} \prod_{i<j} X_{ij} \quad X_{ij} \triangleq \frac{\mathcal{P}(B_{\pi(i)\pi(j)}|A_{ij})\mathcal{P}(B_{\widetilde{\pi}(i)\widetilde{\pi}(j)}|A_{ij})}{\mathcal{Q}(B_{\pi(i)\pi(j)})\mathcal{Q}(B_{\widetilde{\pi}(i)\widetilde{\pi}(j)})}$$

$$= \mathbb{E}_{\widetilde{\pi} \perp\!\!\!\perp \pi} \prod_{O \in \mathcal{O}} X_O \quad X_O \triangleq \prod_{(i,j)\in O} X_{ij}$$

$\mathcal{O}$: disjoint orbits of edge permutation σ^{E} with $\sigma \triangleq \pi^{-1} \circ \widetilde{\pi}$

Second-moment calculation via orbit decomposition

$$\left(\frac{\mathcal{P}(A,B)}{\mathcal{Q}(A,B)}\right)^2 = \left(\mathbb{E}_\pi\left[\frac{\mathcal{P}(A,B|\pi)}{\mathcal{Q}(A,B)}\right]\right)^2$$

$$= \mathbb{E}_{\widetilde{\pi} \perp\!\!\!\perp \pi} \prod_{i<j} X_{ij} \quad X_{ij} \triangleq \frac{\mathcal{P}(B_{\pi(i)\pi(j)}|A_{ij})\mathcal{P}(B_{\widetilde{\pi}(i)\widetilde{\pi}(j)}|A_{ij})}{\mathcal{Q}(B_{\pi(i)\pi(j)})\mathcal{Q}(B_{\widetilde{\pi}(i)\widetilde{\pi}(j)})}$$

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$$\mathbb{E}_{\mathcal{Q}}[X_O] = \begin{cases} \frac{1}{1-\rho^{2|O|}} & \text{Gaussian} \\ 1+\rho^{2|O|} & \text{Erdős-Rényi} \end{cases}$$

Failure of second-moment

We show

$$\mathbb{E}_{\mathcal{Q}}\left[\left(\frac{\mathcal{P}(A,B)}{\mathcal{Q}(A,B)}\right)^2\right] = \begin{cases} 1+o(1) & \text{if } \rho^2 \le \frac{(2-\epsilon)\log n}{n} \\ +\infty & \text{if } \rho^2 \ge \frac{(2+\epsilon)\log n}{n} \end{cases}$$

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Obstruction from short orbits

$$\mathbb{E}_{(A,B)\sim\mathcal{Q}}\left[\left(\frac{\mathcal{P}(A,B)}{\mathcal{Q}(A,B)}\right)^2\right] = \mathbb{E}_{\pi \perp\!\!\!\perp \widetilde{\pi}}\left[\prod_{O\in\mathcal{O}} \mathbb{E}_{\mathcal{Q}}\left[X_O\right]\right] \overset{\widetilde{\pi}=\pi}{\ge} \frac{1}{n!}\left(1+\rho^2\right)^{\binom{n}{2}}$$

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Atypically large magnitude of $\prod_{O\in\mathcal{O}:|O|=k} X_O$ for short orbits of length $k \lesssim \log n \Rightarrow$ second-moment blows up

Truncated second-moment

Let $\mathcal{E}$ denote an event that holds whp under $\mathcal{P}$:

$$\mathbb{E}_{\mathcal{Q}}\left[\left(\frac{\mathcal{P}(A,B)}{\mathcal{Q}(A,B)}\right)^2 \mathbf{1}_{\{\mathcal{E}\}}\right] = O(1) \qquad \Longrightarrow \; \mathrm{TV}(\mathcal{P},\mathcal{Q}) \le 1 - \Omega(1)$$

Strong detection is impossible

$$\mathbb{E}_{\mathcal{Q}}\left[\left(\frac{\mathcal{P}(A,B)}{\mathcal{Q}(A,B)}\right)^2 \mathbf{1}_{\{\mathcal{E}\}}\right] = 1 + o(1) \qquad \Longrightarrow \; \mathrm{TV}(\mathcal{P},\mathcal{Q}) = o(1)$$

Weak detection is impossible

Truncated second-moment: Gaussian model

It suffices to consider $k = 1$:

$$Y \triangleq \prod_{O \in \mathcal{O}: |O|=1} X_O \approx \exp\left(-\rho^2 \binom{n_1}{2} + 2\rho e_{A^\pi \wedge B}(F) \right)$$

