Optimizing the overlap of two independent Erdős-Rényi graphs

Shuyang Gong

School of Mathematical Sciences, Peking University

Janurary, 2024

Joint work with Jian Ding (PKU), Hang Du (MIT) and Rundong Huang (PKU)

Motivations I: random graph matching

- Random Graph Matching is an extensively studied topic in recent years, which lies in the intersection of probability, statistics and theoretical computer science.
- Goal: find a bijection between two vertex sets which maximizes the number of common edges (i.e. minimize the adjacency disagreements)





• Given symmetric $n \times n$ matrices A and B, solve Quadratic Assignment Problem(QAP):

$$\max_{\pi\in\mathsf{S}_n}\sum_{i< j}A_{i,j}B_{\pi(i),\pi(j)}.$$

• Introduced by [Koopmans-Beckmann Econometrica'57] .

COWLES FOUNDATION DISCUSSION PAPER, NO. 4*

Assignment Problems and the Location of Economic Activities**

Ъy

Tjalling C. Koopmans and Martin Beckmann



Optimizing overlap of random graphs

Application 1: protein-to-protein interaction



Figure: Protein-protein interaction

Graph matching for aligning protein-to-protein interaction networks between two 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 under go different deformations



3D shapes \rightarrow geometric graphs (features \rightarrow nodes, distances \rightarrow edges)

- Statistical: two graphs are usually not isomorphic.
- Computational: *n*! bijections. $(100! \approx 10^{158})$
- NP-hard in the worst case: QAP is hard to approximate within exp(polylog(n)) mutiplicative factor.
 [Makarychev-Manokaran-Sviridenko '15]
- Efficient algorithms for average-case analysis are expected.
- Efforts from community on average-case of random graph matching: [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, Ding-Du'22a,22b, Ding-Du-G'22, Ding-Li'22,23, Du-G-Huang'23, Ding-Du-Li'23...]
- It is fair to say that there is still a long way to go to understand the real networks. But it is the first step forward...

Motivation II: random optimization problem

- **Random optimization problem** refers to solving optimization problems where the instance is randomly sampled.
- The problems arise from various fields including computer science, statistical physics, operations research. (e.g. finding maximal independent set in a random graph [Rahman-Virág'17,Wein'22] / finding the groundstate energy of Hamiltonian in spin glass models [Huang-Sellke'22]...)
- Key challenge: non-convexity and high-dimensionality. (case by case analysis)
- Central Question: efficient algorithm exists? information-computation gap?
- Efforts from the community on random optimization problems: [Ding-Du-G'22, Du-G-Huang'23, Gamarnik'21, Garmarnik-Moore-Zdeborová'22, Garmarnik-Kızıldãg-Perkins-Xu'23, Gamarnik-Sudan'14, Garmarnik-Zadik'19, Huang-Sellke'22, Montanari'19, Rahman-Virág'17, Subag'21, Wein'22...]

Mathematical model

- Erdős-Rényi graph G(n, p): Each edge in K_n is preserved with probability p independently.
- Sample two independent Erdős-Rényi graphs $G_1(n, p)$ and $G_2(n, p)$.
- Core quantity $O(\pi)$: the number of common edges of these two graphs under π . Formally,

$$\mathsf{O}(\pi) := \sum_{i < j} \mathsf{G}^{(1)}_{i,j} \mathsf{G}^{(2)}_{\pi(i),\pi(j)} \, ,$$

where $G^{(i)}$ are adjacency matrices.

e.g. $\pi(1) = 1, \pi(2) = 8, \pi(3) = 2, \pi(4) = 7, \pi(5) = 3, \pi(6) = 5, \pi(7) = 4, \pi(8) = 6 \Rightarrow$ we have $O(\pi) = 5$



Our problem

- Q1: what is the typical value of $\max_{\pi \in S_n} O(\pi)$?
- A first moment computation on max_{π∈Sn} O(π) yields an upper bound, e.g. take p = n^{-3/4}, let γ(n) := (1 + ε)2n,

$$\begin{split} \mathbb{P}\left[\max_{\pi\in\mathsf{S}_{n}}\mathsf{O}(\pi) > 2(1+\varepsilon)n\right] &\leq \sum_{\pi\in\mathsf{S}_{n}}\mathbb{P}\left[\mathsf{O}(\pi) \geq 2(1+\varepsilon)n\right] \\ &= n!\mathbb{P}\left[\mathsf{B}\left(\binom{n}{2}, p^{2}\right) > 2(1+\varepsilon)n\right] \\ &\leq n!\exp\left(-2(1+\varepsilon)n\log\left(\frac{2(1+\varepsilon)n}{\binom{n}{2}n^{-3/2}}\right) + 2(1+\varepsilon)n - \binom{n}{2}n^{-3/2}\right) \\ &= n!\exp(-(1+\varepsilon+o(1))n\log n) = o(1)\,. \end{split}$$

• The calculation for other *p* is similar.

