Combinatorial Optimization with Graph Neural Network: Chaining to Learn the Graph Alignment Problem

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Can GNN solve combinatorial optimization problems ?

Combinatorial Optimization and Reasoning with Graph Neural Networks

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GNNs 'solving' the maximum independent set problem

Cracking nuts with a sledgehammer: when modern graph neural networks do worse than classical greedy algorithms

Maria Chiara Angelini[1,2] Federico Ricci-Tersenghi[1,2,3]

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Despite careful attempts, Böther et al. (2022) were incapable of reproducing the results, even reporting that using random weights in the GNN yields similar results as the trained weights. Thus, at this moment this approach should be considered at best inconclusive (...)

from Cappart et al. (2023)


GAP

Graph Alignment Problem (GAP)

Given two $n \times n$ adjacency matrices A and B, the graph alignment problem is to minimize $\|A - PBP^T\|_F$ over all permutation matrices P and where $\|\cdot\|_F$ is the Frobenius norm :

$$\text{GAP} = \min_{\pi \in \mathcal{S}_n} \sum_{i,j} \left(A_{ij} - B_{\pi(i)\pi(j)}\right)^2,$$

where π is the permutation associated to the permutation matrix P. We denote by $\pi^{A \to B}$ a solution to the graph alignment problem.

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For unweighted graphs, the coefficients of the matrices A and B are in $\{0, 1\}$, hence $\pi^{A \to B}$ also solves :

$$\max_{\pi \in \mathcal{S}_n} \sum_{i,j} A_{ij} B_{\pi(i)\pi(j)},$$

which is finding a maximum common subgraph in G_A and G_B, known to be APX-hard.

Measure of performances

For an algorithm producing a candidate permutation π, we measure its performance through two quantities :

- the accuracy defined by

$$\mathbf{acc}(\pi, \pi^{A \to B}) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}(\pi(i) = \pi^{A \to B}(i)). \tag{1}$$

- the number of common edges defined by

$$\mathbf{nce}(\pi) = \frac{1}{2} \sum_{i,j} A_{ij} B_{\pi(i)\pi(j)} \leq \mathbf{nce}(\pi^{A \to B}). \tag{2}$$

Graph alignment is a hard problem

$$\mathrm{GAP} = \max_{\pi \in \mathcal{S}_n} \sum_{i,j} A_{\pi(i)\pi(j)} B_{ij}$$

- Take G_A a graph on n vertices and G_B a path (or a cycle) of length n.

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- Take G_A a graph on n vertices and G_B a union of two clique of sizes $n/2$.

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- Take G_A a graph on n vertices and G_B a union of two clique of sizes $n/2$. Then, GAP is the **minimum bisection problem** on G_A.
- Take $G_A = G_B$, then GAP is the **graph isomorphism problem** solvable in quasipolynomial time Babai (2016).

Synthetic datasets

Random pairs of graphs (G_A, G_B) such that the marginals are the same, i.e. the laws of G_A and G_B are identical but G_A and G_B are correlated. This correlation allows us to control the difficulty of the graph alignment problem. Then a random permutation $\pi^\star \in \mathcal{S}_n$ is applied on the nodes of G_B to get G'_B and the training is done on the generated triplets $(G_A, G'_B, \pi^\star)$.

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3 parameters :
the **number of nodes** n, the **average degree** d and the **noise level** p_{noise}.

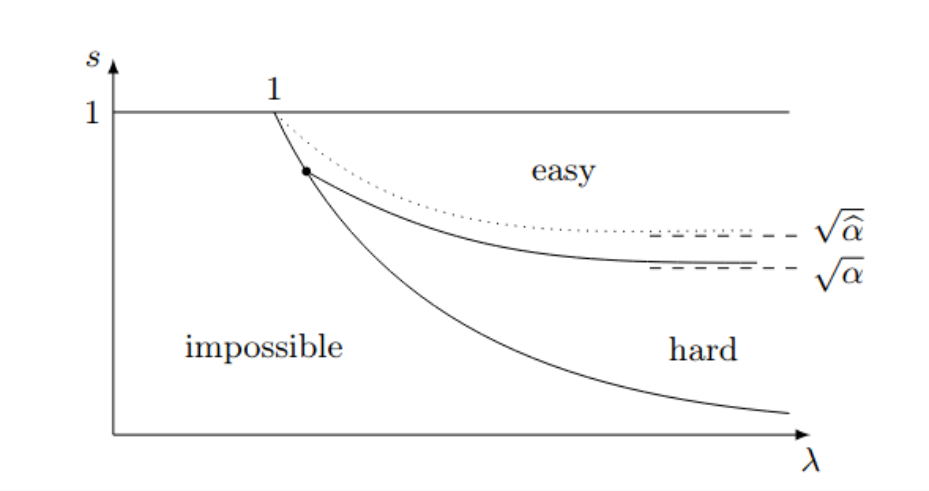
On average, G_A and G_B have $nd/2 = \mathbb{E}[\sum_{ij} A_{ij}/2]$ edges and the noise level p_{noise} controls the number of edges that are different between G_A and G_B so that the average number of common edges is
$(1 - p_{\text{noise}})nd/2 = \mathbb{E}[\sum_{ij} A_{ij}B_{ij}/2]$.


Tell me the truth...I'm...I'm ready to hear it.
You don't need machine learning for that.

Recovering the planted permutation (without learning)

Faster algorithms for the alignment of sparse correlated Erdős-Rényi random graphs

Andrea Muratori[1] and Guilhem Semerjian[2]



Otter's threshold : $\sqrt{\alpha} \approx 0.581$.

