Testing network correlation efficiently via counting trees

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Joint work with
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Graph isomorphism

Given two graphs A and B, decide whether $A \cong B$, i.e., there exists a bijection $\pi : V(A) \to V(B)$ such that

$$(u, v) \in E(A) \Leftrightarrow (\pi(u), \pi(v)) \in E(B)$$

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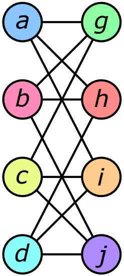
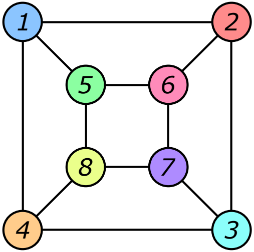
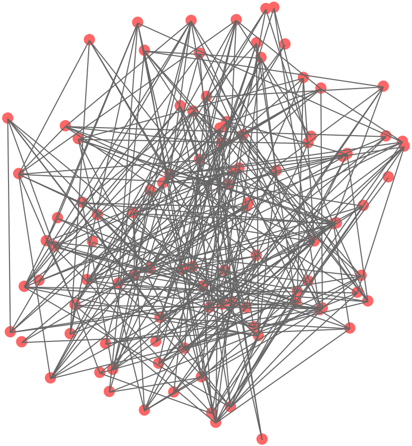
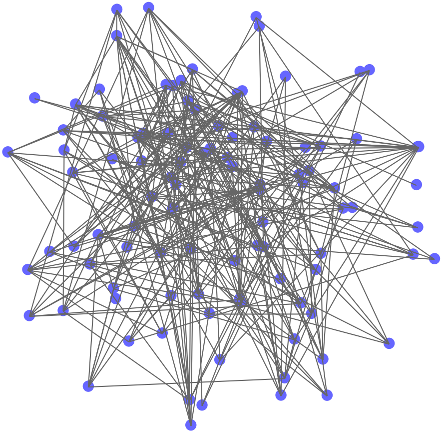




- Not known to be solvable in polynomial time in worst case

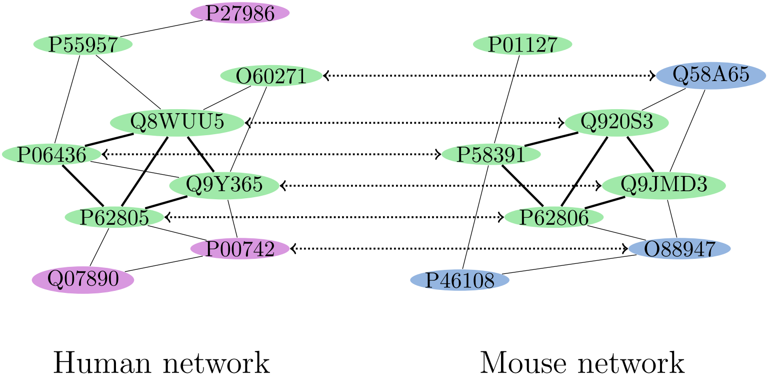
Two key challenges





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

Motivation: Protein-protein interaction network

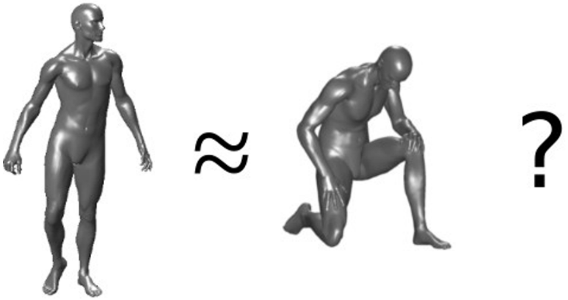


[Kazemi-Hassani-Grossglauser-Modarres '16]

Ontology: Assess the correlation of two biological networks in two different species based on network topology

Motivation: Deformable shape matching

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



Shape REtrieval Contest (SHREC) dataset

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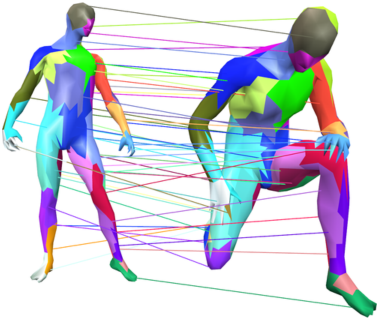


