

Trustworthy AI for Graphs

CPSC483: Deep Learning on Graph-Structured Data

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Readings

- Readings are updated on the website (syllabus page)
- **PyG Lecture Readings:**
 - [Documentation](#)
 - [GitHub](#)
- **Lecture 15 readings:**
 - [Trustworthy Graph Neural Networks](#)
 - [GraphFramEx](#) Evaluation

Outline of Today's Lecture

- 1. Intro to Trustworthy GNN**
- 2. Adversarial Attacks and Robustness of GNNs**
- 3. Explainability for GNNs**

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Trustworthy Graph Learning

- **Trustworthy** AI/GNN includes many components
 - Explainability, fairness, robustness, privacy, ...
 - Algorithms to tackle combination of these aspects
- **Challenges**
 - Role of graph topology is previously unexplored in these problems
 - Comprehensive quantitative evaluation

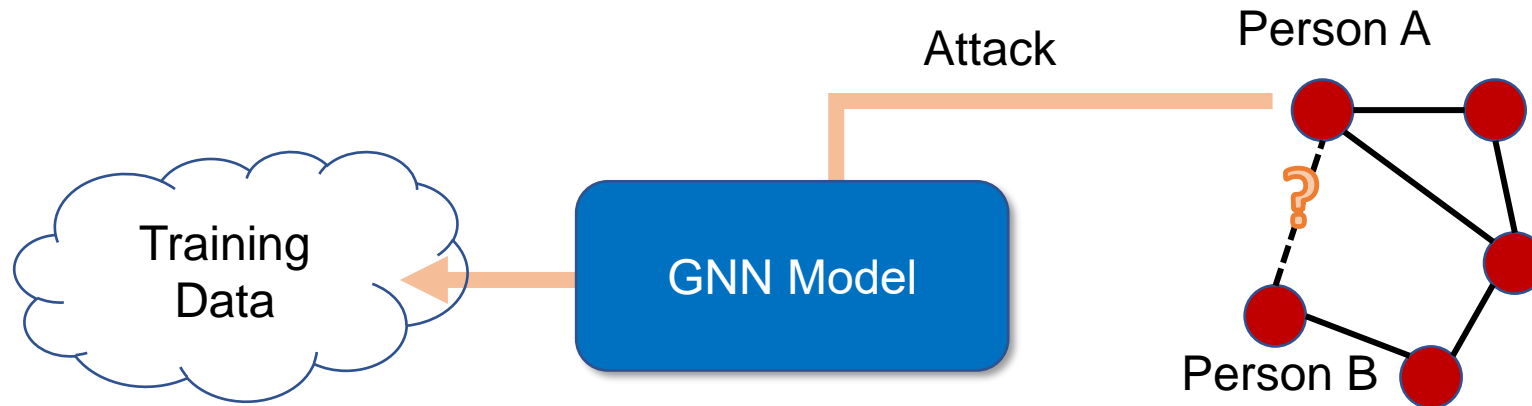
Aspects of Trustworthy GNNs

- **Robustness** (part 2)
- **Explainability** (part 3)
- Privacy
- Fairness
- Accountability
- Environmental well-being
- Others

How does each aspect play a role in gaining trust from users of machine learning models?

Privacy of GNNs

- Prevent private data within GNNs from being leaked
 - Training data
 - Model parameters
- Ex) Query social relations between two people by attacking the GNN model



Privacy of GNNs: Attack

- **Model extraction attacks**
 - Steal architecture and parameters of a GNN model.
- **Membership inference attacks**
 - Infer whether a node/link/graph belongs to the training set of a GNN model.
- **Model inversion attacks**
 - Infer a GNN model's inputs from their corresponding outputs.
- **Other privacy attacks**

Privacy of GNNs: Privacy-Preserving Techniques

- **Federated Learning**

- Calculate gradients on **individuals** using their own data
- Aggregate parameters (e.g. gradients/model weights) on the server

- **Differential Privacy**

- Add noise to data, such that
 - **Meaningless** when viewed individually
 - But approximate the analytics results when **aggregated**
- Noise can cancel out when performing the mean aggregation operation in GNN layers.

- **Insusceptible Training**

Original task loss Attack function: try to distinguish the private labels

$$\min_{\theta} \sum_{v_i \in \mathcal{V}} \mathcal{L}_Y(f_{\theta}(v_i)) + \lambda \mathcal{L}_A(\mathcal{F}_A(v_i))$$

- **Security Computation**

- More related to system/hardware

Privacy-preserving loss: e.g. make the attack function's output probability close to 0.5 for the private labels

Fairness of GNNs

- **Goal:** exclude prejudice or favoritism towards an individual or a group.
 - For example, in a bank's transaction network, the model should not learn to make predictions of loans based on gender, race or other protected characteristics.
- **Prevent Bias & Discrimination**
 - **Bias:** unfair operation in data collection, sampling, measurements, ...
 - **Discrimination:** incorporation of intentional or unintentional human prejudices and stereotyping in deep learning models

Fairness of GNNs: Methods

- **Fair representation learning methods**

- Learn representations, from which one cannot infer sensitive attributes.
- A common technique is **adversarial training**

- **Fair prediction enhancement methods**

- **Data augmentation**

- Perturbation of protected features

- **Fair graph**

- Modify graph structures (e.g. drop edges that may induce bias)

- **Regularisation**

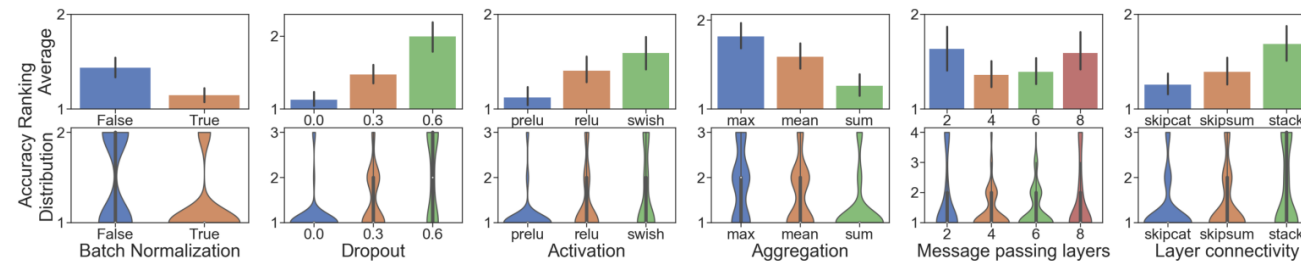
- Ex) any two individuals who are similar should receive similar algorithmic outcome

$$\| \mathbf{Y}[i, :] - \mathbf{Y}[j, :] \|_F^2 \mathbf{S}[i, j] \leq \delta$$

Predictions of node i Similarity between node i and j

Accountability of GNNs

- **Accountability** refers to the extent to which people can trust GNNs by assessing a complex GNN system
- **Benchmarking**: detect violation of utility
 - Architecture design, Model training, Model validation



- **Security evaluation**: detect violation of security
 - Data integrity verification
 - Procedure integrity verification