Ganassali et al. (2021b), Ganassali et al. (2021a), Piccioli et al. (2022), Ding et al. (2021), Mao et al. (2023), Muratori and Semerjian (2024)

Continuous relaxations of GAP (1)

Using basic properties of permutation matrices, we get :

$$\begin{aligned} \|A - PBP^T\|_F^2 &= \|(AP - PB)P^T\|_F^2 \\ &= \|AP - PB\|_F^2 \\ &= \|A\|_F^2 + \|B\|_F^2 - 2\langle AP, PB\rangle. \end{aligned}$$

where $\langle C, D\rangle = \text{trace}(C^T D)$ is the Frobenius inner product.

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Replacing the discrete set of permutations matrices $\mathcal{S}_n$ by the set of doubly stochastic matrices $\mathcal{D}_n$:

- **convex relaxation** :

$$\arg\min_{D \in \mathcal{D}_n} \|AD - DB\|_F^2 = D_{\text{CX}}$$

- **indefinite relaxation** (still NP-hard) :

$$\max_{D \in \mathcal{D}_n} \langle AD, DB\rangle.$$

Continuous relaxations of GAP (2)

- **convex relaxation** :

$$\arg \min_{D \in \mathcal{D}_n} \|AD - DB\|_F^2 = D_{\mathrm{CX}}$$

- **FAQ indefinite relaxation** :

$$\max_{D \in \mathcal{D}_n} \langle AD, DB \rangle .$$

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In both continuous relaxations, we use Frank-Wolfe algorithm and obtain a doubly stochastic matrix in $\mathcal{D}_n$ that needs to be projected to the nearest permutation matrix by solving a linear assignment problem (in $O(n^3)$ time) : for $D \in \mathcal{D}_n$, $\max_{P\in\mathcal{S}_n} \langle P, D\rangle$. We denote by $\mathbf{Proj}(D) \in \mathcal{S}_n$ the resulting projection of D on $\mathcal{S}_n$.

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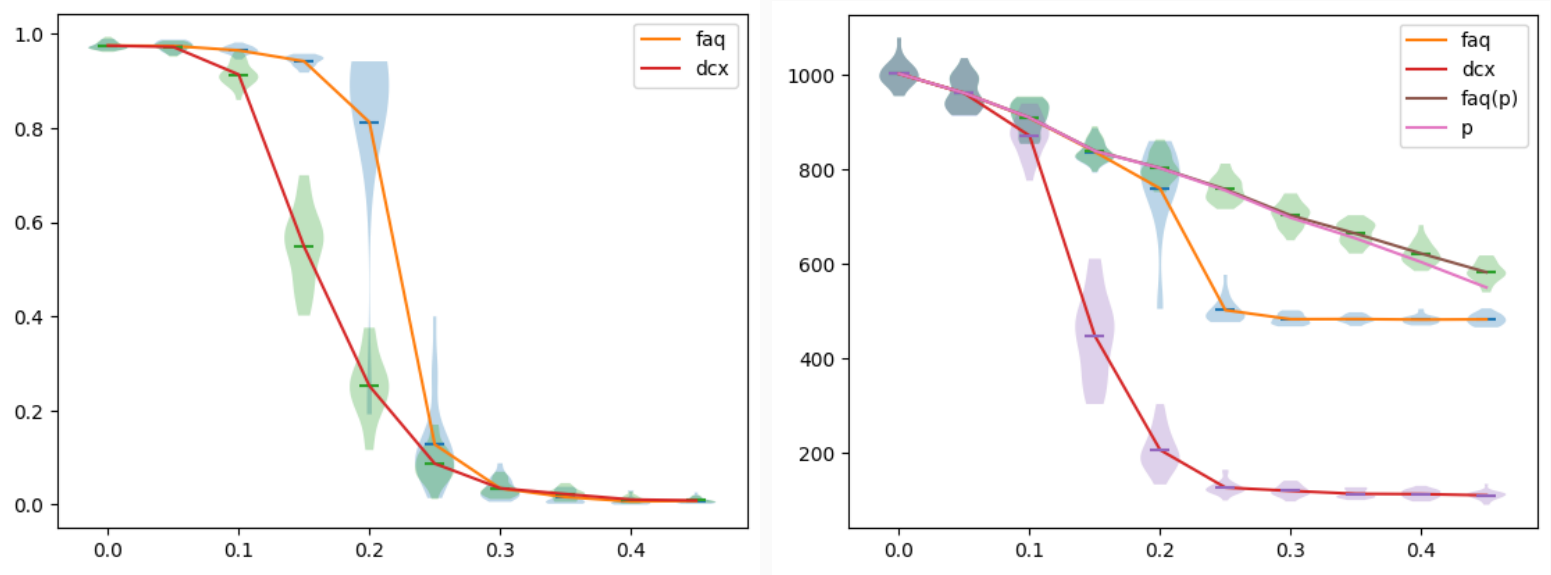
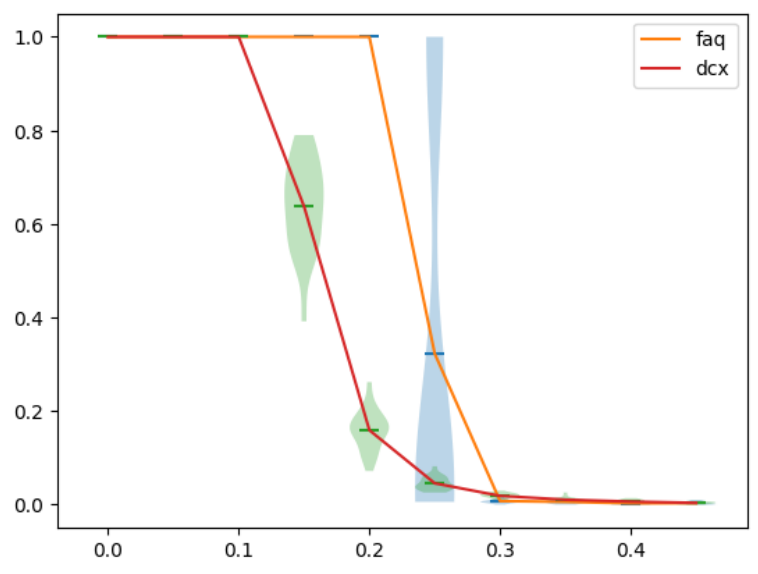
$\textbf{FAQ}(D) \in \mathcal{S}_n$ is the solution obtained with initial condition D and after projection on $\mathcal{S}_n$. There are cases where $\textbf{Proj}(D_{\text{CX}})$ is indeed very far from an optimal solution and $\textbf{FAQ}(D_{\text{CX}})$ gives a better approximation.

