





# Understanding and Improving Graph Injection Attack by Promoting Unnoticeability

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### Graph Neural Networks (GNNs) Are Widely Applied



Model & Inference over the physical world



Protein Interaction Predictions



Besides, GNNs can also process structures like image and text...



Social Network Analysis



Recommender Systems

### **GNNs Are Inherently Vulnerable**







Prediction: Airliner 🤤



### **Adversarial Attacks on GNNs**



(Zügner et al., 2018)

#### **Adversarial Objective:**





### Adversarial Attacks on GNNs



(Zügner et al., 2018)

#### **Adversarial Objective:**

#### **Graph Modification Attack (GMA):**





Sometimes Expensive



# $\min \mathscr{L}_{\mathrm{atk}}(f_{\theta^*}(G')), \text{ s.t.} \|G' - G\| \leq \underbrace{\bigtriangleup}_{\mathrm{perturbation budgets}}$

 $\triangle_A + \triangle_X \le \triangle \in \mathbb{Z}, \ \|A' - A\|_0 \le \triangle_A \in \mathbb{Z}, \ \|X' - X\|_{\infty} \le \epsilon \in \mathbb{R}$ 

Perturbing node features

#### **Adversarial Attacks on GNNs**



(Zügner et al., 2018)

#### **Adversarial Objective:**

#### **Graph Injection Attack (GIA):**





#### $\min \mathscr{L}_{atk}(f_{\theta^*}(G')), \text{ s.t.} \|G' - G\| \leq \Delta$ perturbation budgets

 $X' = \begin{bmatrix} X \\ X_{atk} \end{bmatrix}, A' = \begin{bmatrix} A & A_{atk} \\ A_{atk}^T & O_{atk} \end{bmatrix}, \quad |V_{atk}| \le \triangle \in \mathbb{Z}, \ 1 \le d_u \le b \in \mathbb{Z}, X_u \in \mathcal{D}_X \subseteq \mathbb{R}^d, \forall u \in V_{atk}$ 

Carefully crafted node features

For Node v?

# Let's find out more about GIA!



GIA

#### - through a friendly comparison -





GMA

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### The Power of Graph Injection Attack

**Definition 1 (Threats)** Consider an adversary  $\mathscr{A}$ , given a perturbation budget  $\Delta$ , the threat of  $\mathscr{A}$  to a GNN  $f_{\theta}$  is defined as  $\min_{\|G'-G\|\leq \Delta} \mathscr{L}_{atk}(f_{\theta^*}(G'))$ , i.e., the **optimal objective value**.

**Theorem 1 (GIA is more harmful than GMA)** no isolated nodes, and both GIA and GMA follow the **optimal strategy**, then,  $\forall \triangle_{\text{GMA}} \ge 0, \exists \triangle_{\text{GIA}} \le \triangle_{\text{GMA}},$ 

 $\mathscr{L}_{\text{atk}}(f_{\theta}(G'_{\text{GIA}})) - \mathscr{L}_{\text{atk}}(f_{\theta}(G'_{\text{GMA}})) \leq 0,$ 



Given moderate perturbation budgets  $\Delta_{GIA}$  for GIA and  $\Delta_{GMA}$  for GMA, that is, let  $\Delta_{\text{GIA}} \leq \Delta_{\text{GMA}} \ll |V| \leq |E|$ , for a fixed linearized GNN  $f_{\theta}$  trained on G, assume that G has

where  $G'_{\text{GIA}}$  and  $G'_{\text{GMA}}$  are perturbed graphs generated by GIA and GMA, respectively.

### The Power of Graph Injection Attack



**Definition 2 (Plural Mapping**  $\mathscr{M}_2$ ) A plural mapping  $\mathscr{M}_2$  maps a perturbed graph  $G'_{GMA}$  generated by GMA with only edge addition perturbations<sup>\*</sup>, to a GIA perturbed graph  $G'_{GIA} = \mathscr{M}_2(G'_{GMA})$ , such that:  $f_{\theta}(G'_{GIA})_u = f_{\theta}(G'_{GMA})_u, \forall u \in V.$ 

\*We can also find such mappings for other perturbation actions of GMA.