• For other p (divide into sparse/dense by $\sqrt{\log n/n}$),

regime	$\max_{\pi\inS_n}O(\pi)$
sparse: $\frac{\log n}{n} \ll p \ll \sqrt{\frac{\log n}{n}}$	$n \cdot rac{\log n}{\log(\log n/np^2)}$
dense: $\sqrt{\frac{\log n}{n}} \ll p \le \frac{1}{(\log n)^4}$	$\binom{n}{2}p^2 + \sqrt{n^3p^2\log n}$

- First moment computation \Rightarrow Upper bound w.h.p.
- Right asymptotics?—True.
- Q2: Find a polynomial time algorithm for arg max_π O(π)? (sparse: yes, dense: no)
- Information-Computation gap? (sparse: no, dense: yes)

Sparse regime

Theorem (Ding-Du-G. 22)

For $p = n^{-\alpha + o(1)}$, $1/2 < \alpha \le 1$, there exists a polynomial-time algorithm s.t.

$$\mathbb{P}\left[\mathsf{O}(\pi^*) \geq \frac{1-\epsilon}{2\alpha-1}n\right] = 1 - o(1).$$

Theorem (Du-G.-Huang 23)

For $p = n^{-1/2+o(1)}$ and $p \ll \sqrt{\log n/n}$, for any $\varepsilon > 0$, there exists an $O(n^3)$ -time algorithm such that

$$\mathbb{P}\left[\mathsf{O}(\pi^*) \geq rac{(1-arepsilon)n\log n}{\log\left(\log n/np^2
ight)}
ight] = 1 - o(1)\,.$$

- $n/(2\alpha 1) = (1 + o(1))n \log n / \log (\log n / np^2)$ for $p = n^{-\alpha}$.
- The constructive lower bound matches the $\gamma(n)$ derived in the first moment computation.
- No information-computation gap in the sparse regime.

Shuyang Gong (PKU)

Algorithm

The greedy algorithm in [Ding-Du-G'22], let $\alpha = 3/4 - \delta$, $\frac{1}{2\alpha - 1}n \approx 2n$

- Match the first εn vertices arbitrarily.
- In step k + 1, select unmatched u_k in G_1 . Neighbor of u_k in matched part N_k
- Map N_k by π^*
- For each such pair (s_k, t_k) , check if there exists unmatched v_k in G_2
- If succeed, let $\pi^*(u_k) = v_k$.
- For other α , match a carefully designed tree in each step.



The idea: why the algorithm works?

- Consider the case $\alpha = 3/4 \delta$. Assume independence among the iterative steps.
- $N_k \sim \mathbf{B}(n, p)$.
- Conditioned on N_k . For each v_k in G₂, the number of edges s.t. $v_k \rightarrow \pi^*(N_k)$ obeys $\mathbf{B}(|N_k|, p)$.
- By Poisson approximation,

$$\mathbb{P}[\mathbf{B}(|N_k|,p)\geq 2]=\theta((np^2)^2)=\theta(n^2p^4).$$

- All v_k fail with probability $(1 n^2 p^4)^n \sim \exp(-n^3 p^4) \rightarrow 0$.
- It suffices to tackle the **dependence**.

Key technical input: dealing with correlations

• Consider the (slightly more complicated) case $\alpha = 7/8 - \delta$, $1/(2\alpha - 1) = 4/3$.



To show

$$\mathbb{P}[\boldsymbol{L} \sim \boldsymbol{Q} \,|\, \mathcal{A}_1, \mathcal{A}_2] = (1 + o(1))\mathbb{P}[\boldsymbol{L} \sim \boldsymbol{Q}]\,.$$

• A_1 and A_2 is the set of "failure" and "successful" trees.

LHS equals to

$$\frac{\mathbb{P}[\boldsymbol{L} \sim \boldsymbol{Q}, \mathcal{A}_1 \,|\, \mathcal{A}_2]}{\mathbb{P}[\mathcal{A}_1 \,|\, \mathcal{A}_2]} = \frac{\widehat{\mathbb{P}}[\mathcal{A}_1 \,|\, \boldsymbol{L} \sim \boldsymbol{Q}]}{\widehat{\mathbb{P}}[\mathcal{A}_1]} \mathbb{P}[\boldsymbol{L} \sim \boldsymbol{Q}] \,.$$

- Equivalently, to show the first factor is 1 o(1).
- It means that if we open the edges in L ~ Q, at least one of the "failure" trees emerges.

Key technical input: counting intersection patterns

• The possible intersection patterns:



the blue tree represents $L \sim Q$, the red one is from A_1 .

• (Union bound) count the total number of such intersections:

number of leaves \times number of non-leaves = o(1).