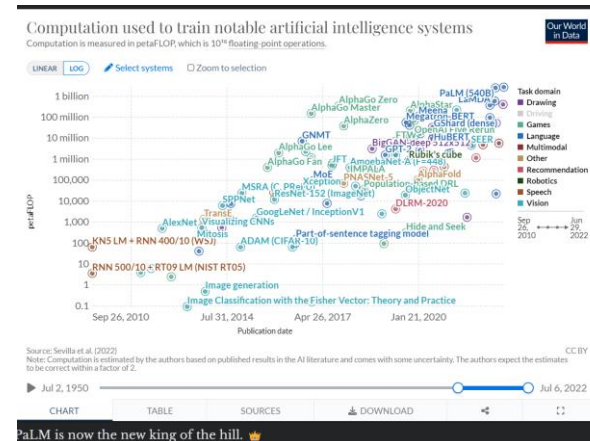
Environmental Well-Being of GNNs

- GNNs should conform to **the fundamental values of the society** in which they are deployed
 - Large-scale graph datasets → GNN execution efficiency
 - Deeper or more complex architectures → GNN's deployment on edge devices
 - The unique characteristics of graph data → specially designed software and hardware



Compute Clusters

Credit: Imaginima/E+/gettyimages



Large model training involves 10^{24} flops

<https://blog.heim.xyz/palm-training-cost/>

tl;dr What would it cost you to train PaLM using cloud computing (and you're not Google)?
Something around **\$9M to \$23M**.

PaLM a 540B state-of-the-art language model

Google recently published a new paper presenting PaLM (their blogpost) – a 540B parameter large language model.

Input: Jennifer looked out her window and sees a really cool cloud below her. She unbuckles her seatbelt and heads to the bathroom. Is Jennifer probably traveling more than 300 miles per hour relative to the earth?

Model Output: 300 miles per hour is about 480 km/h. This is about the speed of a commercial airplane. Clouds are usually below airplanes, so Jennifer is probably on an airplane. The answer is "yes".

540 B parameter pretrained model

<https://blog.heim.xyz/palm-training-cost/>

Environmental Well-Being of GNNs: Methods

- **Scalable GNN**
 - We've already talked about it in [Lecture 6](#)
- **Model compression**
 - Knowledge distillation
 - Model pruning
 - Reducing parameters
 - Model quantisation
- **Efficient frameworks and accelerators**
 - Software: [PyTorch Geometric](#), **Efficient AutoML**
 - Hardware: [EnGN](#), [HyGCN](#)

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2. Adversarial Attacks and Robustness of GNNs

3. Explainability for GNNs

Deep Learning Performance

- Recent years have seen **impressive performance of deep learning models in a variety of applications.**
 - In computer vision, **deep convolutional networks** have achieved human-level performance on ImageNet (image category classification)
- **Are these models ready to be deployed in real world?**

Adversarial Examples

- Deep convolutional neural networks are vulnerable to **adversarial attacks**:
 - Imperceptible noise changes the prediction.



“Panda”

57.7% confidence

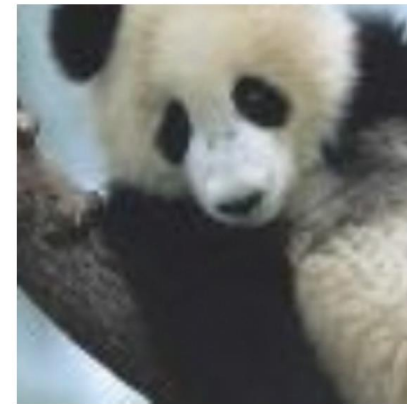
+ .007 ×



Carefully

calculated noise

=



“Gibbon”

93.3% confidence

Goodfellow, I., Shlens, J., & Szegedy, C.. (2014). Explaining and Harnessing Adversarial Examples.

- Adversarial examples are also reported in natural language processing [Jia & Liang et al. EMNLP 2017] and audio processing [Carlini et al. 2018] domains.

Implication of Adversarial Examples

- **The existence of adversarial examples prevents the reliable deployment of deep learning models to the real world.**
 - Adversaries may try to actively hack the deep learning models.
 - The model performance can become much worse than we expect.
- **Deep learning models are often not robust.**
 - It is an active area of research to make these models robust against adversarial examples

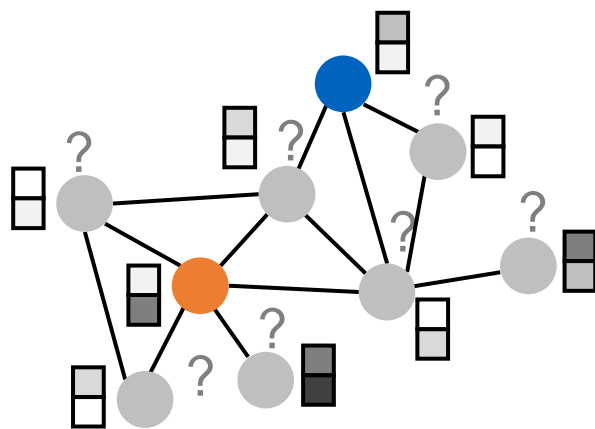
Robustness of GNNs

- **This lecture: How about GNNs? Are they robust to adversarial examples?**
- **Premise:** Common applications of GNNs involve **public platforms** and **monetary interests**.
 - Recommender systems
 - Social networks
 - E-commerce platforms
- **Adversaries have the incentive to** manipulate input graphs and hack GNNs' predictions.

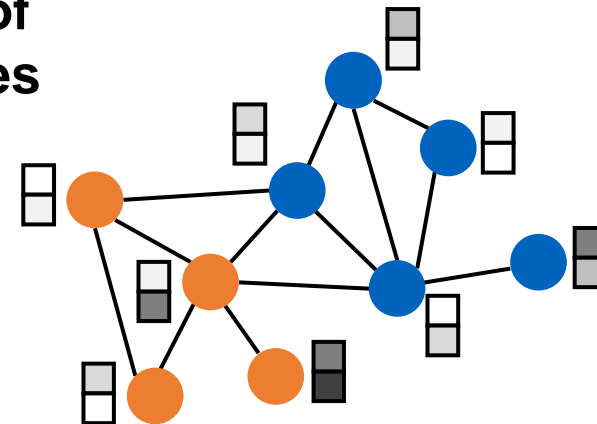
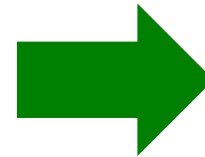
Setting to Study GNNs' Robustness

- To study the robustness of GNNs, we specifically consider the following setting:
 - **Task**: Semi-supervised node classification
 - **Model**: GCN [Kipf & Welling ICLR 2017]

