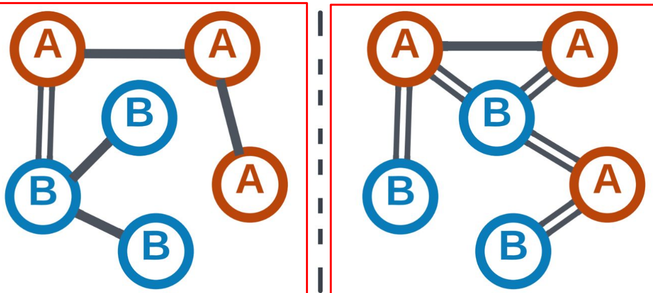
Finding the Missing-half: Graph Complementary Learning for Homophily-prone and Heterophily-prone Graphs

Yizhen Zheng, He Zhang, Vincent Lee, Yu Zheng, Xiao Wang, Shirui Pan

Existing problem



(a) Homophilic-prone Graph

(b) Heterophilic-prone Graph

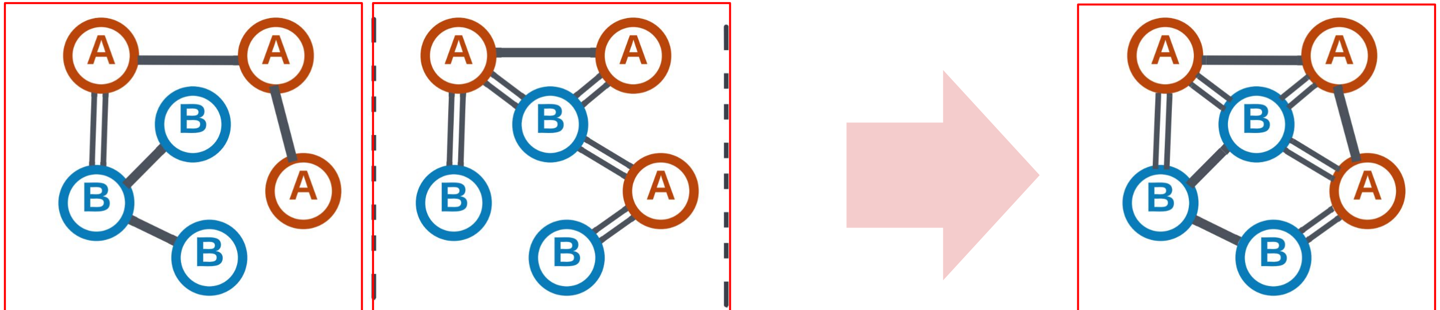
Real-World Graph have only one kind of tendency.

(a) Connecting same class → Homophilic-prone
(b) Connecting different class -> Heterophilic-prone

Existing GNNs only take the original graph during training.

Existing problem

Could we find the missing-half to complement the graph? 🤔



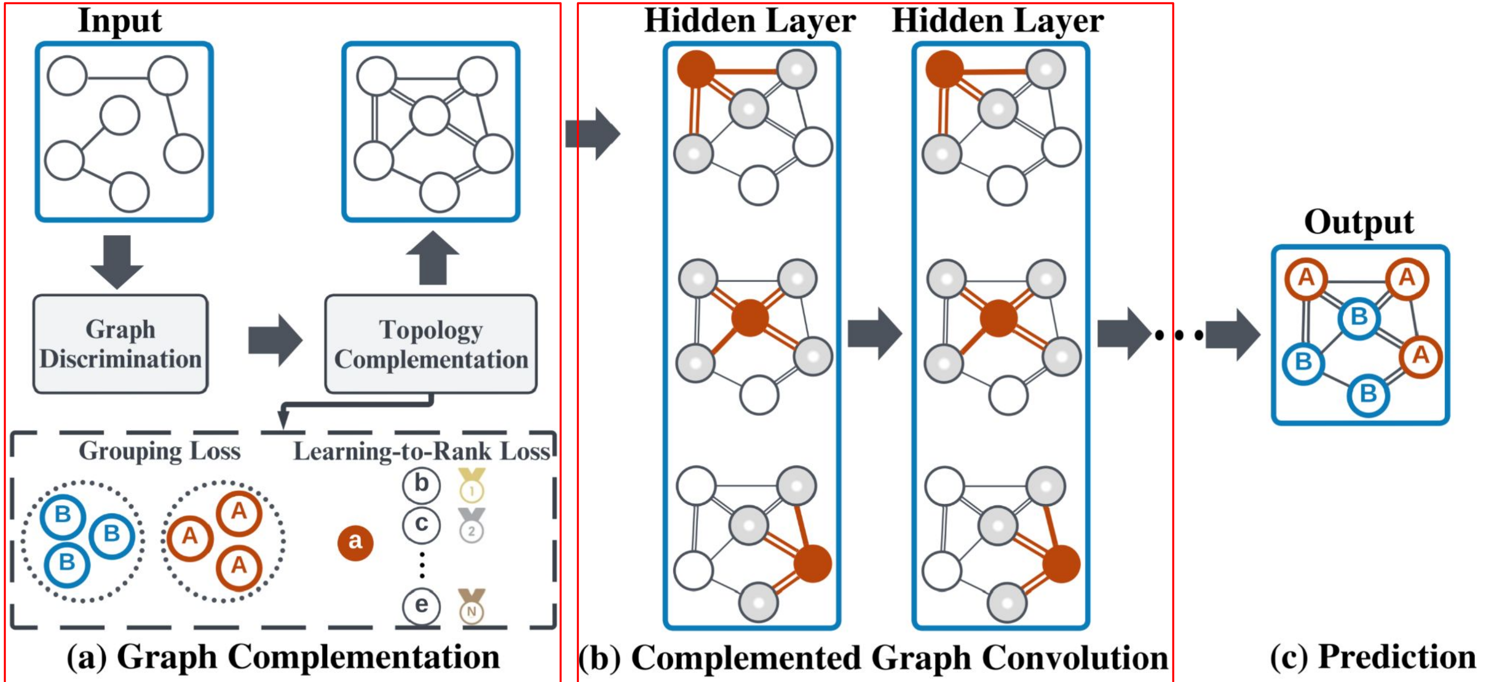
(a) Homophilic-prone Graph

(b) Heterophilic-prone Graph

(c) Complemented Graph

Enriched Structural Information!!