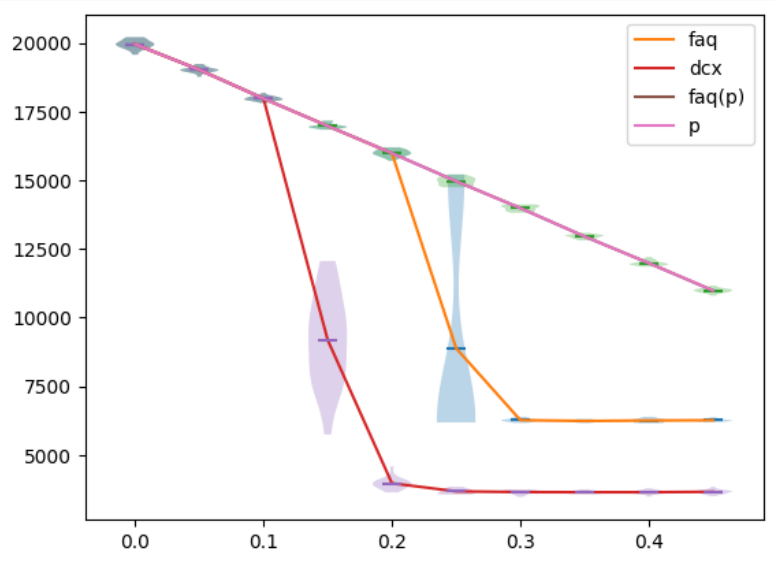
Erdős-Rényi ($n = 500, d = 4$)



Accuracy (left) and number of common edges (right) as a function of noise.

Erdős-Rényi ($n = 500, d = 80$)





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Machine Learning
THE FOOL...
SHEN COMIX

FAQ performs better than GNNs

Our SeedGNN achieves the following matching accuracy (%) on sparse ER graphs ($n = 500$, $p=0.01$, $s=0.8$):

Fraction of Seeds	**0%**	**2%**	**4%**	**6%**	**8%**	**10%**	**12%**	**14%**	**16%**	**18%**	**20%**
SeedGNN	0.3	15.1	47.4	82.8	96.0	96.6	97.0	97.6	97.6	97.6	97.6
1-hop ($T=6$)	0.2	1.5	2.89	4.91	6.0	9.2	12.5	15.3	19.7	23.6	32.3
2-hop ($T=3$)	0.2	2.4	18.0	57.9	81.1	92.1	95.8	96.4	96.4	96.7	97.0
3-hop ($T=2$)	0.3	2.4	7.1	29.7	64.9	90.8	96.0	97.1	97.2	97.4	97.5
PGM	0.2	2.3	6.1	16.3	31.6	54.5	73.3	79.2	86.3	88.9	92.7
SGM	0.3	3.6	8.9	13.8	22.3	36.3	54.5	67.3	84.4	89.6	91.6
MGCN	0.1	2.0	4.0	6.7	8.4	11.1	12.4	14.0	16.3	18.9	20.5

Our SeedGNN achieves the following matching accuracy (%) on dense ER graphs ($n = 500$, $p=0.2$, $s=0.8$):

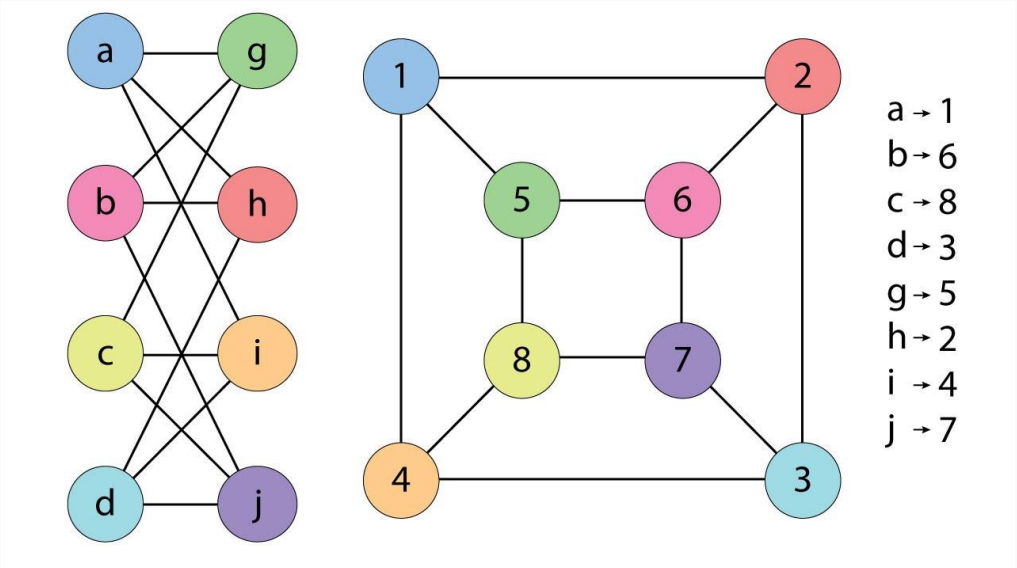
Fraction of Seeds	**0.0**	**0.5%**	**1%**	**1.5%**	**2%**	**2.5%**	**3%**	**3.5%**	**4%**	**4.5%**	**5%**
SeedGNN	0.1	0.7	91.4	100	100	100	100	100	100	100	100
1-hop ($T=6$)	0.1	0.7	2.3	7.4	95.0	100	100	100	100	100	100
2-hop ($T=3$)	0.0	0.7	2.2	5.6	46.6	100	100	100	100	100	100
3-hop ($T=2$)	0.1	0.2	0.38	0.6	0.4	0.54	0.9	1.3	1.2	1.4	2.1
PGM	0.1	0.6	1.8	4.3	19.3	51.2	96.6	100	100	100	100
SGM	0.2	1.5	85.8	100	100	100	100	100	100	100	100
MGCN	0.1	0.7	1.5	1.9	3.7	5.2	6.9	8.0	10.9	12.3	13.7

Yu et al. (2023)

Learning with graph symmetries

Graph isomorphism

$G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic if there is a bijection $V_1 \longrightarrow V_2$ which preserves edges.