?: Unlabeled



Predict labels of unlabeled nodes

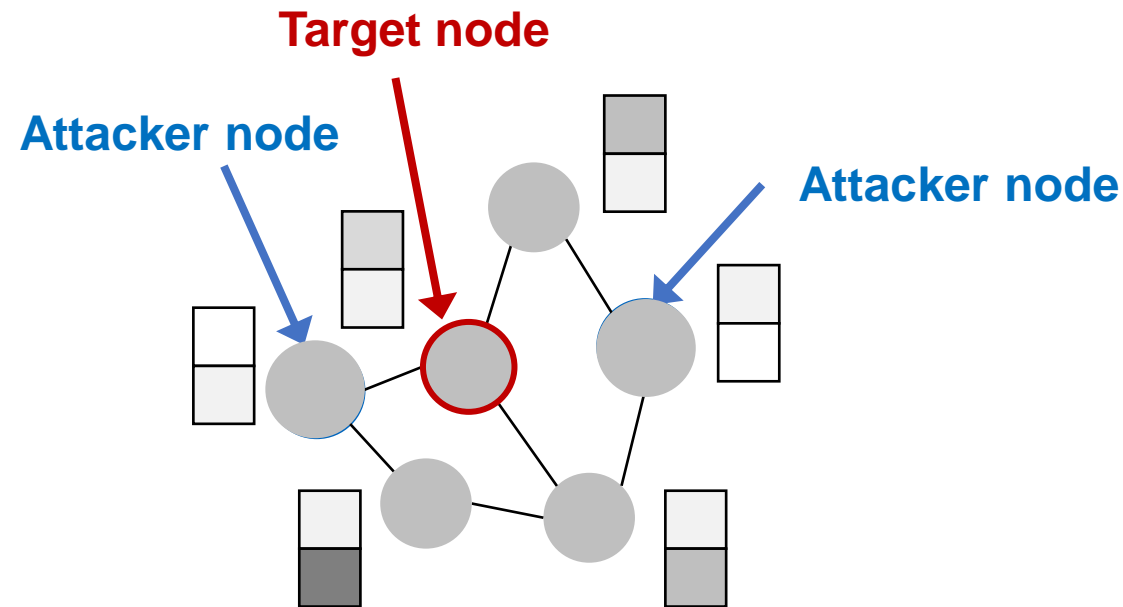


Roadmap

- We first describe several real-world **adversarial attack possibilities**.
- We then review the GCN model that we are going to attack (**knowing the opponent**).
- We mathematically **formalize the attack problem as an optimization problem**.
- **We empirically see how vulnerable GCN's prediction is to the adversarial attack.**

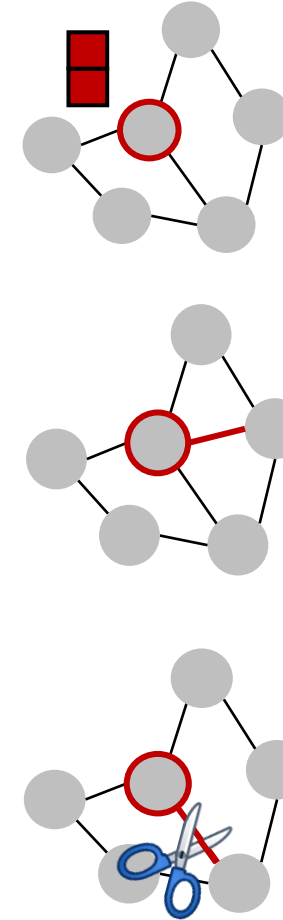
Attack Possibilities

- What are the attack possibilities in real world?
 - **Target node** $t \in V$: node whose label prediction we want to change
 - **Attacker nodes** $S \subset V$: nodes the attacker can modify



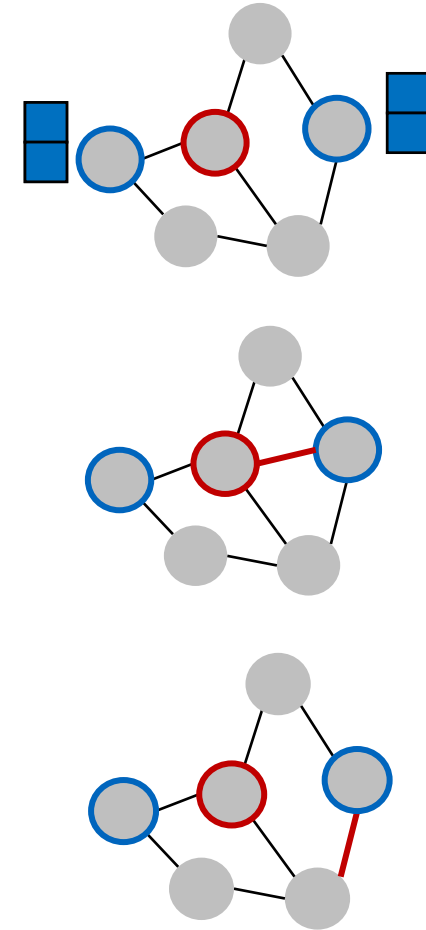
Attack Possibilities: Direct Attack

- **Direct Attack: Attacker** node is the **target** node: $S = \{t\}$
- Modify **target** node feature
 - Change website content
- Add connections to **target**
 - Buy/likes/follows
- Remove connections from **target**
 - Unfollow users



Attack Possibilities: Indirect Attack

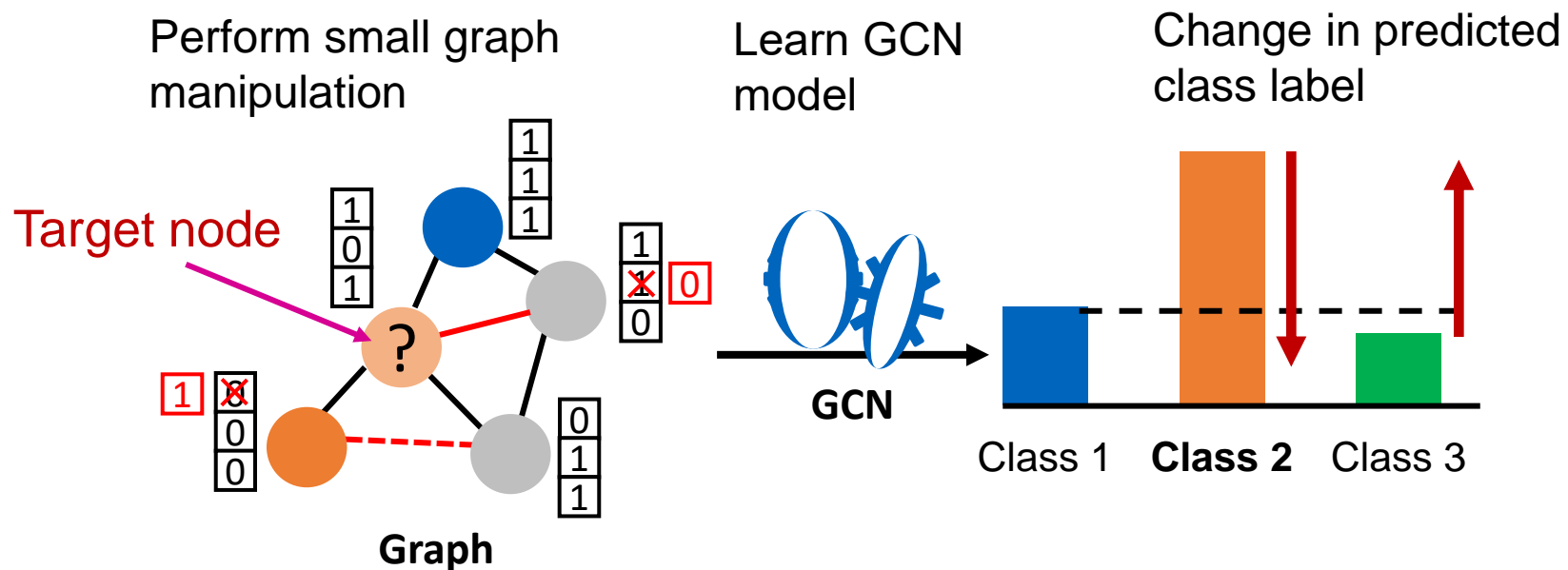
- **Indirect Attack:** The **target** node is not in the **attacker** nodes: $t \notin S$
- Modify **attacker** node features
 - Ex) Hijack friends of targets
- Add connections to **attackers**
 - Ex) Create a link, link farm
- Remove connections from **attackers**
 - Ex) Delete undesirable link



Formalizing Adversarial Attackers

- **Objective for the attacker:**

Maximize (**change of target node label prediction**)
Subject to (**graph manipulation is small**)



If graph manipulation is too large, it will easily be detected. Successful attacks should change the target prediction with “unnoticeably-small” graph manipulation.