# Is The Power of GIA A Free Lunch?

#### It turns out to be NO. 🨅

# The Pitfalls in Graph Injection Attack



Given the example of  $\mathcal{M}_2$ , assume GIA uses PGD to optimize  $X_{w}$ , iteratively, we find:

Illustration of  $\mathcal{M}_2$  mapping

# **Definition 3 (Node-Centric Homophily)** *u* and the aggregated features of its neighbors\*:

$$h_{u} = \operatorname{sim}(r_{u}, X_{u}), \ r_{u} = \sum_{j \in \mathcal{N}(u)} \frac{1}{\sqrt{d_{j}d_{u}}} X_{j},$$

\*We can also define edge-centric homophily, while we will focus on node-centric homophily.

$$sim(X_u, X_w)^{(t+1)} \le sim(X_u, X_w)^{(t)},$$

where t is the number of optimization steps and  $sim(\cdot)$  is the cosine similarity.

The homophily of a node u can be defined with the similarity between the features of node

where  $d_{\mu}$  is the degree of node u and sim(  $\cdot$  ) is a similarity metric, e.g., cosine similarity.

## The Pitfalls in Graph Injection Attack



**Definition 3 (Homophily Defenders)** The homophily defenders can be implemented via edge pruning\*: where  $\left[ \begin{array}{c} u, v \end{array} \right]$  elaborates the pruning condition for edge (u, v).

\*Essentially, homophily defenders can have other implementations than edge pruning.

 $H_{u}^{(k)} = \operatorname{READOUT}(W_{k} \cdot \operatorname{AGG}(\mathbb{I}_{\operatorname{con}}(u, v) \{H_{v}^{(k-1)}\} \mid v \in \mathcal{N}(u) \cup \{u\})),$ 



## The Pitfalls in Graph Injection Attack



Homophily changes before and after attacks

Theorem 2 (GIA loses power when against homophily defenders) Given conditions in Theorem 1, consider a GIA attack, which (i) is mapped by  $\mathcal{M}_2$  from from a GMA attack that only performs edge addition perturbations, and (ii) uses a linearized GNN trained with at least one node from each class in G as the surrogate model, and (iii) optimizes the malicious node features with PGD. Assume that G has no isolated node, and has node features as  $X_u = \frac{C}{C-1}e_{Y_u} - \frac{1}{C-1}\mathbf{1} \in \mathbb{R}^d$  where  $Y_u$  is the label of node u and  $e_{Y_u} \in \mathbb{R}^d$  is a one-hot vector with the  $Y_u$ -th entry being 1 and others being 0. Let the minimum similarity for any pair of nodes connected in G be  $s_G = \min \frac{\sin(X_u, X_v)}{\sin(X_u, X_v)}$  implemented with cosine similarity. For a homophily defender  $g_{\theta}$  that prunes edges (u, v) if  $sim(X_u, X_v) \leq s_G$ , we have:

 $\mathscr{L}_{atk}(g_{\theta}(\mathscr{M}_2(G'_{GMA})))$ 

$$()) - \mathscr{L}_{atk}(g_{\theta}(G'_{GMA})) \ge 0.$$

### **Unnoticeability in Graph Adversarial Attack**





Prediction: Pig Unnoticeable Adversarial noise 🚫 Prediction: Airliner (Szegedy et al., 2014; Goodfellow et al., 2015; Kolter and Madry et al. 2019)







### Homophily Unnoticeable Graph Injection Attack

**Definition 4 (Homophily Unnoticeability)** 

where G' is the perturbed graph generated  $\mathscr{A}$  and  $m(\cdot)$  is a distribution distance measure.

Homophily Unnoticeability measures how likely the new connections between the malicious nodes and target nodes will appear naturally.

Homophily Defender provides efficient check for homophily unnoticeability serving as external examiners.

Let the node-centric homophily distribution for a graph G be  $\mathcal{H}_G$ . Given the upper bound for the allowed homophily distribution shift  $\Delta_{\mathscr{H}} \geq 0$ , an attack  $\mathscr{A}$  is **homophily unnoticeable** if:

 $m(\mathcal{H}_{G}, \mathcal{H}_{G'}) \leq \Delta_{\mathcal{H}},$ 



## Homophily Unnoticeable Graph Injection Attack

**Definition 5 (Harmonious Adversarial Objective (HAO))** Observing the homophily (Definition. 4) is differentiable with respect to X, we can integrate it into the original adversarial objective as\*:

\*We only use HAO to solve for G' while still using the original objective to evaluate the threats.