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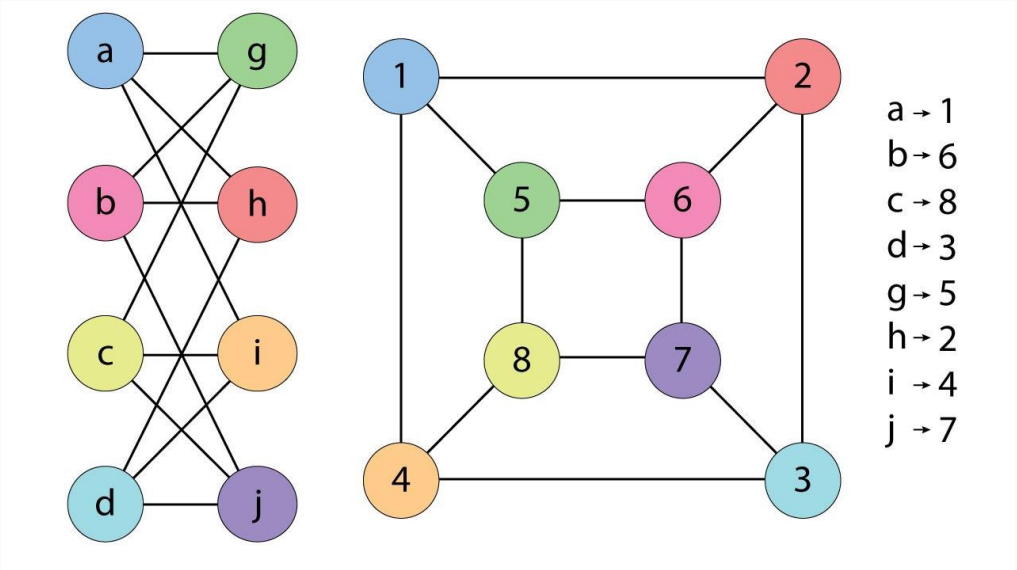

Idea : design a machine learning algorithm whose result does not depend on the representation of the input.

Invariant and equivariant functions

For a permutation $\sigma \in \mathcal{S}_n$, we define ($\mathbb{F} = \mathbb{R}^p$ feature space) :

- for $X \in \mathbb{F}^n$, $(\sigma \star X)_{\sigma(i)} = X_i$
- for $G \in \mathbb{F}^{n \times n}$, $(\sigma \star G)_{\sigma(i_1),\sigma(i_2)} = G_{i_1,i_2}$

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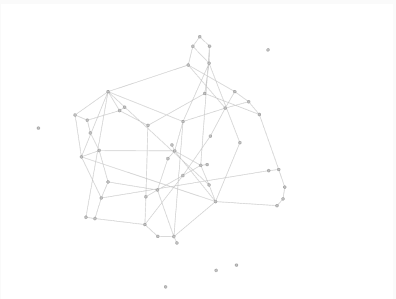
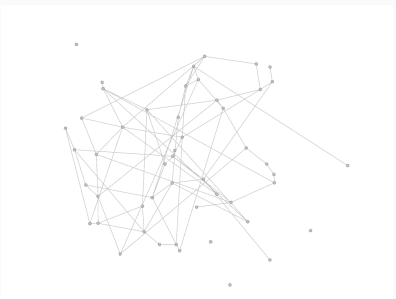
Definition
($k = 1$ or $k = 2$)

A function $f : \mathbb{F}^{n^k} \to \mathbb{F}$ is said to be invariant if $f(\sigma \star G) = f(G)$.

A function $f : \mathbb{F}^{n^k} \to \mathbb{F}^n$ is said to be equivariant if $f(\sigma \star G) = \sigma \star f(G)$.

Learning the graph alignment problem with Siamese GNNs





$$G_1 \in \{0,1\}^{n^2} \xrightarrow{\text{GNN}} E_1 \in \mathbb{R}^{n \times b}$$

$$G_2 \in \{0,1\}^{n^2} \xrightarrow{\text{GNN}} E_2 \in \mathbb{R}^{n \times b}$$

$$E_1 E_2^T \in \mathbb{R}^{n^2}$$

- The same GNN is used for both graphs.
- From the node similarity matrix $E_1 E_2^T$, we extract a mapping from nodes of G_1 to nodes of G_2 (using **Proj** to get a permutation).

Chaining FGNNs

The **second step** takes as input two graphs G_A and G_B as well as a similarity matrix $S^{A\to B}$ and produces two rankings r^A and r^B, one for each graph.

Compute the projected permutation $\pi = \textbf{Proj}(S^{A\to B})$ by solving the linear assignment problem : $\max_{\pi\in\mathcal{S}_n} \sum_i S^{A\to B}_{i\pi(i)}$.

Intuition : the entry $S^{A\to B}_{ij}$ is a measure of the similarity between nodes $i \in G_A$ and $j \in G_B$. Hence π is a mapping from nodes in G_A to nodes in G_B which approximately solves the graph matching problem.

The goal of chaining is to improve incrementally this approximation.