Mathematical Formulation (1)

- **Original graph:**
 - A : adjacency matrix, X : feature matrix
- **Manipulated graph (after adding noise):**
 - A' : adjacency matrix, X' : feature matrix
- **Assumption:** $(A', X') \approx (A, X)$
 - Graph manipulation is **unnoticeably small**.
 - Preserving basic graph statistics (e.g., degree distribution) and feature statistics.
 - Graph manipulation is either **direct** (changing the feature/connection of target nodes) or **indirect**.

Mathematical Formulation (2)

- **Target node:** $v \in V$

- Recall that we only consider semi-supervised node classification settings

- GCN learned over the **graph**

$$\theta^* = \operatorname{argmin}_{\theta} \mathcal{L}_{train}(\theta; \tilde{A}, \tilde{X})$$

What is \tilde{A} and \tilde{X} ?

- GCN's original prediction on the **target node**:

$$c_v^* = \operatorname{argmax}_c f_{\theta^*}(\mathbf{A}, \mathbf{X})_{v,c}$$

Predict the class c_v^* of vertex v that has the highest predicted probability

- GCN's manipulated prediction on the target node

$$c_v^{*'} = \operatorname{argmax}_c f_{\theta^*}(\mathbf{A}', \mathbf{X}')_{v,c}$$

- **We want the prediction to change after the graph is manipulated:**

$$c_v^{*'} \neq c_v^*$$

Mathematical Formulation (3)

- What is $\tilde{\mathbf{A}}, \tilde{\mathbf{X}}$?
- Evasion Attack: $\tilde{\mathbf{A}} = \mathbf{A}, \tilde{\mathbf{X}} = \mathbf{X}$
 - Attacking happens after the GNN model is trained (at test time)
 - Inductive setting
- Poisoning Attack: $\tilde{\mathbf{A}} = \mathbf{A}', \tilde{\mathbf{X}} = \mathbf{X}'$
 - Attacking happens before the GNN model is trained.

Mathematical Formulation (4)

- Change of prediction on target node v :

$$\Delta(v; A', X') =$$

$$\log f_{\theta^*}(A', X')_{v, c_v^{*'}} - \log f_{\theta^*}(A', X')_{v, c_v^*}$$

Predicted (log)
probability of the
newly-predicted
class $c_v^{*'}$



Want to increase
this term

Predicted (log)
probability of the
originally-predicted
class c_v^*



Want to decrease
this term

Mathematical Formulation (5)

- **Final optimization objective:**

$$\begin{aligned} &\operatorname{argmax}_{A', X'} \Delta(v; A', X') \\ &\text{subject to } (A', X') \approx (A, X) \end{aligned}$$

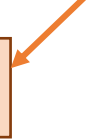
- **Challenges in optimizing the objective**

- Adjacency matrix A' is a discrete object: gradient-based optimization cannot be used.
- Several approximations are proposed to make the optimization.

Nettack: Greedy Scheme

- A **greedy** scheme
- while $|A' - A| + |X' - X| < \delta$
 - Compute a **candidate set** for **struct perturbations** (all should be **unnoticeable**)
 - Pick the one which obtains the **highest** change of predictions
 - Compute a candidate set for **node features perturbations** (all should be **unnoticeable**)
 - Pick the one which obtains the **highest** change of predictions
- Challenges in this scheme:
 - How to make sure the perturbation is **unnoticeable** (budget δ is not enough)?
 - How to efficiently compute the **candidate sets**?
 - How to efficiently get the one which make the **highest change**?

Manipulation budget

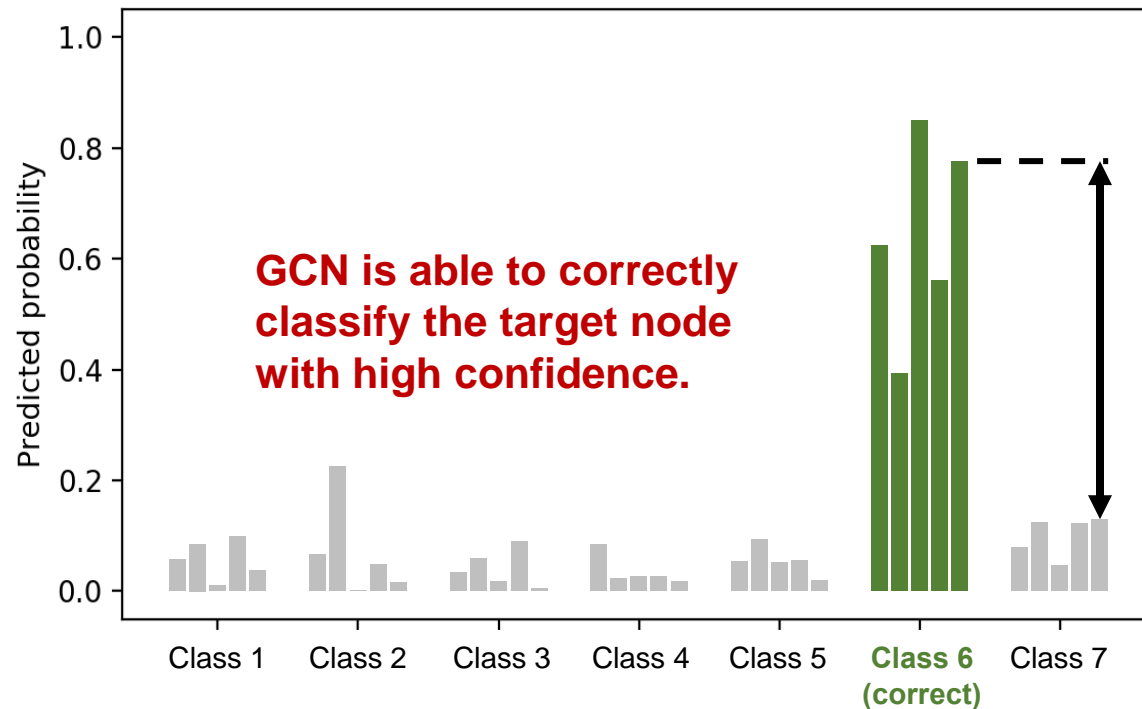


Netattack: Candidate Sets

- Efficiently compute **candidate sets** which make **unnoticeable** changes
- Main idea: use **significance test**
- **Graph structure** preserving perturbations
 - Preserve a graph's degree distribution (usually follow $p(x) \propto x^{-\alpha}$)
 - Can be **incrementally computed (constant time)** during changes
- **Feature statistics** preserving perturbations
 - Preserve feature co-occurrence
 - Can be **precomputed**
- Find more details in [\[Zügner, KDD 2018\]](#)

Experiments: Adversarial Attack (1)

- Semi-supervised node classification with GCN on a paper citation network (2,800 nodes, 8,000 edges).