Shape REtrieval Contest (SHREC) dataset

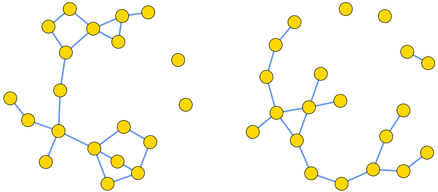
3-D shapes $\rightarrow$ geometric graphs (features $\rightarrow$ nodes, distances $\rightarrow$ edges)
Determine whether two graphs are similar in topologies

Beyond worst-case: noisy graph isomorphism test

Definition

$\mathbb{H}_0$: A and B are independent Erdős-Rényi graphs $\mathcal{G}(n, q)$

$\mathbb{H}_1$: A and $B^\pi = (B_{\pi(i)\pi(j)})$ are correlated $\mathcal{G}(n, q)$ with correlation parameter ρ, conditional on a uniform permutation π



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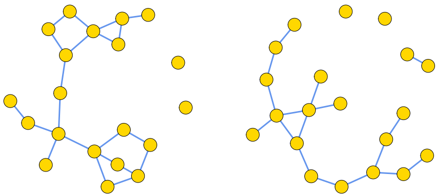

- Hypothesis testing aspect of graph matching (recover π under $\mathbb{H}_1$)
- The inherent edge correlation is obscured by latent node mapping π
- The test needs to rely on graph invariants (e.g. # of edges or triangles)

Key questions

Goal: Design a test statistic $f(A, B)$ with threshold $\tau \in \mathbb{R}$ to achieve consistent detection:

$$\lim_{n\to\infty} \left[\mathbb{P}_{\mathbb{H}_1}\left(f(A,B) < \tau\right) + \mathbb{P}_{\mathbb{H}_0}\left(f(A,B) \geq \tau\right)\right] = 0$$

Two key questions

- What is the statistical detection limit?
- Can we attain the limit in polynomial-time?

Statistical detection limit

Consider an equivalent model: under $\mathbb{H}_1$, A and B are independently subsampled from a common parent graph $\mathcal{G}(n, p)$ with probability s: $q = ps$ and $\rho = \frac{s(1-p)}{1-ps}$

Theorem (Wu-X.-Yu '20)

Consistent detection is possible if and only if

$$s^2 \geq \begin{cases} \frac{2 \log n}{np\left(\log \frac{1}{p} - 1 + p\right)} & \text{if } p = n^{-o(1)} \text{ (dense)} \\ \Theta\left(\frac{1}{np}\right) & \text{if } p = n^{-\Omega(1)} \text{ (sparse)} \end{cases}$$

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- [Ding-Hu' 22] determined the sharp constant in the sparse graph case
- Achieved by computationally intractable statistic:

$$\mathsf{MCS}(A,B) \triangleq \max_{\pi\in\mathcal{S}_n} \sum_{i<j} A_{ij}B_{\pi(i)\pi(j)} \quad \text{(max common subgraph)}$$

- Question: How to test efficiently?

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- Question: How to test efficiently? subgraph count

Testing via subgraph counts

Let $X_H(G)$ denote the number of copies of H in G

- Under $\mathbb{H}_0$: $X_H(A)$ and $X_H(B)$ are independent
- Under $\mathbb{H}_1$: $X_H(A)$ and $X_H(B)$ are correlated

Implication: Test based on the correlation between $X_H(A)$ and $X_H(B)$

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First attempt: H is a single edge [Wu-X.-Yu '20]

$$\frac{X_H(A) - X_H(B)}{\sqrt{n(n-1)q(1-q)}} \approx \begin{cases} \mathcal{N}(0,1) & \text{Under } \mathbb{H}_0 \\ \mathcal{N}(0,1-\rho) & \text{Under } \mathbb{H}_1 \end{cases}$$

$\Rightarrow$ consistent detection demands $\rho \to 1$

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Lesson: need to count more "distinguishing" subgraph

Counting a flock of black swans

Counting a family $\mathcal{H}$ of rare subgraphs [Barak-Chou-Lei-Schramm-Sheng'19]