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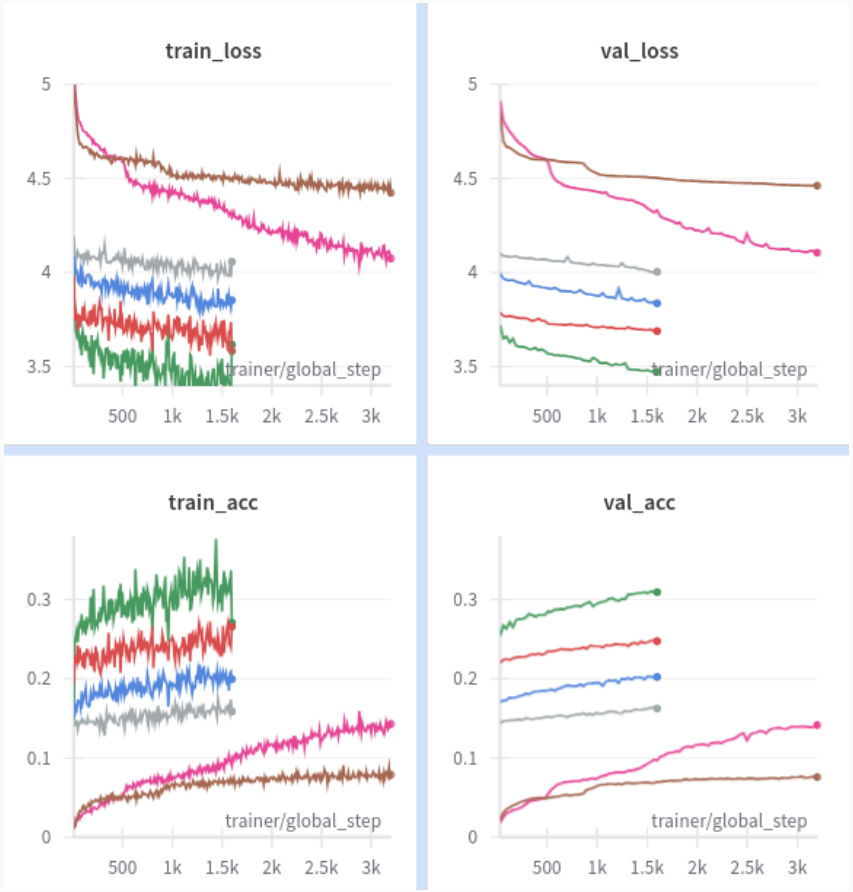
The goal of chaining is to improve incrementally this approximation.

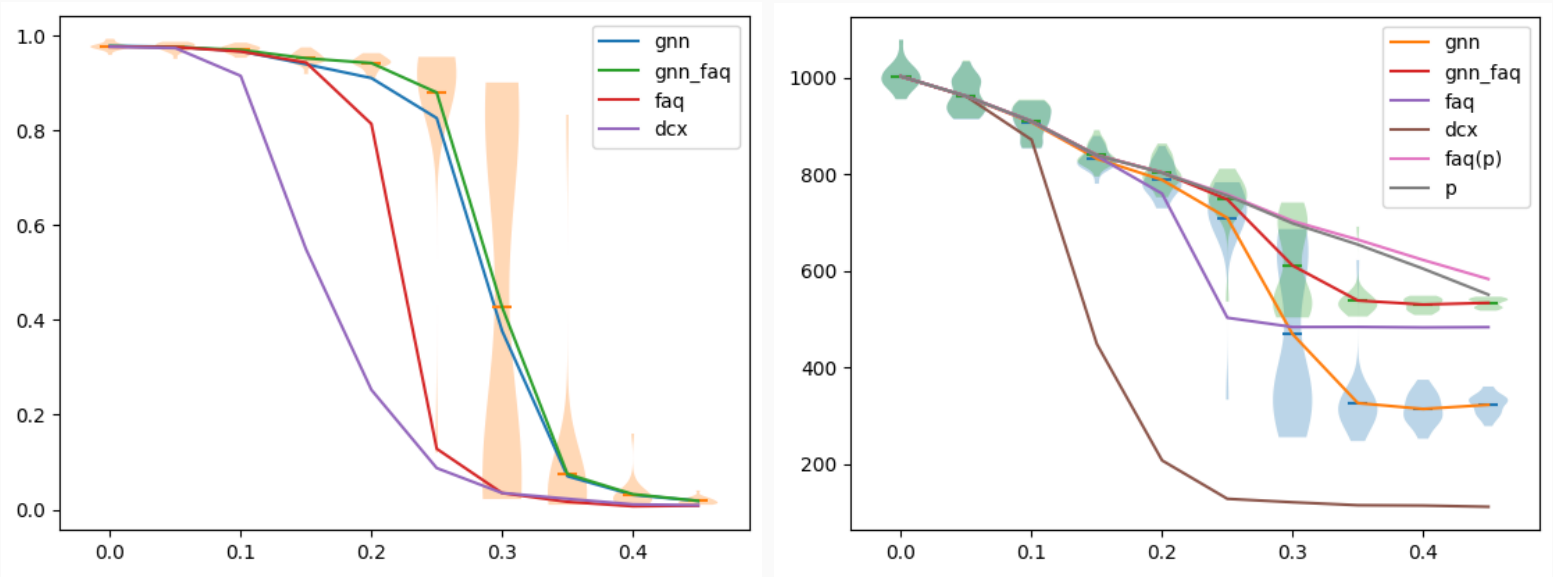
For this, we need to transfer the information contained in π into node features for both graphs : compute a score for each node i in the graph A by $s(i) = \sum_j A_{ij} B_{\pi(i)\pi(j)}$. We can then sort the nodes in A in decreasing order of their scores $s(i)$ and obtain a ranking $r^A \in \mathcal{S}_n$ for the nodes in A. In order to get the ranking r^B, we use the permutation $\pi : G_A \to G_B$ as follows : $r^B_i = \pi\left(r^A_i\right)$.