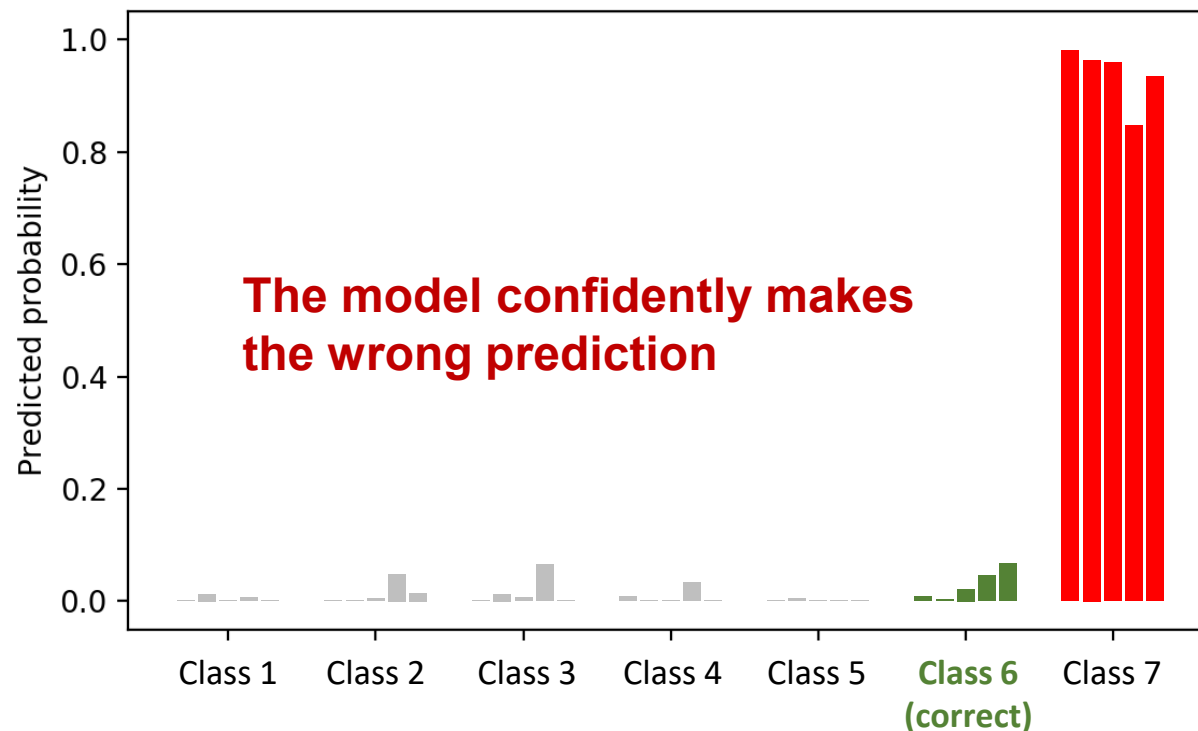


Predicted probabilities over 5 re-trainings
(without graph manipulation, i.e., clean graph)

Classification margin
> 0: Correct classification
< 0: Incorrect classification

Experiments: Adversarial Attack (2)

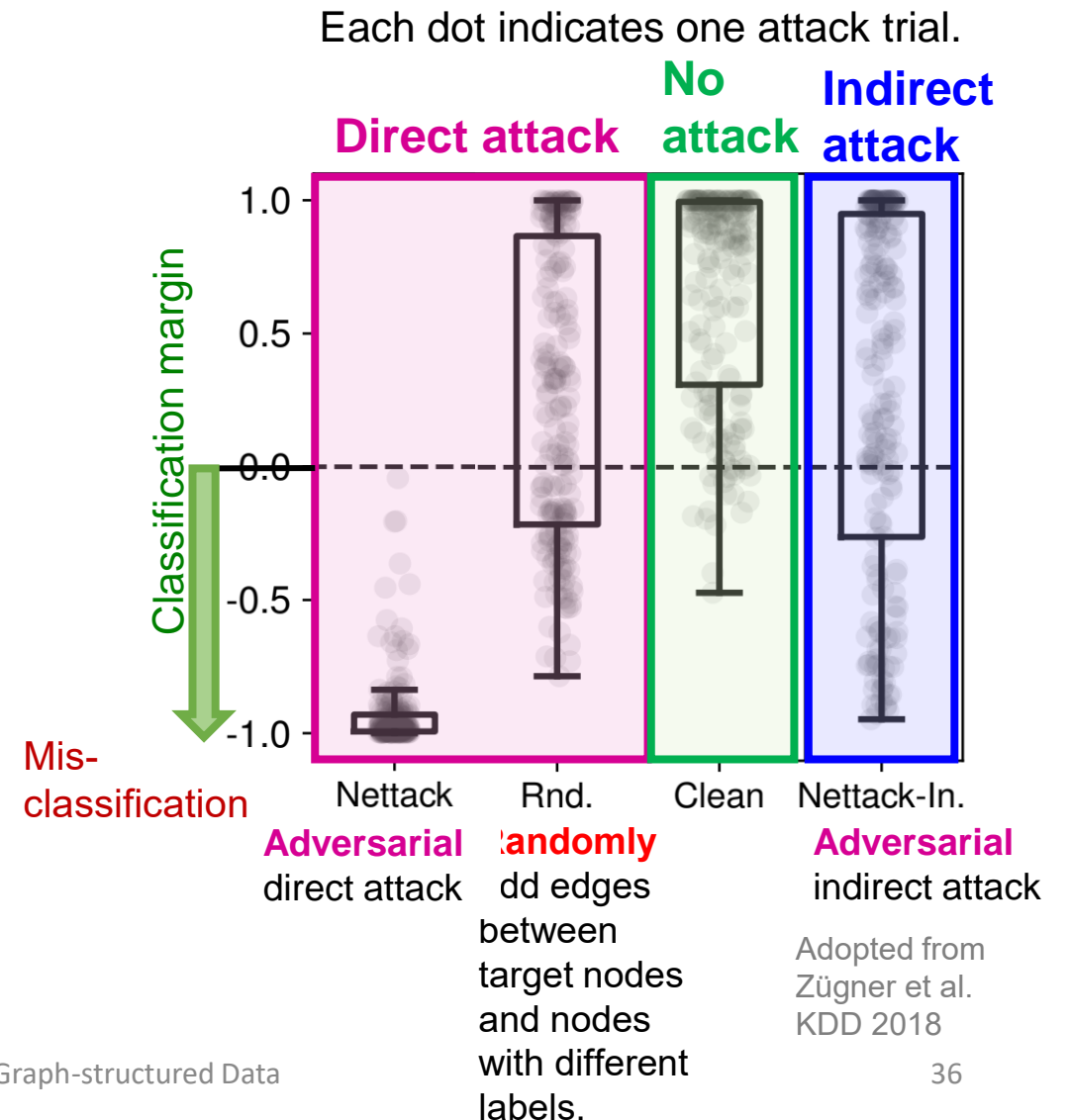
- GCN's prediction after carefully modifying just 5 edges attached to the target node (**direct adversarial attack**).



Predicted probabilities over 5 re-trainings
(with adversarial attacks)

Experiments: Attack Comparison

- **Adversarial direct attack** is the strongest attack, significantly worsening GCN's performance (compared to **no attack**).
- **Random** attack is much weaker than **adversarial** attack.
- **Indirect attack** is more challenging than direct attack.