- F is the set of fixed points of $\sigma \triangleq \pi^{-1} \circ \widetilde{\pi}$ and $n_1 = |F|$
- $e_{A^\pi \wedge B}(F) \triangleq \sum_{(i,j) \in F} A_{\pi(i)\pi(j)} B_{ij}$

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- Under $\mathcal{P}$: $e_{A^\pi \wedge B}(S)$ concentrates on $\rho\binom{|S|}{2}$ uniformly over all S when $|S|$ is large

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- Under $\mathcal{P}$: $e_{A^\pi \wedge B}(S)$ concentrates on $\rho\binom{|S|}{2}$ uniformly over all S when $|S|$ is large
- On this typical event $\mathcal{E}$ under $\mathcal{P}$, when $|F|$ is large,

$$\mathbb{E}_{\mathcal{Q}}\left[Y \mathbf{1}_{\{\mathcal{E}\}}\right] \lesssim e^{-\rho^2\binom{n_1}{2}} \mathbb{E}_{\mathcal{Q}}\left[e^{2\rho e_{A^\pi \wedge B}(F)} \mathbf{1}_{\left\{e_{A^\pi \wedge B}(F) \le \rho\binom{n_1}{2}\right\}}\right]$$

$$\approx \exp\left(\frac{\rho^2}{2}\binom{n_1}{2}\right) \quad \text{(Gain a factor of 2)}$$

Truncated second-moment: dense Erdős-Rényi

Again it suffices to consider $k = 1$:

$$Y \triangleq \prod_{O \in \mathcal{O}:|O|=1} X_O \approx \left(\frac{1}{p}\right)^{2e_{A^\pi \wedge B}(F)}$$

- Under $\mathcal{P}$: $e_{A^\pi \wedge B}(S)$ concentrates on $\binom{|S|}{2} ps^2$ uniformly over all S when $|S|$ is large
- On this typical event $\mathcal{E}$ under $\mathcal{P}$, when $|F|$ is large,

$$\mathbb{E}_{\mathcal{Q}}\left[Y \mathbf{1}_{\{\mathcal{E}\}}\right] \lesssim \mathbb{E}_{\mathcal{Q}}\left[\left(\frac{1}{p}\right)^{2e_{A^\pi \wedge B}(F)} \mathbf{1}_{\left\{e_{A^\pi \wedge B}(F) \le \binom{|F|}{2} ps^2\right\}}\right]$$

Truncated second-moment: sparse Erdős-Rényi

Need to consider $k = \Theta(\log n)$. It can be shown

- Long orbits:

$$\mathbb{E}_{\mathcal{Q}}\left[\prod_{|O|>k} X_O\right] \le \left(1+\rho^k\right)^{\frac{n^2}{k}} = 1 + o(1)$$

- Short incomplete orbits:

$$\mathbb{E}_{\mathcal{Q}}\left[X_O \mid O \not\subset E\left(A \wedge B^\pi\right)\right] \le 1$$

- Short complete orbits:

$$X_O = \left(\frac{1}{p}\right)^{2|O|}, \quad \forall O \subset E\left(A \wedge B^\pi\right)$$

Suffices to consider subgraph $H_k \triangleq \cup_{O:|O|\le k, O\subset E(A\wedge B^\pi)} O$

Truncated second-moment: sparse Erdős-Rényi

- If $nps^2 \le 1 - \omega(n^{-1/3})$:

$$\mathcal{E} \triangleq \{A \wedge B^\pi \text{ is a pseudoforest}\}$$

- If $nps^2 \le \lambda^* - \epsilon$:

$$\mathcal{E} \triangleq \{\text{The subgraph density of } A \wedge B^\pi \text{ is smaller than } \gamma(\lambda^*)\}$$

Then

$$\mathbb{E}_{\mathcal{Q}}\left[\prod_{O \in \mathcal{O}} X_O \mathbf{1}_{\{\mathcal{E}\}}\right] \le (1+o(1))\,\mathbb{E}_{\mathcal{Q}}\left[\left(\frac{1}{p}\right)^{2e(H_k)} \mathbf{1}_{\{H_k \text{ is admissible}\}}\right]$$

$$= (1+o(1)) \sum_{H \in \mathcal{H}_k} s^{2e(H)} \quad \text{(generating function)}$$