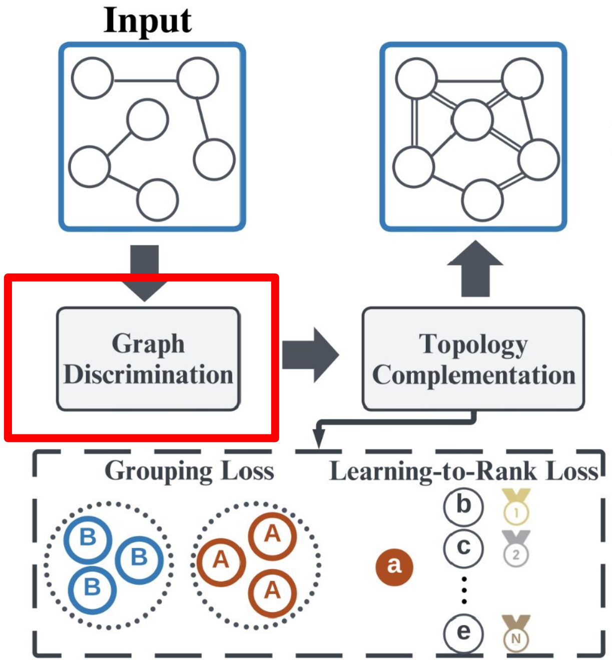
The GOAL Framework



Find the missing-half

New Conv for Complemented Graph

The GOAL Framework

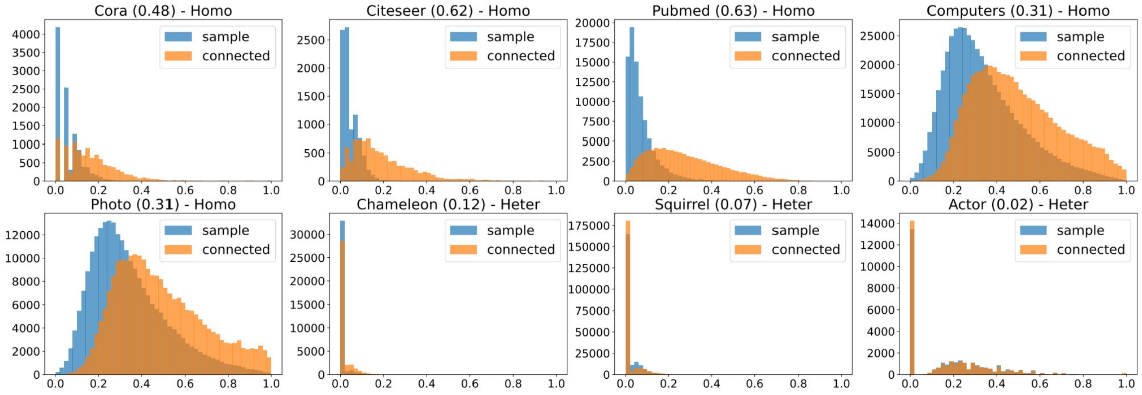


(a) Graph Complementation

Find the missing-half

Graph Discrimination:

Find which part is missing for a graph?



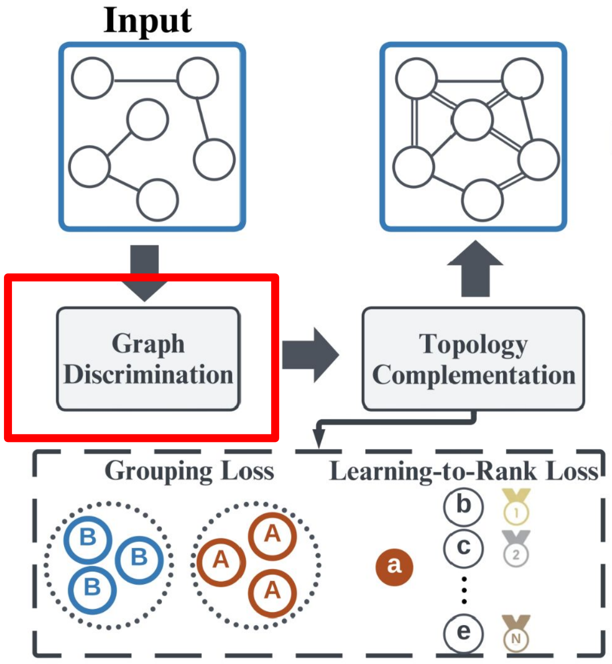
Average Cosine Similarity

(Random sampled pairs)

VS

(Connected node pairs)

The GOAL Framework

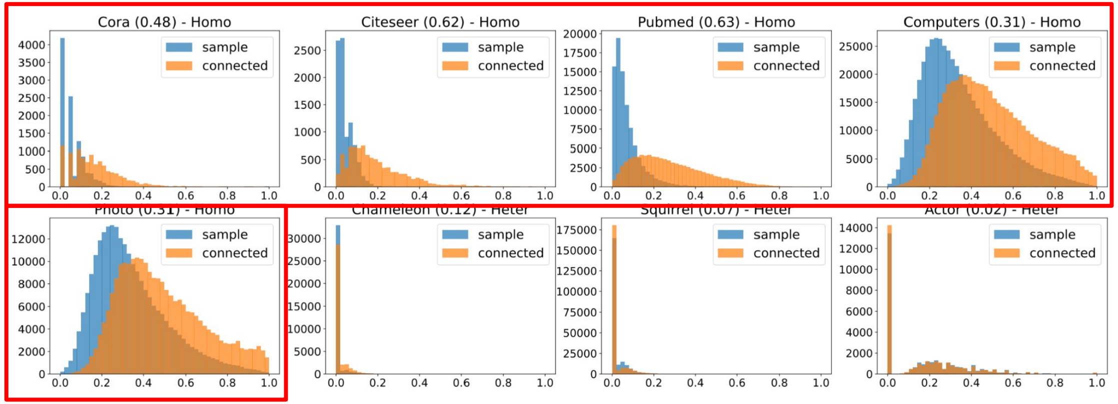


(a) Graph Complementation

Find the missing-half

Graph Discrimination:

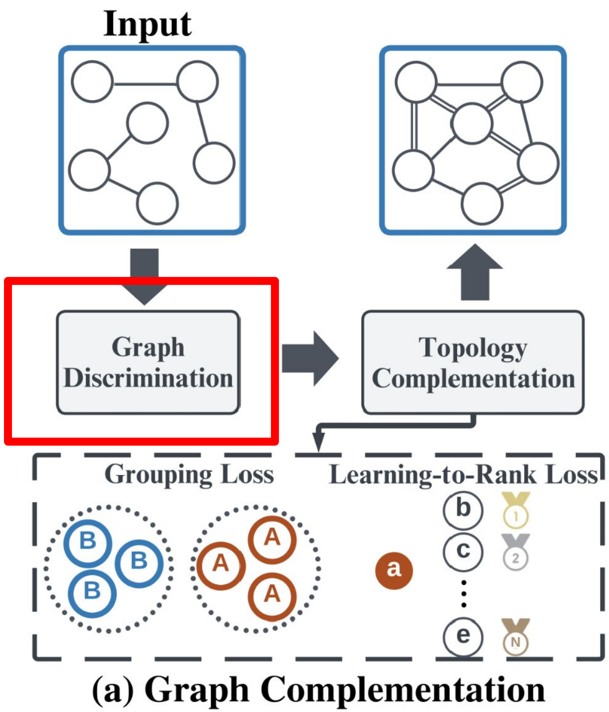
Find which part is missing for a graph?



Homophilic-prone graph

Connected different from Sampled!

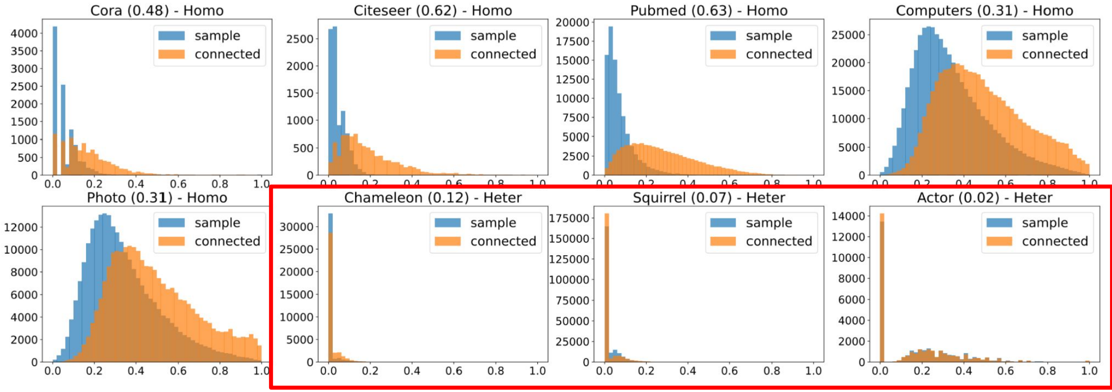
The GOAL Framework



Find the missing-half

Graph Discrimination:

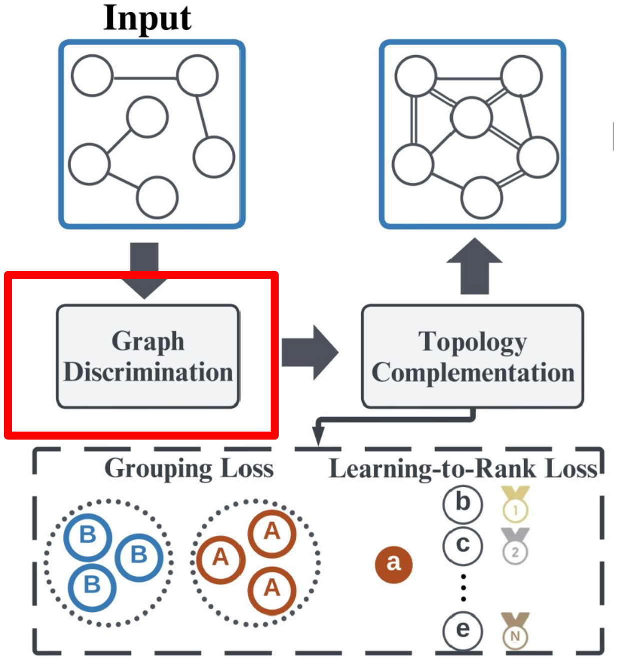
Find which part is missing for a graph?



Heterophilic-prone graph

Connected similar to Sample!

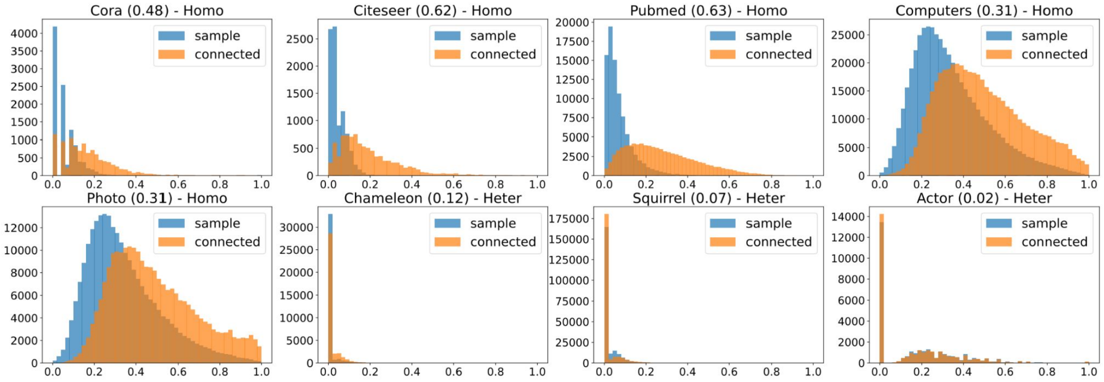
The GOAL Framework



(a) Graph Complementation

Find the missing-half

Graph Discrimination:
Find which part is missing for a graph?



