# From tree matching to graph alignment 

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The graph isomorphism problem
Definition: Given two graphs $G=(V, E), G^{\prime}=\left(V^{\prime}, E^{\prime}\right)$, is there a graph isomorphism, i.e. a bijection $f: V \rightarrow V^{\prime}$ such that $(i, j) \in E \Leftrightarrow(f(i), f(j)) \in E^{\prime}$ ?

$\rightarrow$ Classical problem in NP, thought to be neither in P, nor NP-complete

## Graph alignment

Relaxed version: bijection $f$ between vertices $V$ of $G$ and $V^{\prime}$ of $G^{\prime}$ that preserves most edges


Formally, $f$ minimizes $\sum_{i, j \in V}\left|\mathbb{I}_{(i, j) \in E}-\mathbb{I}_{(f(i), f(j)) \in E^{\prime}}\right|$
$\rightarrow$ An instance of the NP-hard quadratic assignment problem: $\max _{\Pi} \operatorname{Trace}\left(A \Pi A^{\prime} \Pi^{\top}\right)$ where $\Pi$ runs over permutation matrices

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- Align meshes of 3D images of hearts to transfer segmentation into distinct parts from image of reference heart
- Align graphs between words in languages $A$ and $B$ to construct dictionary between the two languages


## Generative, probabilistic models of graphs

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$$
\begin{aligned}
& G_{2}^{\prime} \sim \mathcal{G}(n, p) \\
& \rightarrow \mathbb{P}\left((i, j) \in E_{1} \cap E_{2}^{\prime}\right)=p * s, \\
& \rightarrow \mathbb{P}\left((i, j) \in E_{1},(i, j) \notin E_{2}^{\prime}\right)=p(1-s)
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$\rightarrow \mathbb{P}\left((i, j) \in E_{1} \cap E_{2}^{\prime}\right)=p * s$,
$\rightarrow \mathbb{P}\left((i, j) \in E_{1},(i, j) \notin E_{2}^{\prime}\right)=p(1-s)$
- Shuffle labels of nodes of $G_{2}^{\prime}$ uniformly at random to form $G_{2}$

Formally: random permutation $\sigma$; Adjacency matrix $A_{2}=\Pi_{\sigma} A_{2}^{\prime} \Pi_{\sigma}^{\top}$

## Goal: recover permutation $\sigma$ from graphs $G_{1}$ and $G_{2}$

Exact recovery of permutation $\sigma$ :

- Information-theoretically feasible iff $n p s=\log n+\omega(1)$
[Cullina-Kyavash'16]
- Polynomial-time feasible if $n p \geq \log ^{\alpha}(n)$ and $1-s \leq \log ^{-\beta}(n)$ [Ding et al.'18]
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This work: polynomial-time recovery, in sparse regime $n p=O(1)$.
$\rightarrow$ We relax objective from exact recovery to partial recovery:

Construct permutation $\hat{\sigma}$ from $G_{1}, G_{2}$ such that $\operatorname{overlap}(\hat{\sigma}):=\frac{1}{n} \sum_{i=1}^{n} \mathbb{I}_{\sigma_{i}=\hat{\sigma}_{i}}=\Omega(1)$

## Main result

## Theorem

Let $p=\lambda / n$ for fixed $\lambda \in\left(1, \lambda_{0}\right]$. There exists $s^{*}(\lambda)<1$ such that for all $s \in\left(s^{*}(\lambda), 1\right]$, the Neighborhood Tree Matching Algorithm (NTMA) returns a permutation $\hat{\sigma}$ achieving positive overlap with high probability.


## Outline

- Tree matching weights
- NTMA algorithm
- Matching weights for pairs of random trees
- Proof outline and experiments


## Tree matching weights

## Definition

Given two rooted trees $\mathcal{T}, \mathcal{T}^{\prime}$ and integer $d \geq 0$, matching weight $\mathcal{W}_{d}\left(\mathcal{T}, \mathcal{T}^{\prime}\right)$ : largest number of leaves of all rooted sub-trees $\mathcal{T}^{\prime \prime}$ of both $\mathcal{T}$, $\mathcal{T}^{\prime}$ of depth $d$.


Example of two trees $\mathcal{T}, \mathcal{T}^{\prime}$ with $\mathcal{W}_{3}\left(\mathcal{T}, \mathcal{T}^{\prime}\right)=7$, where an optimal $t \in \mathcal{A}_{3}$ is drawn in red.