Training procedure



Training chained GNNs. Each color corresponds to a different training and GNN.

Erdős-Rényi ($n = 500, d = 4$)



Accuracy (left) and number of common edges (right) as a function of noise.

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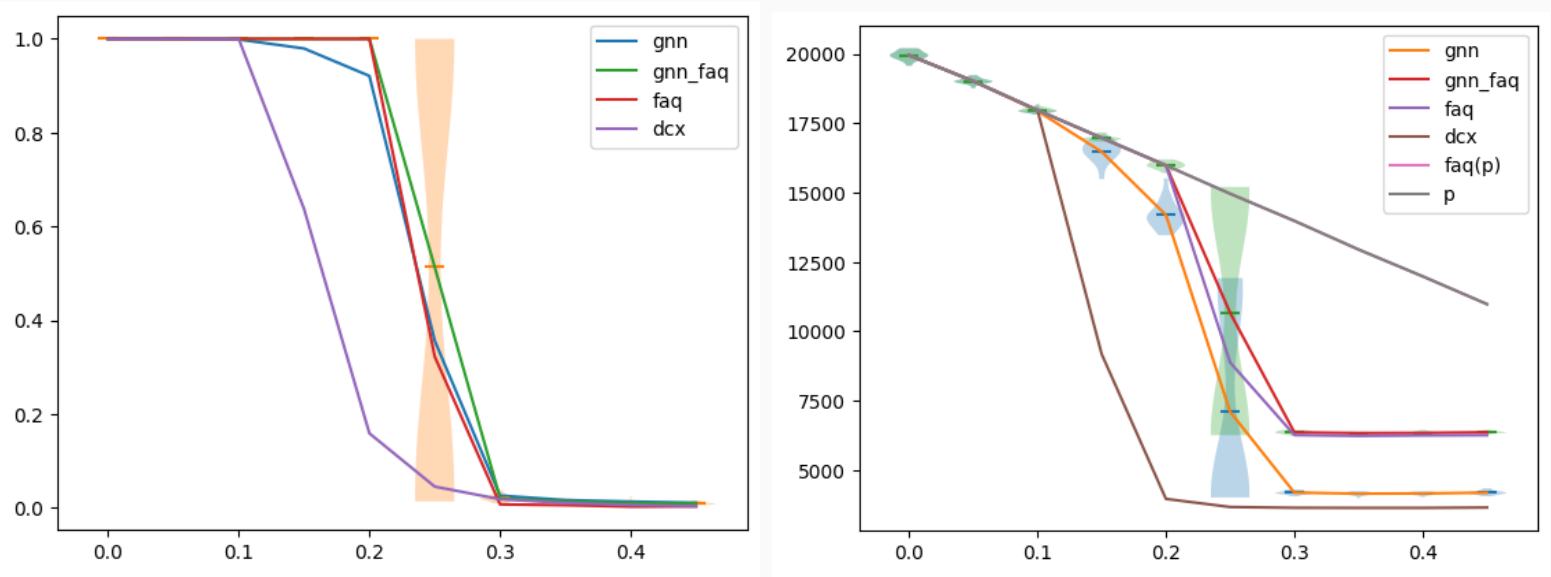

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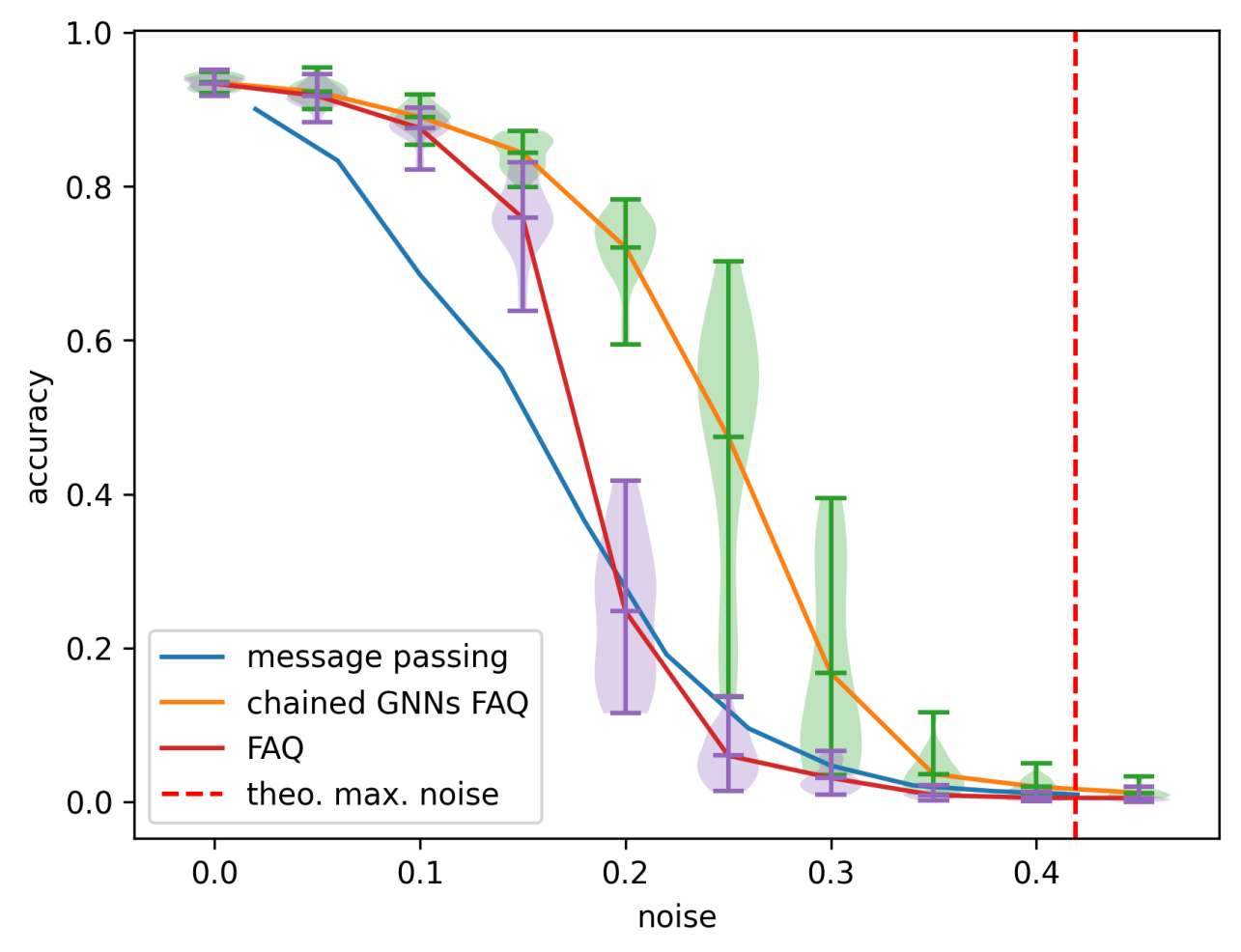
Erdős-Rényi ($n = 1000, d = 3$, training 0.25)