Jan. 2024

Theorem (Du-G.-Huang 23, informational result)

For p in the dense regime, we have

$$\frac{\max_{\pi\in\mathsf{S}_n}\mathsf{O}(\pi)-\binom{n}{2}p^2}{\sqrt{n^3p^2\log n}}\stackrel{\text{prob.}}{\to}1\,.$$

• Second moment method: $X_{\varepsilon} := \sum_{\pi \in S_n} \mathbf{1}_{O(\pi) > \binom{n}{2} p^2 + \sqrt{(1-\varepsilon)n^3 p^2 \log n}}.$

$$\mathbb{P}\left[\max_{\pi\in\mathsf{S}_n}\mathsf{O}(\pi) > \binom{n}{2}\rho^2 + \sqrt{(1-\varepsilon)n^3\rho^2\log n}\right] \geq \frac{(\mathbb{E}X_{\varepsilon})^2}{\mathbb{E}X_{\varepsilon}^2} = \exp(-o(n\log n)).$$

- Idea: concentration of maximum.
- Talagrand's concentration inequality:

$$\mathbb{P}\left[\left|\max_{\pi\in S_n} O(\pi) - \mathbb{E}\max_{\pi\in S_n} O(\pi)\right| \geq \sqrt{\varepsilon n^3 p^2 \log n}\right] \leq \exp\left(-c(\varepsilon)n \log n\right) \,.$$

Theorem (Du-G.-Huang 23, computational result)

There exists an $O(n^3)$ -time algorithm $\mathcal A$ which outputs a π^* such that

$$\mathbb{P}\left[\frac{\mathsf{O}\left(\pi^*\right)-\binom{n}{2}p^2}{\sqrt{n^3p^2\log n}} \geq \sqrt{8/9} - \varepsilon\right] = 1 - o(1).$$

Theorem (Du-G.-Huang 23, hardness result)

For p in the dense regime, for all $\varepsilon > 0$, there exists a constant $c = c(\varepsilon) > 0$ such that for any online algorithm A,

$$\mathbb{P}\left[\frac{O\left(\mathcal{A}(\mathsf{G}_1,\mathsf{G}_2)\right)-\binom{n}{2}p^2}{\sqrt{n^3p^2\log n}}\geq\sqrt{8/9}+\varepsilon\right]=\exp(-c(\varepsilon)n\log n).$$

No online algorithm above $\sqrt{8/9}!$ — Hardness result.

• Main tool: Branching-OGP structure[Huang-Sellke'22].

Shuyang Gong (PKU)

The Branching OGP

- Define tree \mathbb{T} with leave set \mathbb{L} .
- Construct leave-indexed correlated instances $\{(G_1^{(u)}, G_2)\}_{u \in \mathbb{L}}$.
- Each ray represents an instance. $G_1^{(u)}$ and $G_1^{(v)}$ share $\rho_{|u \wedge v|}$ Bernoulli variables. $(\rho_1 < \rho_2 < \rho_3)$
- Impossible for all $O(\pi_i)$ above $\sqrt{8/9} + \varepsilon$.
- Run online algorithm on all instances. Prove by contradiction.



- How about $p = \theta(\sqrt{\log n/n})$?
- When $1/2 < \alpha < 1$, is there a polynomial-time algorithm with fixed power that finds (near) optimal matchings?
- For other graph model (with more general edge weights), determine the maximal overlap.

Take-home messages

- In sparse regime, no information computation gap.
- In dense regime, information computation gap emerges with a threshold $\sqrt{8/9}.$

Related papers:

- DDG22 Jian Ding, Hang Du and Shuyang Gong, A Polynomial-time Approximation Scheme for the Maximal Overlap Between Two Independent Erdős-Rényi Graphs. To appear in *Random Structures and Algorithms*.
- DGH23 Hang Du, Shuyang Gong and Rundong Huang, The Algorithmic Phase Transition of Random Graph Alignment Problem, *arXiv:2307.06590*.

[BCPP98] Rainer E Burkard, Eranda Cela, Panos M Pardalos, and Leonidas S Pitsoulis. The quadratic assignment problem. In handbook of combinatorial optimization, pages 1713-1809. *Springer*, 1998. [DDG22] Jian Ding, Hang Du and Shuyang Gong, A Polynomial-time Approximation Scheme for the Maximal Overlap Between Two Independent Erdős-Rényi Graphs. To appear in *Random Structures and Algorithms*.

[DGH23+]Hang Du, Shuyang Gong and Rundong Huang, The Algorithmic Phase Transition of Random Graph Alignment Problem, *arXiv:2307.06590*. [HS22] B. Huang and M. Sellke, "Tight Lipschitz Hardness for optimizing Mean Field Spin Glasses," *2022 IEEE 63rd Annual Symposium on Foundations of Computer Science (FOCS), Denver, CO, USA, 2022, pp. 312-322, doi: 10.1109/FOCS54457.2022.00037*.

[PRW94] Panos M. Pardalos, Franz Rendl, and Henry Wolkowicz. The quadratic assignment problem: A survey and recent developments.