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Recursive computation: $\mathcal{W}_{d}\left(\mathcal{T}, \mathcal{T}^{\prime}\right)=\max \sum_{(i, u) \in m} \mathcal{W}_{d-1}\left(\mathcal{T}_{i}, \mathcal{T}_{u}^{\prime}\right)$
where max over matchings $m$ between neighbors $i$ of $\rho(\mathcal{T})$ and $u$ of $\rho\left(\mathcal{T}^{\prime}\right)$, and $\mathcal{T}_{i}$ : tree rooted at $i$ obtained from $\mathcal{T}$ by removing edge $(\rho(\mathcal{T}), i)_{\bar{\Xi}}$

## A first attempt

Match vertices $i$ of $G_{1}$ and $u$ of $G_{2}$ whose respective $d$-neighborhoods:

- are trees $\mathcal{T}_{1}, \mathcal{T}_{2}$
- with large matching weight $\mathcal{W}_{d}\left(\mathcal{T}_{1}, \mathcal{T}_{2}\right)$


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Problem: false positives caused by nearby nodes


## Neighborhood tree matching algorithm



Pair of nodes $(i, u) \in V_{1} \times V_{2}$ whose $d$-neighborhood in $G_{1}$, resp. $G_{2}$ is a tree:

- if $\exists j, j^{\prime} \stackrel{1}{\sim} i, v, v^{\prime} \stackrel{2}{\sim} u$ such that $\mathcal{W}_{d}\left(\mathcal{T}_{j \rightarrow i}, \mathcal{T}_{v \rightarrow u}\right), \mathcal{W}_{d}\left(\mathcal{T}_{j^{\prime} \rightarrow i}, \mathcal{T}_{v^{\prime} \rightarrow u}\right)>\tau$, add pair $(i, u)$ to set $\mathcal{S}$
- Then for $d=\Theta(\log n), \tau=\Theta\left((\lambda s)^{d}\right)$, with high probability:
$\frac{1}{n} \sum_{i \in V_{1}} \mathbb{I}_{(i, \sigma(i)) \in \mathcal{S}}=\Omega(1)$,
$\frac{1}{n} \sum_{i \in V_{1}} \mathbb{I}_{\exists u \neq \sigma(i):(i, u) \in \mathcal{S}}=o(1)$.


## Matching weights for independent random trees

$\mathcal{T}, \mathcal{T}^{\prime}$ : two independent Galton-Watson branching random trees, with offspring distribution Poisson $(\lambda)$.

Theorem
For $\lambda \in\left(1, \lambda_{0}\right]$ and $s \in\left(s^{*}(\lambda), 1\right]$, then there exists $\gamma<\lambda s$ such that $\mathcal{W}_{d}\left(\mathcal{T}, \mathcal{T}^{\prime}\right) \ll \gamma^{d}$ as $d \rightarrow \infty$.

Proof: Probabilistic bounds on $\mathcal{W}_{d}\left(\mathcal{T}, \mathcal{T}^{\prime}\right)$ established by induction on $d$.

Arguments for main result: local structure of graphs $G_{1}, G_{2}$

- Local neighborhood of $i \in V_{1}$ in $G_{1}$ : Poisson $(\lambda)$ Galton-Watson branching process.
- Local structure of union graph $G_{1} \cup G_{2}^{\prime}$ : three-type branching process
- Local structure of intersection graph $G_{1} \cap G_{2}^{\prime}$ : $\operatorname{Poisson}(\lambda s)$ Galton-Watson branching process.



## Arguments, continued

$\rightarrow$ For $u=\sigma(i), \mathcal{W}_{d}\left(\mathcal{T}_{i}, \mathcal{T}_{u}\right) \geq$ size at generation $d$ of Poisson $(\lambda s)$
Galton-Watson branching tree, hence $\approx(\lambda s)^{d}$
$\rightarrow$ For nodes $i, u$ "far apart" in union graph, $\mathcal{W}_{d}\left(\mathcal{T}_{i}, \mathcal{T}_{u}\right) \approx \mathcal{W}_{d}\left(\mathcal{T}, \mathcal{T}^{\prime}\right)$ for
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Several other cases need to be dealt with...



Mean score of NTMA-2 for $\lambda=2.1, d=5$ (25 iterations per value of $n$ ).


## Conclusions and outlook

- Graph alignment: important unsupervised learning problem with many applications
- NTMA: first method proven to succeed at partial alignment in relevant regime of sparse graphs
- To be done: boundaries of phases in $(\lambda, s)$ diagram, in particular IT-feasibility and poly-time feasibility of partial alignment (see [Hall-M'20]: partial alignment IT-feasible for $n q s=\Theta(1), 1-s=\Omega(1))$
- Extend NTMA for better scalability and handling of denser graphs (with more cycles)