- H is rare: $\mathbb{E}\left[X_H(A)\right] = O(1) \Rightarrow$ unlikely to co-occur under $\mathbb{H}_0$
- $\mathcal{H}$ needs to be "rich" to ensure co-occurrence under $\mathbb{H}_1$
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Construction of $\mathcal{H}$ based on random d-regular graphs of size $K = \rho^{-C}$
$\Rightarrow$ correctly tell $\mathbb{H}_0$ vs. $\mathbb{H}_1$ w.p. 0.9 in time n^K, if

$$\rho = \Omega(1) \quad \text{and} \quad nq \in \left[n^{\epsilon}, n^{1/153}\right] \cup \left[n^{2/3}, n^{1-\epsilon}\right]$$

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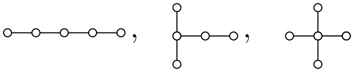
Limitations:

- nq needs to fall into specific range and does not cover sparse graphs
- The test error is not vanishing
- The runtime grows polynomially at rate of $\rho^{-C} \Rightarrow$ too expensive for large networks

Our idea: counting large trees

Our strategy: count a family $\mathcal{T}$ of trees of K edges with K growing in n

e.g. $K = 4, \quad \mathcal{T} = \Big\{$  $\Big\}$

- $\#$ of vertices $= \#$ of edges $+1 \Rightarrow$ abundant even in sparse graphs
- $\mathcal{T}$ is "rich": $|\mathcal{T}|$ grows exponentially in K
- Tree structure allows for efficient counting even when K grows in n

An obstacle: subgraph counts for different trees are still too correlated, especially when $nq \geq 1$

Our solution: counting signed trees

Counting signed trees

- Centered adjacency matrices: $\overline{A} = A - \mathbb{E}[A]$ and $\overline{B} = B - \mathbb{E}[B]$

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$$f_{\mathcal{T}}(A, B) \triangleq \sum_{H \in \mathcal{T}} \mathsf{aut}(H) W_H(\overline{A}) W_H(\overline{B}),$$

where $\mathsf{aut}(H)$ is the number of automorphism of H, and

$$W_H(M) \triangleq \sum_{S \cong H} \prod_{(i,j) \in S} M_{ij} \quad \text{(signed subgraph count)}$$

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- Crucial orthogonal property:

$$\mathbb{E}\left[W_H(\overline{A}) W_{H'}(\overline{A})\right] = 0 \Longleftrightarrow H \ncong H'$$

Statistical guarantee

Theorem (Mao-Wu-X.-Yu '21)

Suppose

$$nq \geq n^{-o(1)}, \quad \rho^2 > \alpha, \quad \omega(1) \leq K = O\left(\frac{\log n}{\log \log n}\right).$$

Then the testing error satisfies

$$\mathbb{P}_{\mathbb{H}_1}\left(f_{\mathcal{T}}(A,B) \leq \tau\right) + \mathbb{P}_{\mathbb{H}_0}\left(f_{\mathcal{T}}(A,B) \geq \tau\right) = o(1),$$

where $\tau = C\mathbb{E}_{\mathbb{H}_1}\left[f_{\mathcal{T}}(A,B)\right]$ *for any fixed constant* $0 < C < 1$.

- $\alpha \approx 0.33833$ is Otter's constant given by $|\mathcal{T}| \approx (1/\alpha)^K$
- $nq \geq n^{-o(1)}$ applies to very sparse regime and is necessary for existence of trees with $K = \omega(1)$ edges

Proof sketch: mean and variance calculations

$$f_{\mathcal{T}}(A,B) \triangleq \sum_{H \in \mathcal{T}} \mathsf{aut}(H) W_H(\overline{A}) W_H(\overline{B}), \; W_H(M) \triangleq \sum_{S \cong H} \prod_{(i,j) \in S} M_{ij}$$

- $\mathbb{E}_{\mathbb{H}_0}[f_{\mathcal{T}}(A,B)] = 0$ and by the orthogonal property,

$$\text{(SNR)} \quad \frac{(\mathbb{E}_{\mathbb{H}_1}[f_{\mathcal{T}}(A,B)])^2}{\mathrm{Var}_{\mathbb{H}_0}[f_{\mathcal{T}}(A,B)]} = \rho^{2K} |\mathcal{T}| \approx \left(\frac{\rho^2}{\alpha} \right)^K$$

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- To drive the SNR to ∞, need $\rho^2 > \alpha \approx 0.33833$
- Further show

$$\frac{(\mathbb{E}_{\mathbb{H}_1}[f_{\mathcal{T}}(A,B)])^2}{\mathrm{Var}_{\mathbb{H}_1}[f_{\mathcal{T}}(A,B)]} \to \infty$$

  Needs delicate analysis of correlations between subgraph counts

Computational guarantees

Efficient tree counts via color coding

How to compute $W_H(M) \triangleq \sum_{S \cong H} \prod_{(i,j) \in S} M_{ij}$ efficiently?