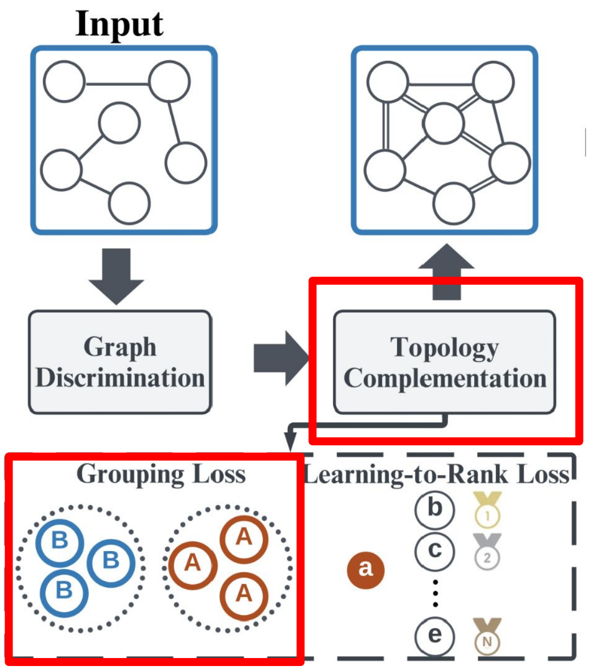
K-S statistics (evaluation of distribution difference) > 0.2

→ homophilic-prone graph

→ need to find heterophilic-prone structure

→ Vice versa

The GOAL Framework

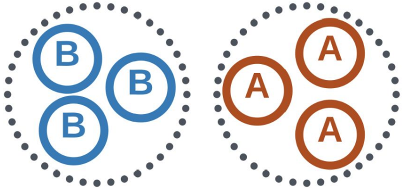


(a) Graph Complementation

Find the missing-half

Topology Complementation:
Find the missing-half graph structure.

Grouping Loss

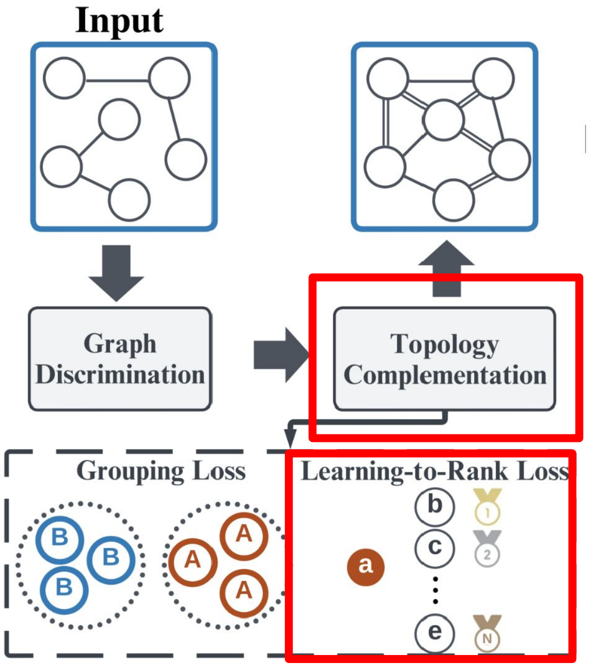


Maximise same class node similarity
Minimise different class node similarity

$$\mathcal{L}_{pos} = -log(sig(\frac{\sum_{(i,j)\in\mathbb{P}} \mathbf{Z}_{gc}^{T}[v_i] \cdot \mathbf{Z}_{gc}[v_j]}{|\mathbb{P}|}) + \epsilon),$$

$$\mathcal{L}_{neg} = -log(1 - sig(\frac{\sum_{(i,j)\in\mathbb{N}} \mathbf{Z}_{gc}^{T}[v_i] \cdot \mathbf{Z}_{gc}[v_j]}{|\mathbb{N}|} + \epsilon)),$$

The GOAL Framework



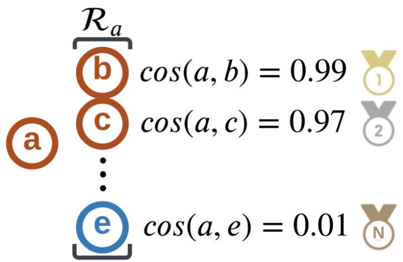
(a) Graph Complementation

Find the missing-half

Topology Complementation:

Find the missing-half graph structure.

Learning-to-rank loss



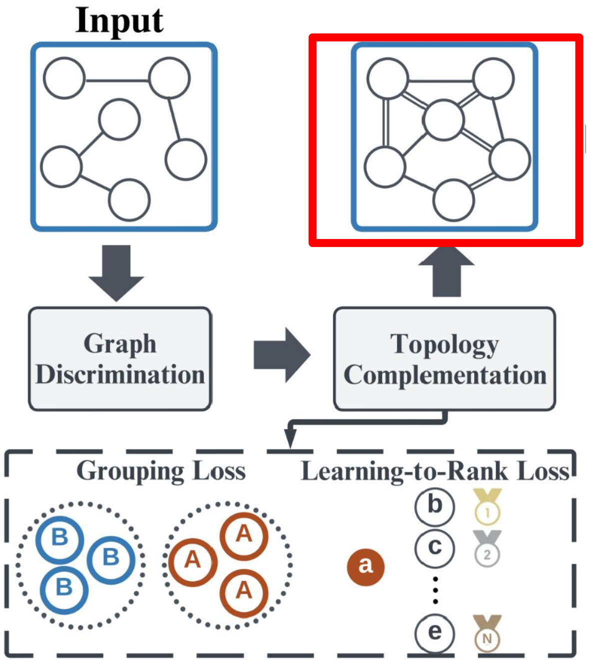
For node a

→ most similar k same class nodes

→ least similar k different class nodes

A 2k list → put nodes in correct rank

The GOAL Framework



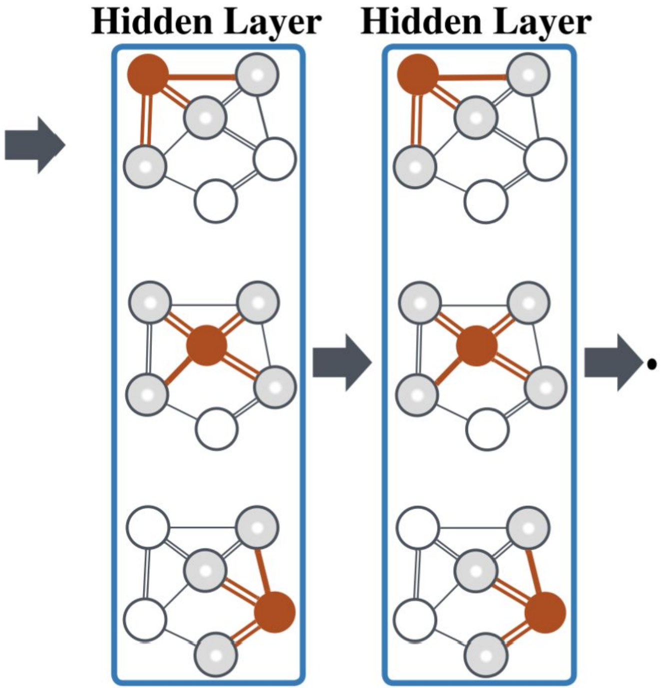
(a) Graph Complementation

Find the missing-half

Topology Complementation:
Find the missing-half graph structure.