Training : optimal noise level

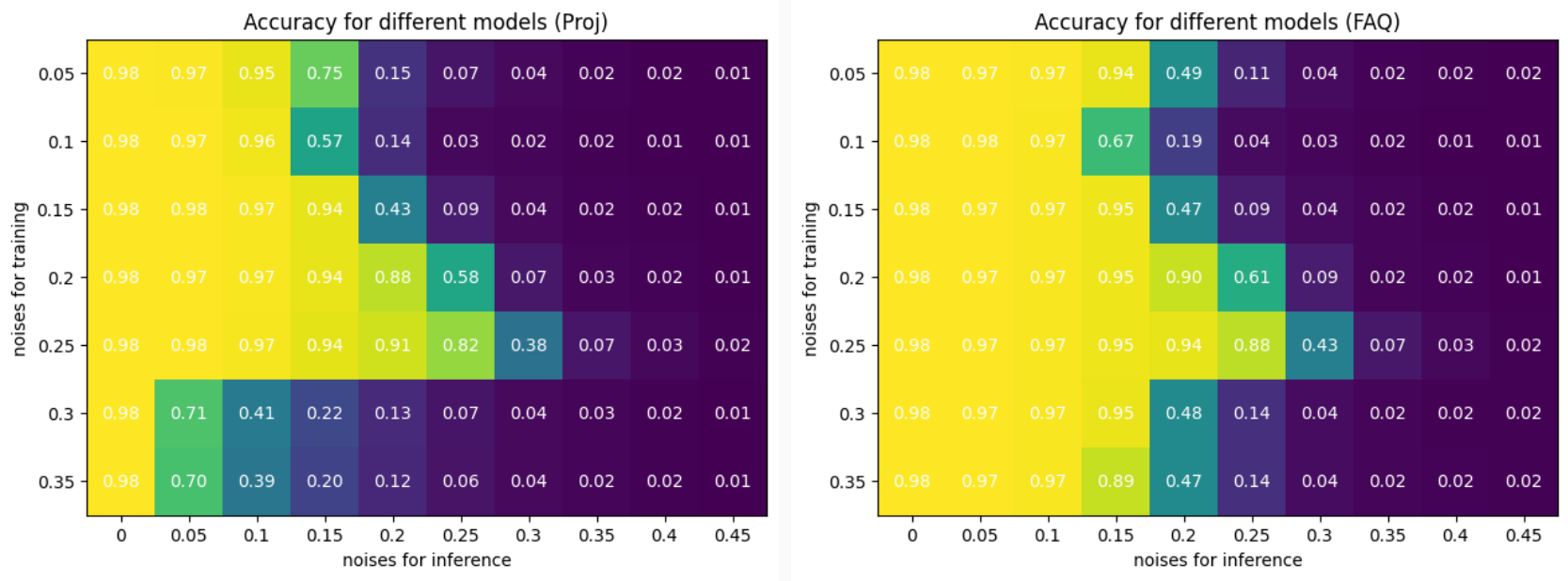


Figure 2 – Each line corresponds to a chained FGNN trained at a given level of noise and evaluated across all different level of noises. Performances are **acc** for sparse Erdős-Rényi (ER 4) with last operation **Proj** (left) or **FAQ** (right).