**Theorem 3 (HAO re-empowers GIA)** Given conditions in Theorem 2, we have  $m(\mathcal{H})$ 

 $\mathscr{L}_{\text{atk}}(g_{\theta}(G'_{\text{HAO}})) - \mathscr{L}_{\text{atk}}(g_{\theta}(G'_{\text{GIA}})) \leq 0,$ 

where  $G'_{HAO}$  and  $G'_{GIA}$  are perturbed graphs generated by GIA with and without HAO, respectively.

$$\min_{\|G'-G\|\leq \Delta} \mathscr{L}^h_{\mathrm{atk}}(f_{\theta^*}(G')) = \mathscr{L}_{\mathrm{atk}}(f_{\theta^*}(G')) - \lambda C(G, G'),$$

where C(G, G') is a regularization term based on homophily and  $\lambda \geq 0$  is the corresponding weight.

$$(G', \mathcal{H}_{G'_{HAO}}) \leq m(\mathcal{H}_{G}, \mathcal{H}_{G'_{GIA}})$$
, hence:



## Homophily Unnoticeable Graph Injection Attack



Homophily changes



**Theorem 3 (HAO re-empowers GIA)** Given conditions in Theorem 2, we have  $m(\mathcal{H}_G, \mathcal{H}_{G'_{HAO}}) \leq m(\mathcal{H}_G, \mathcal{H}_{G'_{GIA}})$ , hence:  $\mathscr{L}_{atk}(g_{\theta}(G'_{HAO})) - \mathscr{L}_{atk}(g_{\theta}(G'_{GIA})) \leq 0$ ,

where  $G'_{\text{HAO}}$  and  $G'_{\text{GIA}}$  are perturbed graphs generated by GIA with and without HAO, respectively.



### HAO Re-empowers GIA

injection strategies can further advance the state of the art.

#### **Homo:** Homophily Defenders

Vanilla: Vanilla GNNs, e.g., GCN, GAT, GraphSage.

**Robust:** Robust GNN models, or GNN models with robust tricks such as layer normalisation, or adversarial training.

**Combo:** Robust GNN models with robust tricks such as layer normalisation, or adversarial training.

	HAO	Cora (↓)			Citeseer(↓)			Computers( $\downarrow$ )			Arxiv(↓)		
		Homo	Robust	Combo	Homo	Robust	Combo	Homo	Robust	Combo	Homo	Robust	Comb
Clean		85.74	86.00	87.29	74.85	75.46	75.87	93.17	93.17	93.32	70.77	71.27	71.4
PGD PGD	$\checkmark$	$\begin{array}{c} 83.08\\52.60\end{array}$	$\begin{array}{c} 83.08\\ 62.60\end{array}$	$85.74 \\ 77.99$	$\begin{array}{c} 74.70 \\ 69.05 \end{array}$	$74.70 \\ 69.05$	$75.19 \\ 73.04$	$\begin{array}{c} 84.91 \\ 79.33 \end{array}$	$84.91 \\ 79.33$	$\begin{array}{c} 91.41 \\ 87.83 \end{array}$	$\begin{array}{c} 68.18 \\ 55.38 \end{array}$	$\frac{68.18}{62.89}$	71.1
MetaGIA <sup>†</sup> MetaGIA <sup>†</sup> AGIA <sup>†</sup> AGIA <sup>†</sup>	√ √	$83.61 \\ 49.25 \\ 83.44 \\ \underline{47.24}$	$83.61 \\ \underline{69.83} \\ 83.44 \\ 61.59$	85.86 76.80 85.78 <b>75.25</b>	$74.70\\68.04\\74.72\\70.24$	$74.70\\68.04\\74.72\\70.24$	75.15 arrow 71.25 arrow 75.29 arrow 71.80	84.91 78.96 85.21 <u>75.14</u>	$84.91 \\78.96 \\85.21 \\\underline{75.14}$	$91.41 \\ 90.25 \\ 91.40 \\ \underline{86.02}$	$68.47 \\ 57.05 \\ 68.07 \\ 59.32$	$68.47 \\ 63.30 \\ 68.07 \\ 65.62$	71.0 69.9 71.0 69.9
TDGIA TDGIA ATDGIA ATDGIA	√ √	83.44 56.95 83.07 <b>42.18</b>	$83.44 \\ 73.38 \\ 83.07 \\ 70.30$	$85.72 \\79.45 \\85.39 \\\underline{76.87}$	$74.76 \\ 60.91 \\ 74.72 \\ \underline{61.08} \\$	74.76 <b>60.91</b> 74.72 <u>61.08</u>	75.26 72.51 75.12 <b>71.22</b>	88.32 <b>74.77</b> 86.03 80.86	88.32 <b>74.77</b> 86.03 80.86	91.40 90.42 91.41 <b>84.60</b>	$\begin{array}{r} 64.49 \\ \underline{49.36} \\ 66.95 \\ 45.59 \end{array}$	64.49 60.72 66.95 63.30	70.9 <b>63.5</b> 71.0 <u>64.3</u>
MLP			61.75	·····		65.55	·····		84.14			52.49	