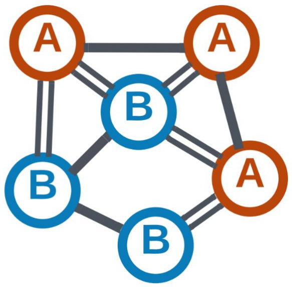
Two losses to train a MLP
→
Generate node embeddings
→
Find each node most similar/least similar neighbours (cosine sim)
→
Connect them
→
Done!

The GOAL Framework



(b) Complemented Graph Convolution

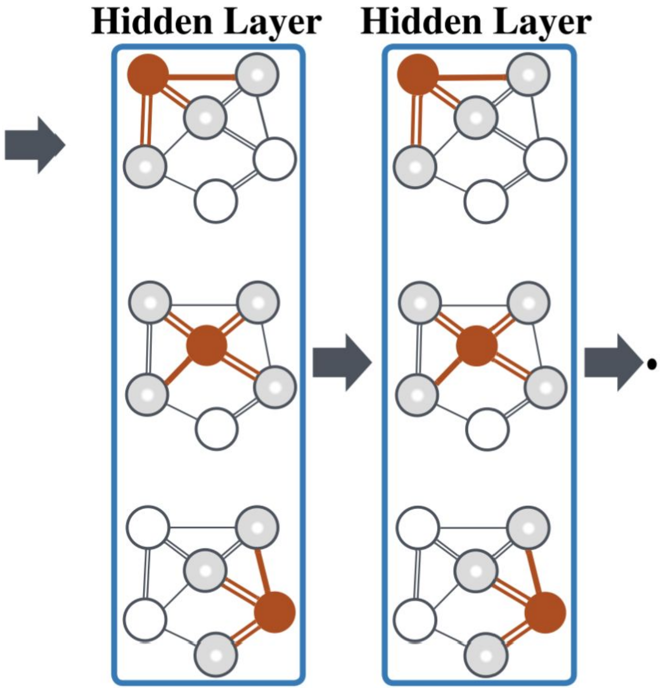
New Conv for Complemented Graph



(c) Complemented Graph

How to design a new graph convolution → handle complemented graphs with both homophily- and heterophily-prone topology? 🤔

The GOAL Framework



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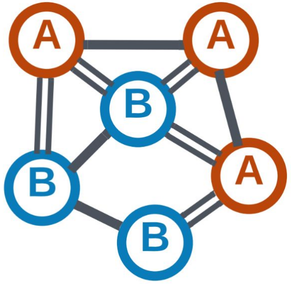
New Conv for Complemented Graph

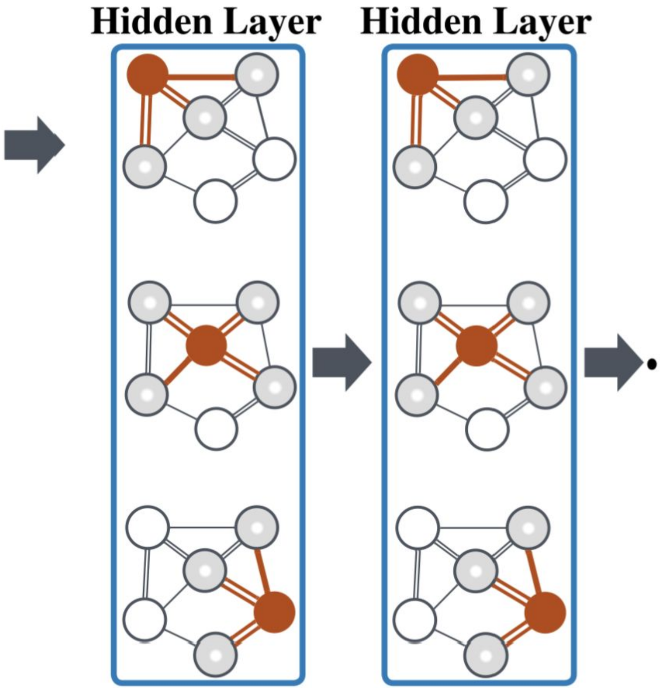


(c) Complemented Graph

Straightforward Solution:

Maximise similarity for **homophilic-connected** nodes
Minimise similarity for **heterophilic-connected** nodes

The GOAL Framework



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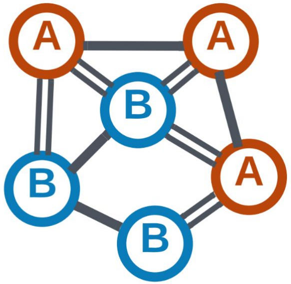


(c) Complemented Graph

Two Objectives

Maximise sim for **homophilic-connected**

$$\mathcal{O}_o = \min_{\mathbf{H}}\{tr(\mathbf{H}^T(\mathbf{I} - \hat{\mathbf{A}}_o)\mathbf{H})\}$$