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- Exhaustive search takes n^K time: super poly-time when $K \to \infty$
- Our solution: color coding [Alon-Yuster-Zwick '95]
  1. Assign random color μ to each vertex from color set $[K+1]$ uniformly
  2. Define *colorful* subgraph count

$$Y_H(M,\mu) \triangleq \sum_{S \cong H} \mathbf{1}_{\{S \text{ has } K+1 \text{ distinct colors}\}} \prod_{(i,j)\in S} M_{ij}$$

     Key implication: $\mathbb{E}_\mu \left[Y_H(M,\mu) \right] = r W_H(M)$, where $r = \frac{(K+1)!}{(K+1)^{K+1}}$

  3. Generate $1/r$ independent random colorings μ_t so that

$$W_H(M) \approx \sum_{t=1}^{1/r} Y_H(M,\mu_t) \triangleq \widehat{W}_H(M)$$

$Y_H(M,\mu)$ can be computed via dynamic programming in $n^2 e^{O(K)}$

Computational guarantees

Define an approximate statistic:

$$\widetilde{f}_{\mathcal{T}} \triangleq \sum_{H \in \mathcal{T}} \mathsf{aut}(H) \widehat{W}_H(\overline{A}) \widehat{W}_H(\overline{B})$$

Theorem (Mao-Wu-X.-Yu '21)

Under both $\mathbb{H}_0$ and $\mathbb{H}_1$,

$$\frac{\widetilde{f}_{\mathcal{T}} - f_{\mathcal{T}}}{\mathbb{E}_{\mathbb{H}_1}[f_{\mathcal{T}}]} \xrightarrow{L_2} 0.$$

Moreover, $\widetilde{f}_{\mathcal{T}}$ can be computed in time $n^{2+o(1)}$.

Implication: $\widetilde{f}_{\mathcal{T}}$ satisfies the same statistical guarantee as $f_{\mathcal{T}}$

Statistical-computational gap

Statistical-computational gap

- Statistical limit: $\rho \approx \frac{1}{nq}$
- Tree counting limit: $\rho^2 > \alpha \approx 0.33833$
- There is a large computational gap, especially when the graphs are dense

Key question: Can we close the computational gap?

Statistical-computational gap

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Key question: Can we close the computational gap?

No, based on the low-degree hardness conjecture [Hopkins '18, Kunisky-Wein-Bandeira '19]: computationally hard when $\rho \leq \frac{1}{\text{polylog}(n)}$

Signed tree counting as a low-degree projection

- Space of functions on the hypercube $\{0,1\}^{2\binom{n}{2}}$ endowed with

$$\langle f, g \rangle \triangleq \mathbb{E}_{\mathbb{H}_0}\left[f(A,B)g(A,B)\right]$$

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- Orthonormal polynomial basis [O'Donnell '4]

$$\phi_{\mathsf{S}}(A,B) \triangleq \sigma^{-|S_1|-|S_2|} \prod_{(i,j)\in S_1} \overline{A}_{ij} \prod_{(k,\ell)\in S_2} \overline{B}_{k\ell}, \quad \mathsf{S} \triangleq (S_1, S_2)$$

where $\sigma^2 = q(1-q)$

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- Low-degree projection of likelihood ratio $L(A,B) = \frac{\mathbb{P}_{\mathbb{H}_1}(A,B)}{\mathbb{P}_{\mathbb{H}_0}(A,B)}$

$$f_{\mathcal{H}}(A,B) \triangleq \sum_{H\in\mathcal{H}} \sum_{S_1: S_1\cong H} \sum_{S_2: S_2\cong H} \langle L, \phi_{\mathsf{S}}\rangle \, \phi_{\mathsf{S}}$$

for given collection $\mathcal{H}$ of unlabeled graphs

Low-degree hardness

- "Optimal" degree-$2K$ polynomial of (A, B):

$$f^* = \underset{f:\ \text{degree}(f) \le 2K}{\arg\max} \frac{\left(\mathbb{E}_{\mathbb{H}_1}\left[f\right]\right)^2}{\mathbb{E}_{\mathbb{H}_0}\left[f^2\right]}$$