 $\downarrow$  The lower number indicates better attack performance. <sup>†</sup>Runs with SeqGIA framework on Computers and Arxiv.

We evaluate with **38** defense models and report the *maximum* mean test robustness from multiple runs.

#### Table 1: Performance of non-targeted attacks against different models

# HAO significantly improves the performance of *all* attacks on *all* datasets up to 30%. Adaptive

### HAO Re-empowers GIA

injection strategies can further advance the state of the art.

#### **Homo:** Homophily Defenders

Vanilla: Vanilla GNNs, e.g., GCN, GAT, GraphSage.

**Robust:** Robust GNN models, or GNN models with robust tricks such as layer normalisation, or adversarial training.

**Combo:** Robust GNN models with robust tricks such as layer normalisation, or adversarial training.

	HAO	Computers( $\downarrow$ )			Arxiv(↓)			Aminer(↓)			Reddit(↓)		
		Homo	Robust	Combo	Homo	Robust	Combo	Homo	Robust	Combo	Homo	Robust	Comb
Clean		92.68	92.68	92.83	69.41	71.59	72.09	62.78	66.71	66.97	94.05	97.15	97.1
PGD PGD	$\checkmark$	$\begin{array}{c} 88.13 \\ 71.78 \end{array}$	$\begin{array}{c} 88.13 \\ 71.78 \end{array}$	$\begin{array}{c} 91.56 \\ 85.81 \end{array}$	69.19 <b>36</b> . <b>06</b>	69.19 <b>37</b> . <b>22</b>	$\begin{array}{c} 71.31 \\ 69.38 \end{array}$	$\begin{array}{c} 53.16\\ 34.62 \end{array}$	$\begin{array}{c} 53.16\\ 34.62 \end{array}$	$\begin{array}{c} 56.31\\ 39.47\end{array}$	$\frac{92.44}{56.44}$	$\frac{92.44}{86.12}$	93.0 <b>84</b> .9
MetaGIA <sup>†</sup> MetaGIA <sup>†</sup> AGIA <sup>†</sup> AGIA <sup>†</sup>	√ √	87.67 <u>70.21</u> 87.57 <b>69.96</b>	87.67 <u>71.61</u> 87.57 <b>71.58</b>	$91.56 \\ 85.83 \\ 91.58 \\ 85.72$	$69.28 \\ 38.44 \\ 66.19 \\ 38.84$	$\begin{array}{r} 69.28 \\ \underline{38.44} \\ 66.19 \\ 38.84 \end{array}$	71.22 $48.06$ $70.06$ $68.97$	$\begin{array}{c} 48.97 \\ 41.12 \\ 50.50 \\ 35.94 \end{array}$	$48.97 \\ 41.12 \\ 50.50 \\ 35.94$	$52.35 \\ 45.16 \\ 53.69 \\ 42.66$	92.40 <b>46.75</b> 91.62 80.69	92.40 90.06 91.62 88.84	93.9 90.7 93.6 90.4
TDGIA TDGIA ATDGIA ATDGIA	√ √	$87.21 \\ 71.39 \\ 87.85 \\ 72.00$	$87.21 \\ 71.62 \\ 87.85 \\ 72.53$	91.56 <b>77.15</b> 91.56 <u>78.35</u>	$\begin{array}{r} 63.66 \\ 42.56 \\ 66.12 \\ \underline{38.28} \end{array}$	$\begin{array}{c} 63.66 \\ 42.56 \\ 66.12 \\ 40.81 \end{array}$	71.06 42.53 71.16 39.47	51.34 25.78 50.87 22.50	51.34 25.78 50.87 22.50	$54.82 \\ \underline{29.94} \\ 53.68 \\ 28.91$	$\begin{array}{c} 92.19 \\ 78.16 \\ 91.25 \\ 64.09 \end{array}$	92.19 <b>85.06</b> 91.25 89.06	93.6 <u>88.6</u> 93.0 88.9
MLP		·····	84.11		·····	52.49			32.80			70.69	