$\mathcal{H}_k$: The set of all admissible H_k

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$\mathcal{H}_k$: The set of all admissible H_k

Key remaining challenge: enumerate $\mathcal{H}_k$ using orbit structure

Analysis

- Proof of detection thresholds
- Proof of partial recovery thresholds
- Proof of exact recovery thresholds

Proof of partial recovery thresholds: Positive results

- Gaussian or dense Erdős-Rényi: analyzing MLE (QAP)

$$\widehat{\pi}_{\mathrm{ML}} \in \arg\max_{\pi \in \mathcal{S}_n} \sum_{i<j} A_{ij} B_{\pi(i)\pi(j)}$$

- Sparse Erdős-Rényi: Analyze densest subgraph in intersection graph $A^{\pi} \wedge B$

Proof of negative results: Gaussian model

1. Characterization of mutual info by truncated 2nd moment method:

$$I(\pi^*; A, B) = \binom{n}{2} I(\rho) - \mathsf{KL}(\mathcal{P} \| \mathcal{Q}) \approx \binom{n}{2} I(\rho)$$

where $I(\rho) = \frac{1}{2} \log \frac{1}{1-\rho^2}$ is the mutual info between two ρ-correlated standard Gaussians

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2. An area theorem based on I-MMSE formula [Guo-Shamai-Verdú '05]

$$I(\pi^*; A, B) = \frac{1}{2} \int_0^{\rho^2} \frac{\mathsf{mmse}_\theta(A^{\pi^*} | A, B)}{(1-\theta)^2} d\theta$$

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3. Impossibility of estimating A^{π^*} in squared error
$\Longrightarrow$ Impossibility of estimating π^* in overlap

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2. An "approximate" area theorem: Find an interpolating model P_θ such that $P_0 = Q$ and $P_1 = P$, and

$$I(\pi^*; A, B) \approx \binom{n}{2} I(p, s) - s \int_0^1 \theta \cdot \mathsf{mmse}_\theta(A^{\pi^*} | A, B) \mathrm{d}\theta$$

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Analysis

- Proof of detection thresholds
- Proof of partial recovery thresholds
- Proof of exact recovery thresholds

Proof of exact recovery thresholds: Positive results

- Decompose the likelihood difference via edge orbits

$$\left\langle A^{\pi} - A^{\pi^*}, B \right\rangle = \sum_{O \in \mathcal{O} \setminus \mathcal{O}_1} \underbrace{\sum_{(i,j) \in O} A_{\pi(i)\pi(j)} B_{ij}}_{X_O} - \sum_{O \in \mathcal{O} \setminus \mathcal{O}_1} \underbrace{\sum_{(i,j) \in O} A_{\pi^*(i)\pi^*(j)} B_{ij}}_{Y_O}$$

- Apply large deviation analysis:
  - For π far away from π^*: bound $\sum_O X_O$ and $\sum_O Y_O$ separately
  - For π close to π^*: bound $\sum_O (X_O - Y_O)$ directly
- The contribution of longer edge orbits can be effectively bounded by that of the 2-edge orbits

$$M_{|O|} \triangleq \mathbb{E}\left[\exp(tX_O)\right] \le M_2^{|O|/2}, \quad \forall |O| \ge 2$$

Proof of exact recovery thresholds: Negative results

- Suffices to show the failure of MLE
- The bottleneck happens when π' differs from π by a 2-node orbit (i,j), for which the likelihood difference simplifies to

$$\left\langle A^{\pi} - A^{\pi^*}, B \right\rangle = -\sum_{k \in [n]\setminus\{i,j\}} \left(A_{\pi^*(i)\pi^*(k)} - A_{\pi^*(j)\pi^*(k)} \right) \left(B_{ik} - B_{jk} \right)$$

- Prove the existence of (i,j) for which $\langle A^{\pi} - A^{\pi^*}, B \rangle \geq 0$ whp

Concluding remarks

		Partial recovery & detection	Almost exact recovery	Exact recovery
p	$n^{-o(1)}$	$nps^2 = \frac{2\log n}{\log(1/p)-1+p}$		$\frac{nps^2}{(1-\sqrt{p})^2\log n} = 1$
	$n^{-\alpha}$	$nps^2 = \lambda^*$	$nps^2 = \omega(1)$	
Gaussian		$\frac{n\rho^2}{\log n} = 4$		

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