Varying the number of steps in chaining

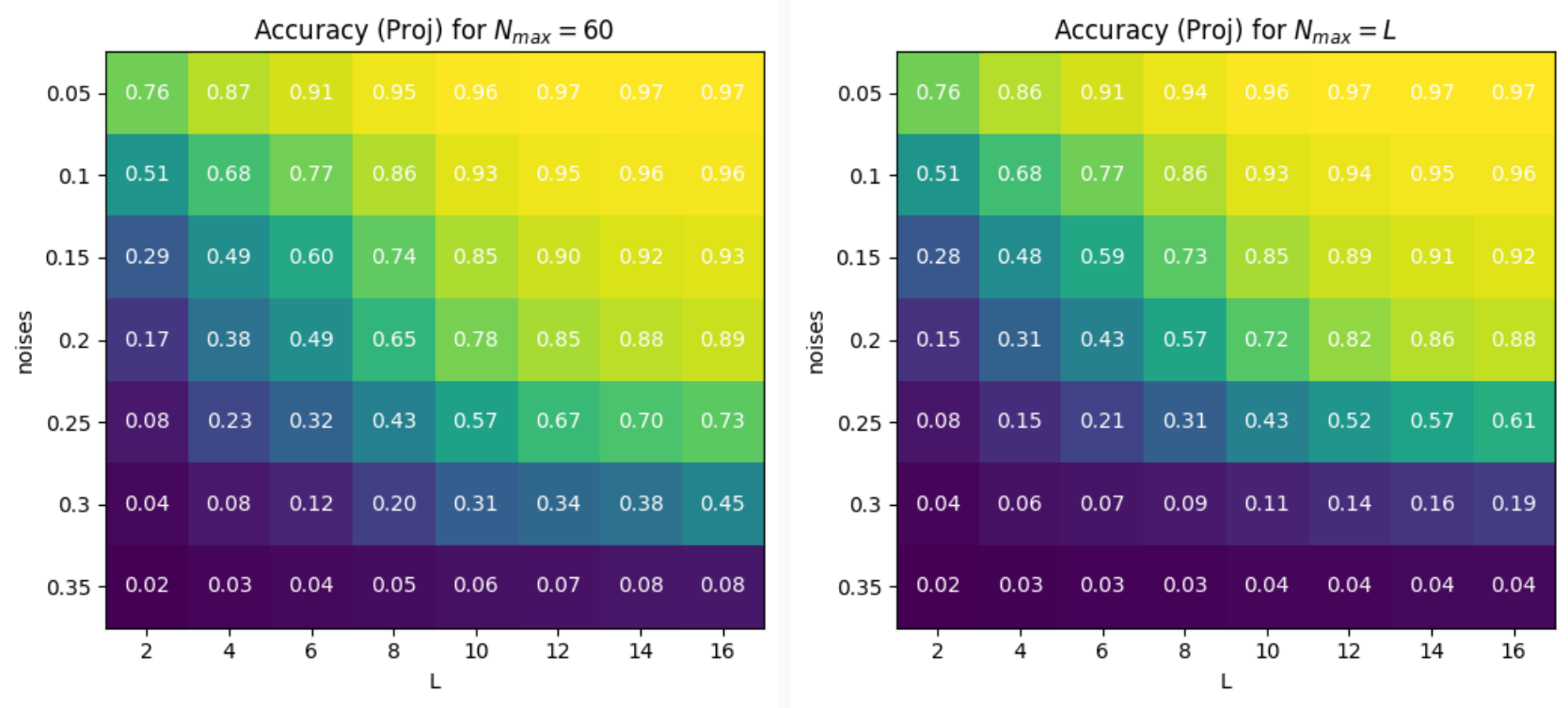
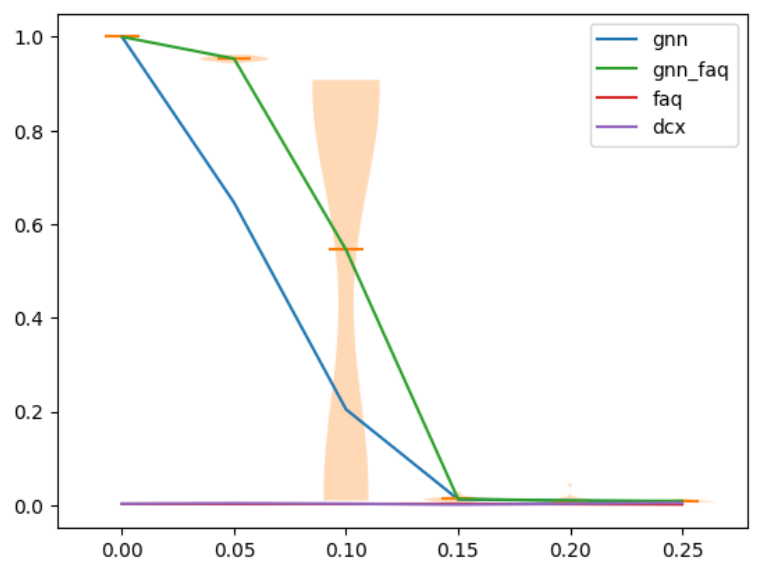
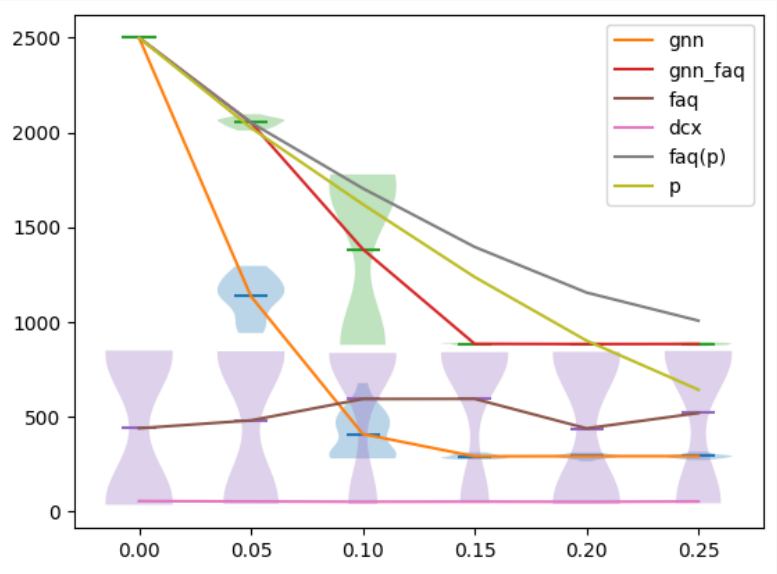


Figure 3 – Accuracy for a chained FGNN on sparse Erdős-Rényi graphs (trained at optimal noise level). Each column corresponds to a different L, with **looping** and $N_{\max} = 60$ on the left and no looping, $N_{\max} = L$ on the right. Each line corresponds to a different noise level for inference.

Regular ($n = 500, d = 10$)





Accuracy (left) and number of common edges (right) as a function of noise.

Conclusion

- General problem : how to learn a permutation ?
- What is the role of chaining ?
  It allows us to use GNNs in an iterative algorithm
  Similar to diffusions, can it be interpreted as a denoising ?
- GNNs chaining is working for correlated random graphs !
- Results with GNNs corroborate theoretical predictions.
- New hard instances (regular graphs) are solved with GNNs (and I do not know of any alternative solutions).

Thank You!

Références

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