 $\downarrow$  The lower number indicates better attack performance. <sup>†</sup>Runs with SeqGIA framework.

We evaluate with **38** defense models and report the *maximum* mean test robustness from multiple runs.

#### Table 2: Performance of targeted attacks against different models

# HAO significantly improves the performance of *all* attacks on *all* datasets up to 15%. Adaptive



#### HAO Re-empowers GIA

strategies can further advance the state of the art.

Model	$\mathbf{Cora}^{\dagger}$	Citeseer <sup>†</sup>	<b>Computers</b> <sup>†</sup>	$\mathbf{Arxiv}^{\dagger}$	<b>Arxiv</b> <sup>‡</sup>	<b>Computers</b> <sup>‡</sup>	<b>Aminer</b> <sup>‡</sup>	<b>Reddit</b> <sup>‡</sup>
Clean	84.74	74.10	92.25	70.44	70.44	91.68	62.39	95.51
PGD	61.09	54.08	61.75	54.23	36.70	62.41	26.13	62.72
+HAO	56.63	48.12	59.16	45.05	28.48	59.09	22.15	56.99
MetaGIA	$\overline{60.56}$	53.72	$\overline{61.75}$	$\overline{53.69}$	28.78	62.08	$\overline{32.78}$	60.14
+HAO	58.51	47.44	60.29	48.48	24.61	58.63	29.91	54.14
AGIA	60.10	54.55	60.66	48.86	32.68	$\overline{61.98}$	31.06	59.96
+HAO	53.79	48.30	58.71	48.86	29.52	58.37	26.51	56.36
TDGIA	66.86	52.45	66.79	49.73	31.68	62.47	32.37	57.97
+HAO	65.22	46.61	65.46	49.54	22.04	59.67	22.32	54.32
ATDGIA	61.14	$\overline{49.46}$	65.07	46.53	32.08	64.66	24.72	$\overline{61.25}$
+HAO	58.13	<b>43.41</b>	63.31	<b>44.40</b>	29.24	59.27	<b>17.62</b>	56.90

 Table 9: Full Averaged performance across all defense models

The lower is better. <sup>†</sup>Non-targeted attack. <sup>‡</sup>Targeted attack.

We evaluate with 38 defense models and report the mean test robustness of all models from multiple runs.

# HAO consistently improves the performances of *all* attacks on *all* datasets up to 5%. Adaptive injection



Varying  $\lambda$  in HAO



### Summary

We provide a formal comparison between GIA and GMA in a unified setting and find that GIA can be provably more harmful than GMA due to its high flexibility (Theorem 1).

However, the flexibility of GIA will cause severe damage to the homophily which makes GIA easily defendable by homophily defenders (Theorem 2).

To mitigate the issue, we introduce the concept of homophily unnoticeability and a novel objective HAO to conduct homophily unnoticeable attacks (Theorem 3).









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### **Future Navigations**





If you focus on other domains: more unnoticeability constraints & the corresponding external examiners...





I NANK YOU!

If you focus on graph domain: more advanced injection strategies, more downstream tasks, more attack scenarios, more robust GNNs...

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*Figure source: navigate360* 