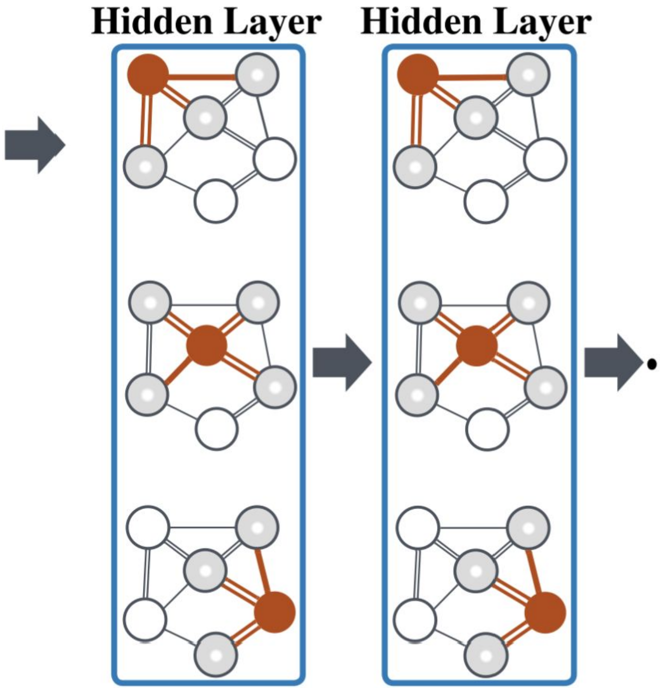
$$= \frac{1}{2}\sum_{(i,j)\in\mathcal{E}}^{E} \boxed{\hat{\mathbf{A}}_o}[i,j] \parallel \mathbf{H}_i - \mathbf{H}_j \parallel^2,$$

Minimise sim for **heterophilic-connected**

$$\mathcal{O}_t = \min_{\mathbf{H}}\{tr(\mathbf{H}^T(\mathbf{I} + \hat{\mathbf{A}}_t)\mathbf{H})\}$$

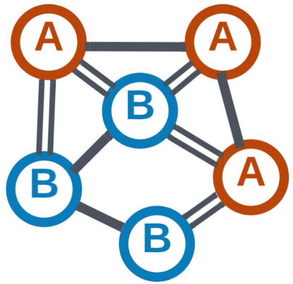
$$= \frac{1}{2}\sum_{(i,j)\in\mathcal{E}}^{E} \boxed{\hat{\mathbf{A}}_t}[i,j] \parallel \mathbf{H}_i + \mathbf{H}_j \parallel^2,$$

The GOAL Framework



(b) Complemented Graph Convolution

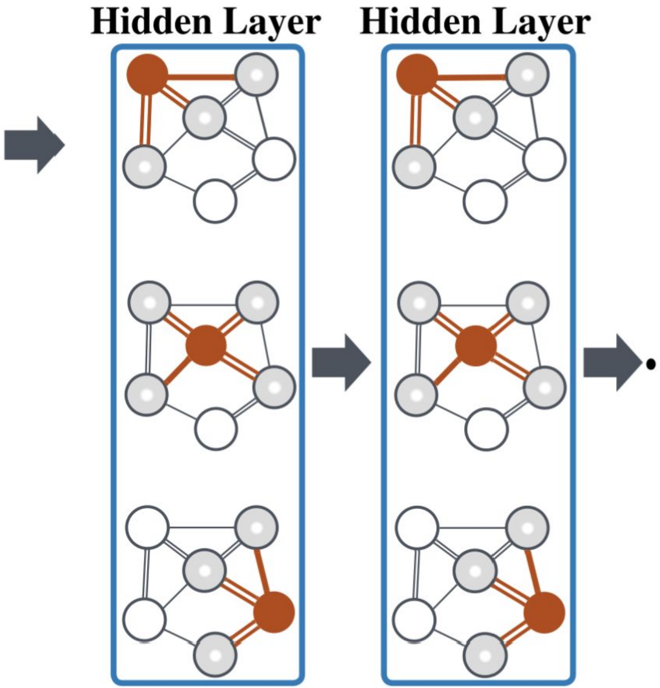
New Conv for Complemented Graph



(c) Complemented Graph

A step forward: **any other objective**? 🤔

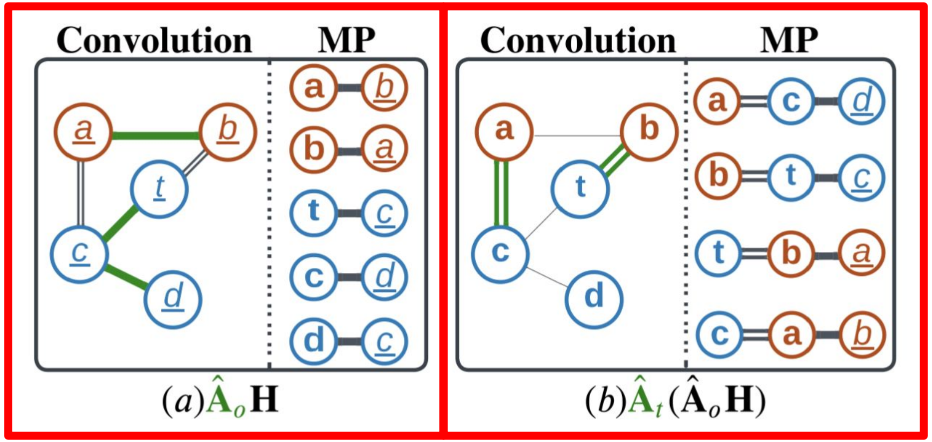
The GOAL Framework



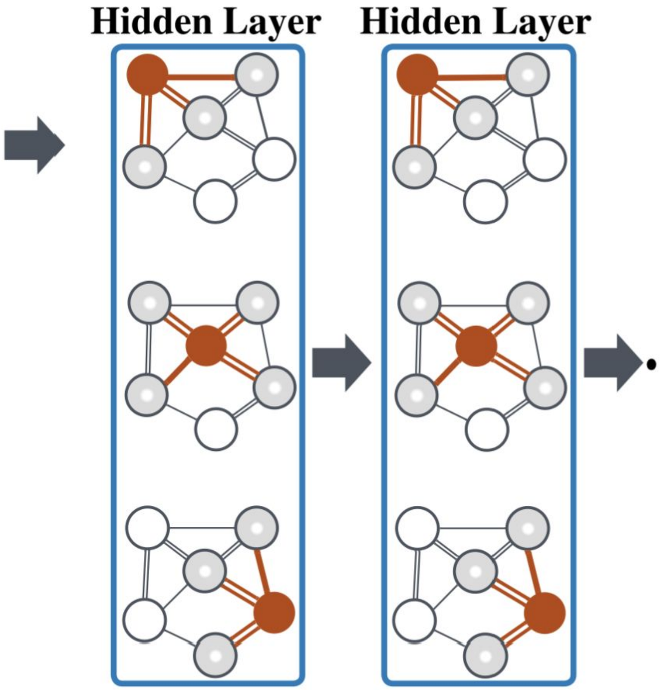
(b) Complemented Graph Convolution

New Conv for Complemented Graph

$\hat{\mathbf{A}}_t \hat{\mathbf{A}}_o$ The **heterophilic neighbors of homophilic neighors** → still heterophilic-prone