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2. Adversarial Attacks and Robustness of GNNs

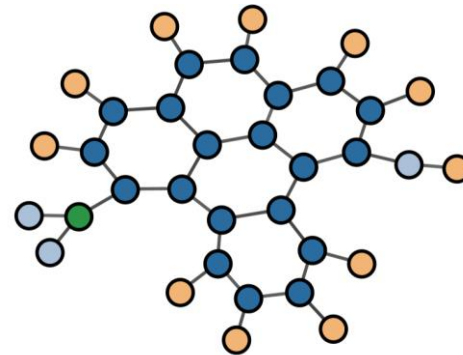
3. Explainability for GNNs

Explainability: Motivation (1)

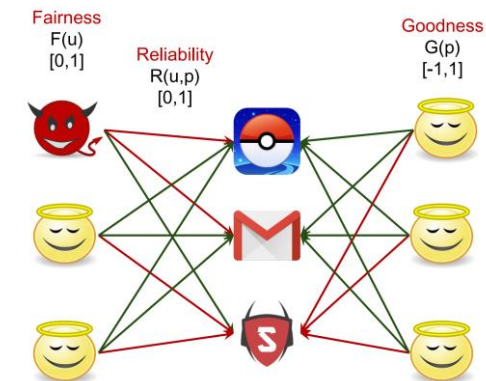
- Example questions after training GNNs:
 - Why is an item recommended to a user?
 - Why is the molecule mutagenic?
 - Why is the user classified as fraudulent?
- How to let the domain experts understand and trust the GNN model?



Recommender System



Mutagenic Molecule



Fraudulent Detection

Explainability: Motivation (2)

- **Example questions after training GNNs:**
 - Why is an item recommended to a user?
Explain link prediction
 - Why is the molecule mutagenic?
Explain graph classification
 - Why is the user classified as fraudulent?
Explain node classification
- **Need to provide explanations to GNN models!**

Deep Learning Explainability Methods: Examples

- **Proxy Model**

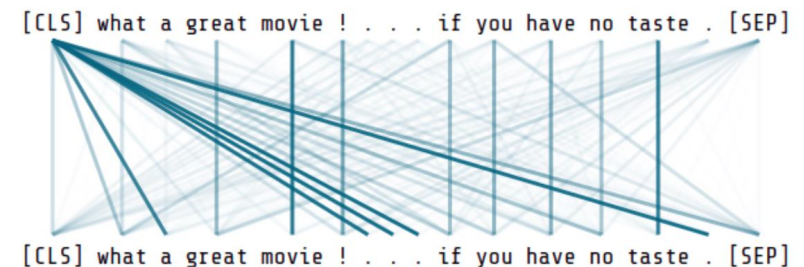
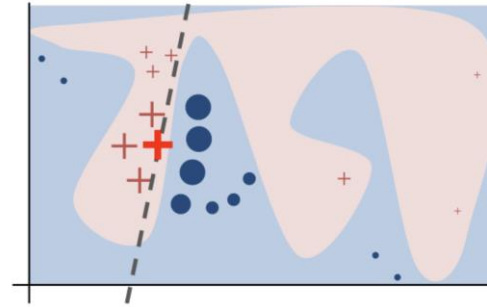
- Learn a inherently interpretable model locally approximating the original model (e.g. a linear model, interpret by weights).

- **Saliency Maps**

- Compute gradients of outputs w.r.t. input pixels.

- **Attention Mechanisms**

- Visualize attention weights in a attention models

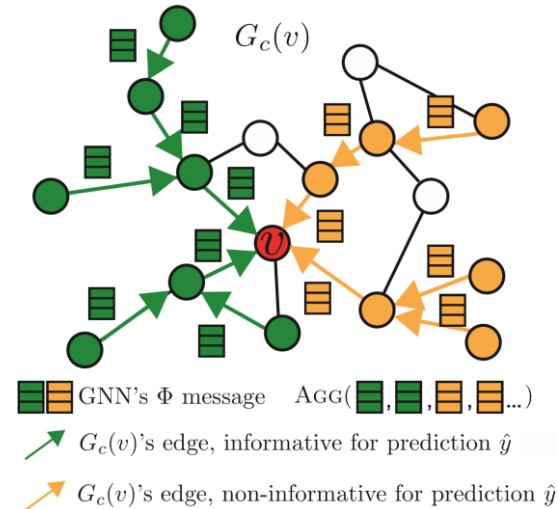


Challenges of Applying these Methods to Graphs

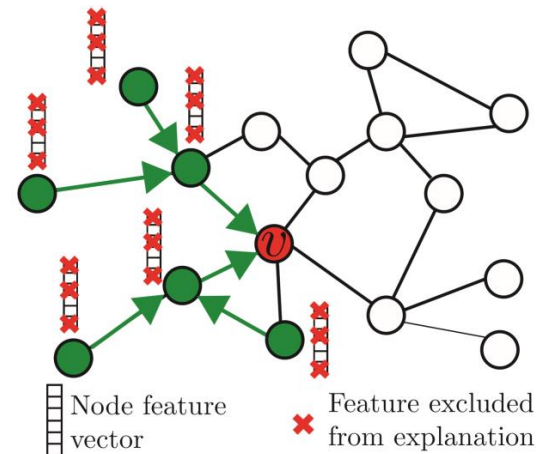
- Why is it non-trivial to apply these explainability methods to graph structure?
 - predictions on graphs are induced by a complex combination of nodes and paths of edges between them (not only nodes).

How to explain a GNN

- Message passing structure
- The importance of node features



Structural explanation

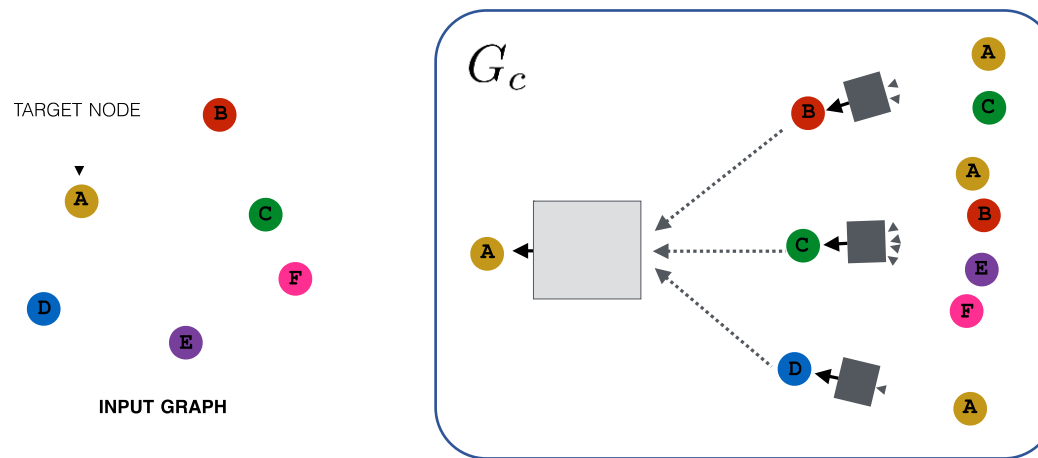


Feature explanation

- GNNExplainer explain both aspects **simultaneously**

GNNExplainer Input

- Without loss of generality, consider node classification task:

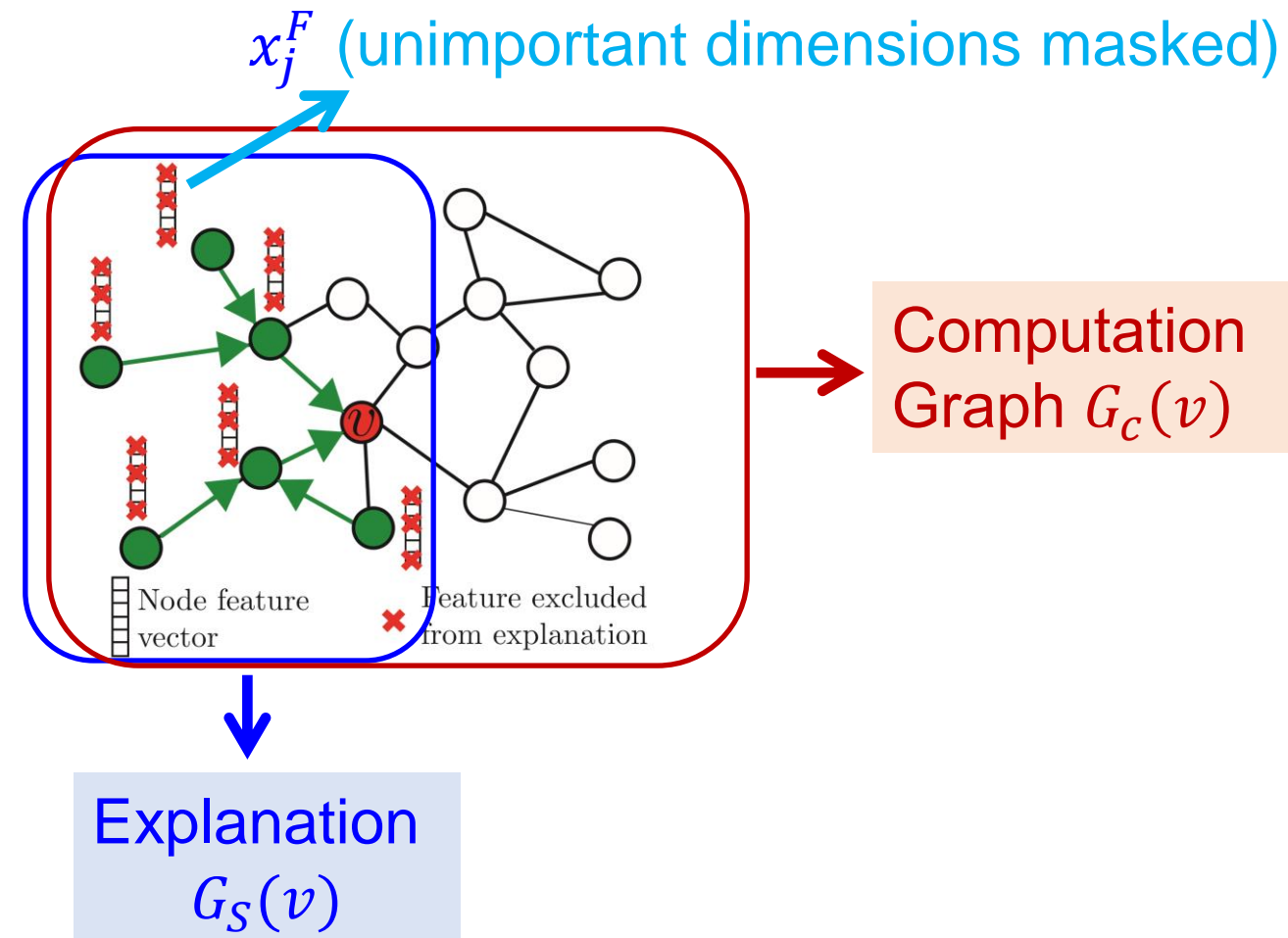


Suppose GNN predicts label \hat{y} for node v

- Input computation graph: $G_c(v)$
- Adjacency matrix of G_c : $A_c(v) \in \{0,1\}^{n \times n}$
- Node Feature: $X_c(v) = \{x_j | v_j \in G_c(v)\}$

GNNExplainer Output

- GNN model ϕ learns $P_{\phi}(Y \mid A_c(v), X_c(v))$
- Y denotes predicted label of v
- **GNNExplainer** outputs (A_S, X_S^F)
- Graph G_S with adjacency matrix A_S is a subgraph of graph with adjacency matrix $A_c(v)$ (omit v)
- $X_S^F = \{x_j^F \mid v_j \in G_S\}$ are features for G_S
- Mask F masks out unimportant dimensions



Explain by Mutual Information

- **Mutual information (MI)**

- A measure of the mutual correlation between the two random variables.
- Good explanation should have **high correlation** with model prediction
- **Relation to entropy:**

$$MI(X; Y) = H(X) - H(X|Y) = H(Y) - H(Y|X)$$

- GNNExplainer **Objective:**

- **Maximize MI** between **label** and **explanation**

$$\max_{G_S} MI(\mathbf{Y}; (\mathbf{A}_S, \mathbf{X}_S)) = H(Y) - H(\mathbf{Y} | \mathbf{A} = \mathbf{A}_S, \mathbf{X} = \mathbf{X}_S^F)$$

Explain by Optimization

- By **relation to entropy**:
equivalent to minimize conditional entropy

$$\max_{A_S} MI(Y|(A_S, X_S)) = \min_{A_S} H(Y|A = A_S, X = X_S^F)$$


Subgraph Feature subset

- Finding A_S that minimizes the conditional entropy is **computationally expensive!**
 - Exponentially many possible A_S
- **Solution**: Treat explanation as a distribution of “**plausible explanations**”, instead of a single graph
 - Optimize the expected explanation
 - **Benefit 1**: captures multiple possible explanations for the same node
 - **Benefit 2**: turns discrete optimization to continuous

GNNExplainer Model

- continuous relaxation

- Optimize the expected adjacency matrix A_S
expectation of explanations

$$\min_{\mathcal{A}} \mathbb{E}_{A_S \sim \mathcal{A}} H(Y|A = A_S, X = X_S)$$

- View $\mathbb{E}_{A_S \sim \mathcal{A}}$ as an adjacency matrix where entries are continuous

- Approximation

$$\min_{\mathcal{A}} H(Y|A = \mathbb{E}_{\mathcal{A}}[A_S], X = X_S)$$

- Optimize the expectation by masking

Element-wise multiply

- Use $A_C \odot \text{Mask}$ to represent $\mathbb{E}_{\mathcal{A}}[A_S]$

- If Mask_{ij} close to 1, keep edge (i, j) ; if close to 0, drop edge (i, j) .