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where $\mathcal{H}^*$ consists of all unlabeled graphs induced by K edges

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- $$\frac{(\mathbb{E}_{\mathbb{H}_1}[f])^2}{\mathbb{E}_{\mathbb{H}_0}[f^2]} = \sum_{H \in \mathcal{H}^*} \rho^{2|E(H)|} \le \sum_{k=1}^{K} (4ek)^k \rho^{2k} = O(1)$$

provided that $\rho^2 \lesssim \frac{1}{K}$

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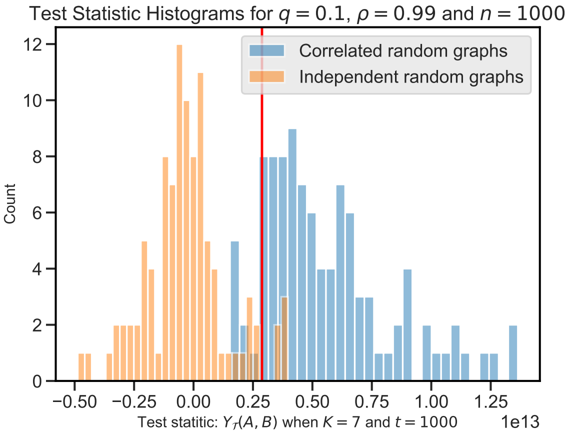
- Low-degree hardness conjecture [Hopkins '18, Kunisky-Wein-Bandeira '19]: All degree-$\log n$ polynomials fail when $\rho \le \frac{1}{\text{polylog}(n)}$

Simulation study

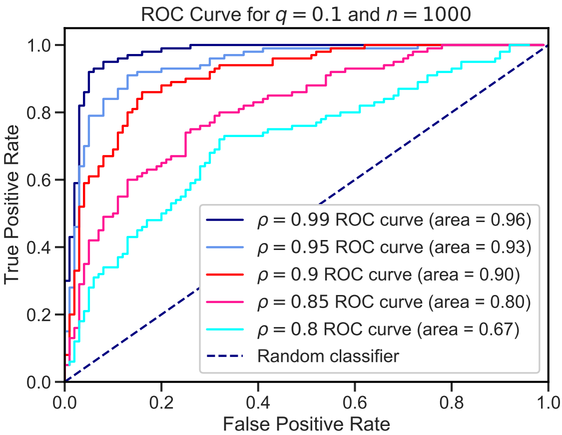
Simulation results

$n = 1000,\ K = 7,\ \rho = 0.99$



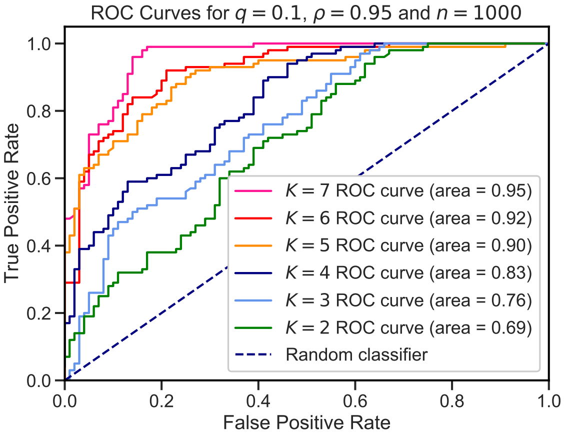
Type-I and type-II error are around 5% and 9%

$n = 1000$ and $K = 6$



Consistent with theoretical prediction: need $\rho \gtrsim |T|^{-\frac{1}{2K}} \approx 0.82$ for SNR exceeding 1, as $|\mathcal{T}| = 11$ when $K = 6$.

$n = 1000,\ q = 0.1,\ \rho = 0.95$



Performance of tree counting statistic improves as tree size K increases

Concluding remarks

- Efficient test via counting signed trees up to Otter's constant
- Low-degree hardness conjecture: no efficient test when $\rho \leq \frac{1}{\mathrm{polylog}(n)}$

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