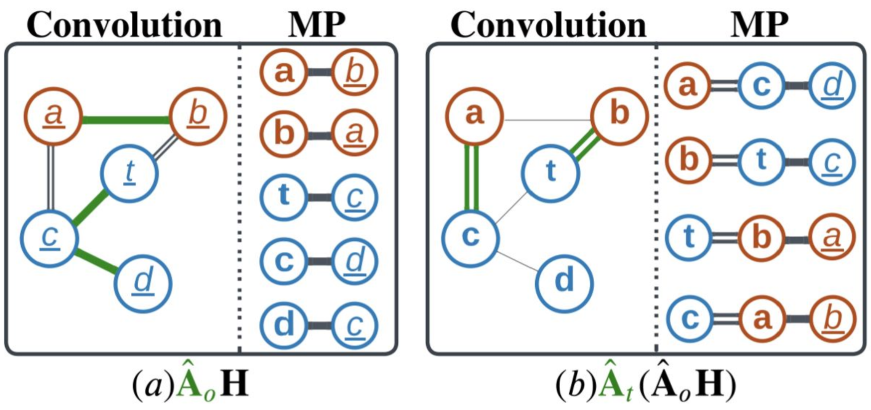


The GOAL Framework



(b) Complemented Graph Convolution

New Conv for Complemented Graph

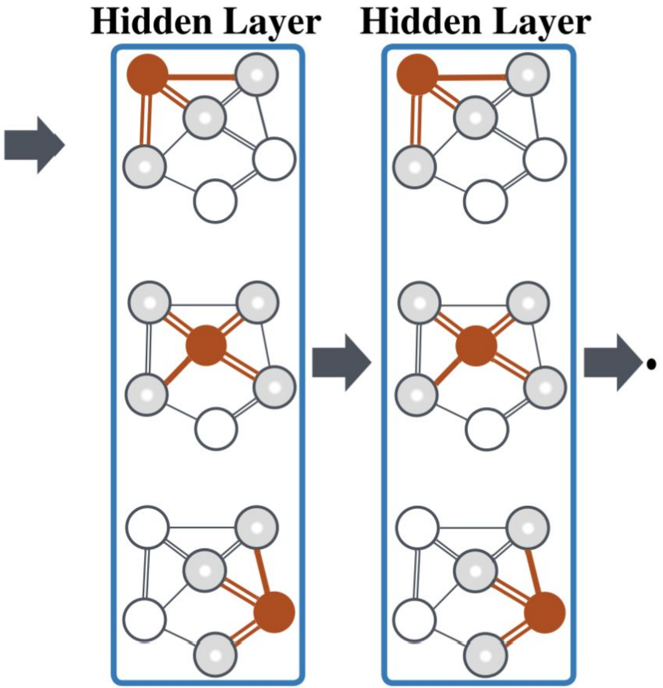


Minimise sim for extended heterophilic neighbors

$$\mathcal{O}_c = \min_{\mathbf{H}}\{tr(\mathbf{H}^T(\mathbf{I}+\hat{\mathbf{A}}_{to})\mathbf{H})\}; \hat{\mathbf{A}}_{to} = \hat{\mathbf{A}}_t\hat{\mathbf{A}}_o$$

$$= \frac{1}{2}\sum_{(i,j)\in\mathcal{E}}^{E} \hat{\mathbf{A}}_{to}[i,j] \parallel \mathbf{H}_i + \tilde{\mathbf{H}}_j \parallel^2 .$$

The GOAL Framework



(b) Complemented Graph Convolution

New Conv for Complemented Graph

Combine all objectives → we finally derive the new convolution

$$\mathbf{H}^{l+1} = \sigma((\alpha \mathbf{I} + \beta \hat{\mathbf{A}}_o - \gamma \hat{\mathbf{A}}_t - \delta \hat{\mathbf{A}}_{to})\mathbf{H}^l \mathbf{W}^l), \quad (8)$$

Experiment

Table 1. Node classification for eight baselines on eight datasets.

	Cora	Citeseer	Pubmed	Computer	Photo	Chameleon	Squirrel	Actor
MLP	72.09 ± 0.32	71.67 ± 0.40	87.47 ± 0.14	83.59 ± 0.89	90.49 ± 0.20	46.55 ± 0.42	30.67 ± 0.52	28.75 ± 0.88
GCN	87.50 ± 1.04	75.11 ± 1.12	87.20 ± 0.52	83.55 ± 0.38	89.30 ± 0.82	62.72 ± 2.09	47.26 ± 0.34	29.98 ± 1.18
GAT	88.25 ± 1.22	75.75 ± 1.23	85.88 ± 0.38	85.36 ± 0.50	90.81 ± 0.22	62.19 ± 3.78	51.80 ± 1.04	28.17 ± 1.19
APPNP	88.36 ± 0.61	76.03 ± 1.27	86.21 ± 0.25	88.32 ± 0.36	94.44 ± 0.36	50.88 ± 1.18	33.58 ± 1.00	29.82 ± 0.82
GraphSage	88.01 ± 1.29	75.17 ± 1.35	87.39 ± 0.84	88.54 ± 0.69	94.23 ± 0.62	58.82 ± 2.29	41.19 ± 0.75	31.76 ± 0.73
ChebyNet	87.49 ± 0.90	75.50 ± 0.87	89.05 ± 0.29	89.77 ± 0.36	95.02 ± 0.41	59.98 ± 1.54	40.18 ± 0.55	35.85 ± 1.05
GPR-GNN	88.65 ± 0.75	75.70 ± 0.81	88.53 ± 0.30	87.63 ± 0.48	94.60 ± 0.30	67.96 ± 2.55	49.52 ± 5.00	30.78 ± 0.61
JKNET	86.99 ± 1.60	75.38 ± 1.30	88.64 ± 0.51	86.97 ± 0.56	92.68 ± 0.58	64.63 ± 3.08	44.91 ± 1.94	28.48 ± 1.25
GOAL	$\mathbf{88.75 \pm 0.87}$	$\mathbf{77.15 \pm 0.95}$	$\mathbf{89.25 \pm 0.55}$	$\mathbf{91.33 \pm 0.38}$	$\mathbf{95.60 \pm 0.44}$	$\mathbf{71.65 \pm 1.66}$	$\mathbf{60.53 \pm 1.60}$	$\mathbf{36.46 \pm 1.02}$

Achieve best performance on all datasets.

Notably → almost 9% better than the best baseline on Squirrel.

Experiment

ICML
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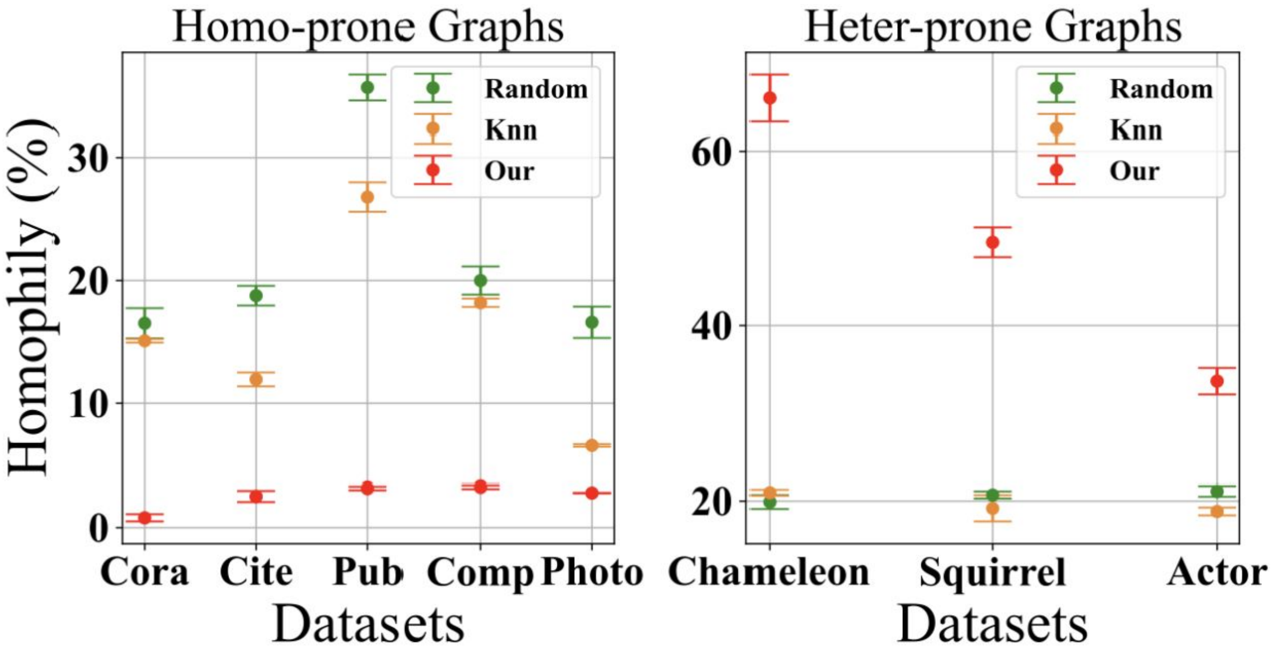
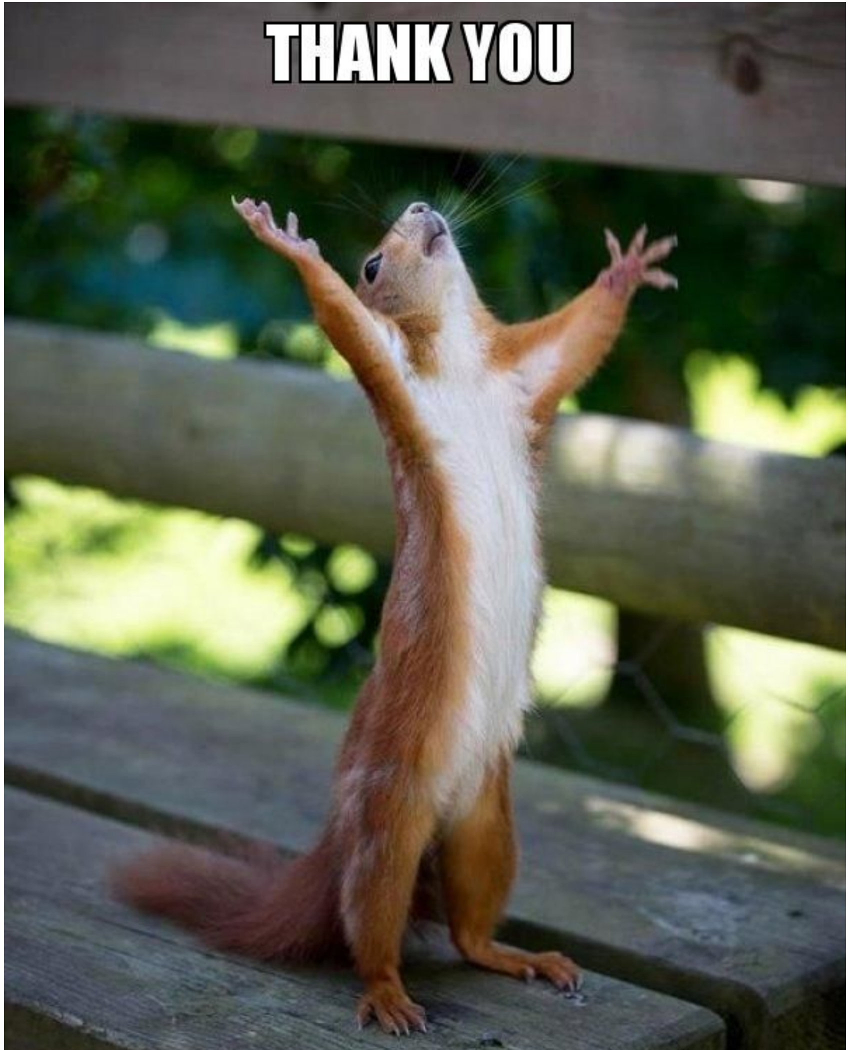


The generated topology is way better than random and knn connection



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