GNNExplainer Model

- Let $\text{Mask} = \sigma(\mathbf{M})$ be the adjacency mask
 - Continuous relaxation: $\sigma(\mathbf{M}) \in \mathbb{R}$ instead of binary
 - **Sigmoid** function σ squashes \mathbf{M} into $[0, 1]$
 - Masking: Element-wise multiply $\sigma(\mathbf{M})$ by \mathbf{A}_c
- Assume edges are independent

$$P_{\mathcal{A}}(\mathbf{A}_S) = \prod_{e=(j,k) \in G_c(v_i)} \mathbf{A}_S[j, k]$$

- Objective:

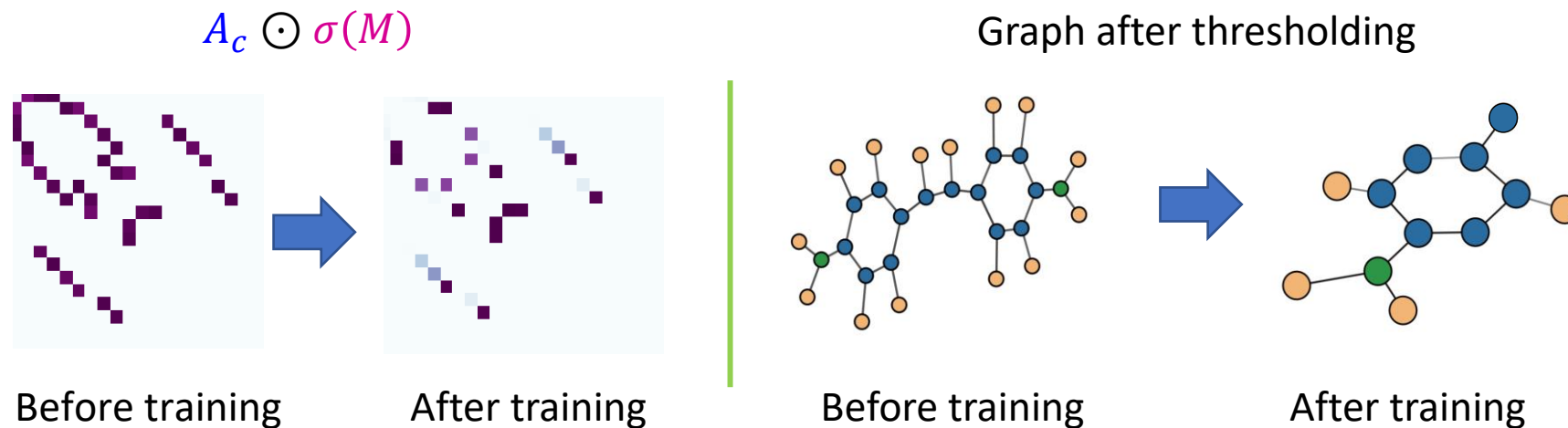
$$\min_{\mathbf{M}} -H(\log P_{\phi}(Y = y | G = \mathbf{A}_c \odot \sigma(\mathbf{M}), X = X_S))$$

GNNExplainer Model

- Optimize M :

$$\min_M -H(\log P_{\phi}(Y = y | A = A_c \odot \sigma(M), X = X_S))$$

- $A_c \odot \sigma(M)$ is the relaxed adjacency matrix
- Threshold $A_c \odot \sigma(M)$ to get G_S
- Example:



Feature Explanation

- Similarly select features by **masking**

$$X_S^F = \{x_j^F \mid v_j \in G_S\}, \quad x_j^F = [x_{j,t_1}, \dots, x_{j,t_k}]$$

For the **selected dimensions**, $\sigma(F_{t_i}) \rightarrow 1$

- **Problem**: Zero value could be important!
- **Solution**: Measure feature importance by how much drop in model confidence when features are replaced with random values.
(See paper for details)

Regularization Constraints

- Optimize feature and adjacency masks jointly with regularization

- **Concise explanation**

- Mask size: $\text{Sum}(\sigma(M))$
- Feature size: $\text{Sum}(\sigma(F))$

- **Final Objective**

$$\min_M -H(\log P_{\phi}(Y = y | G = A_c \odot \sigma(M), X = X_S^F)) + \lambda_1 \underbrace{\text{Sum}(\sigma(M)) + \lambda_2 \text{Sum}(\sigma(F))}_{\text{Sum of entries in feature and adjacency masks}}$$

- Threshold $A_c \odot \sigma(M)$ to get the explanation G_S

GNNExplainer Model

- **Task extensions**

- Link prediction: optimize mask on union of 2 node neighborhoods
- Graph classification: optimize mask on graph

- **Can adapt to different architectures**

- Graph Attention Networks
- Gated Graph Sequence
- Graph Networks
- GraphSAGE
- Jumping Knowledge Networks

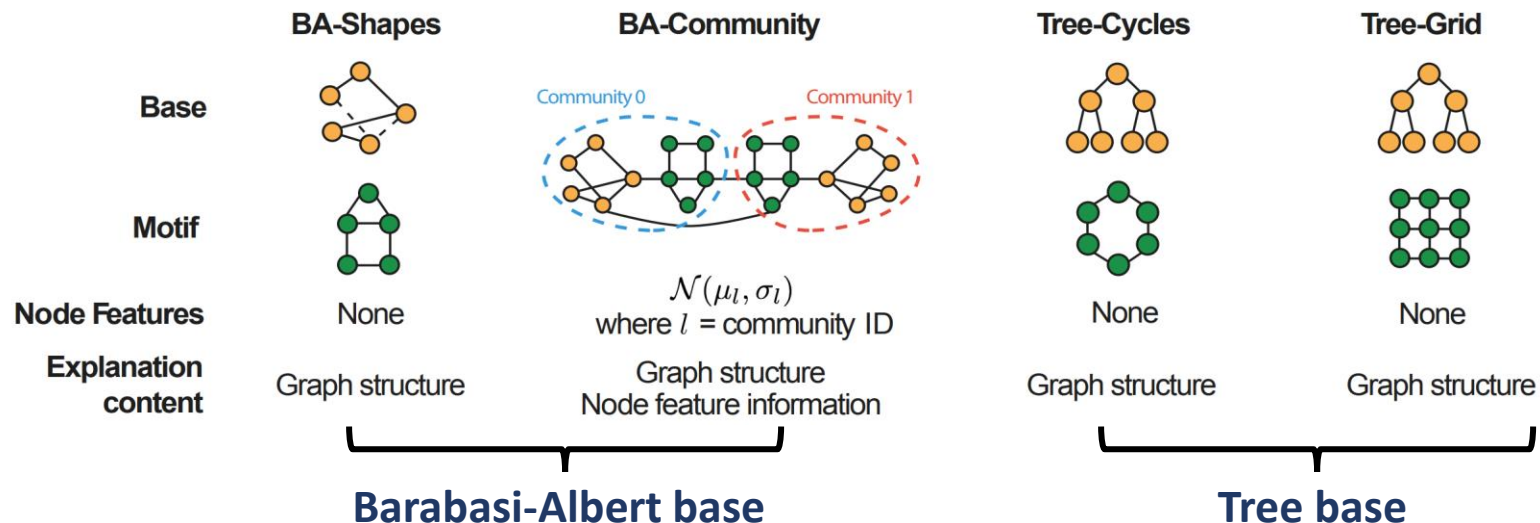
We use GNN
general formulation

Experiments: Baselines

- GNN saliency map based on gradients of output score w.r.t. inputs
- Attention values based on Graph Attention Networks (GAT)
 - Edge importance indicated by average attention weights across layers for each edge

Experiments: Datasets (1)

- Synthetic task: **is a node part of a given motif?**
 - 100 Motifs are randomly attached to nodes in base graphs (500 nodes)
 - **Node classification (structural roles)**



Experiments: Datasets (2)

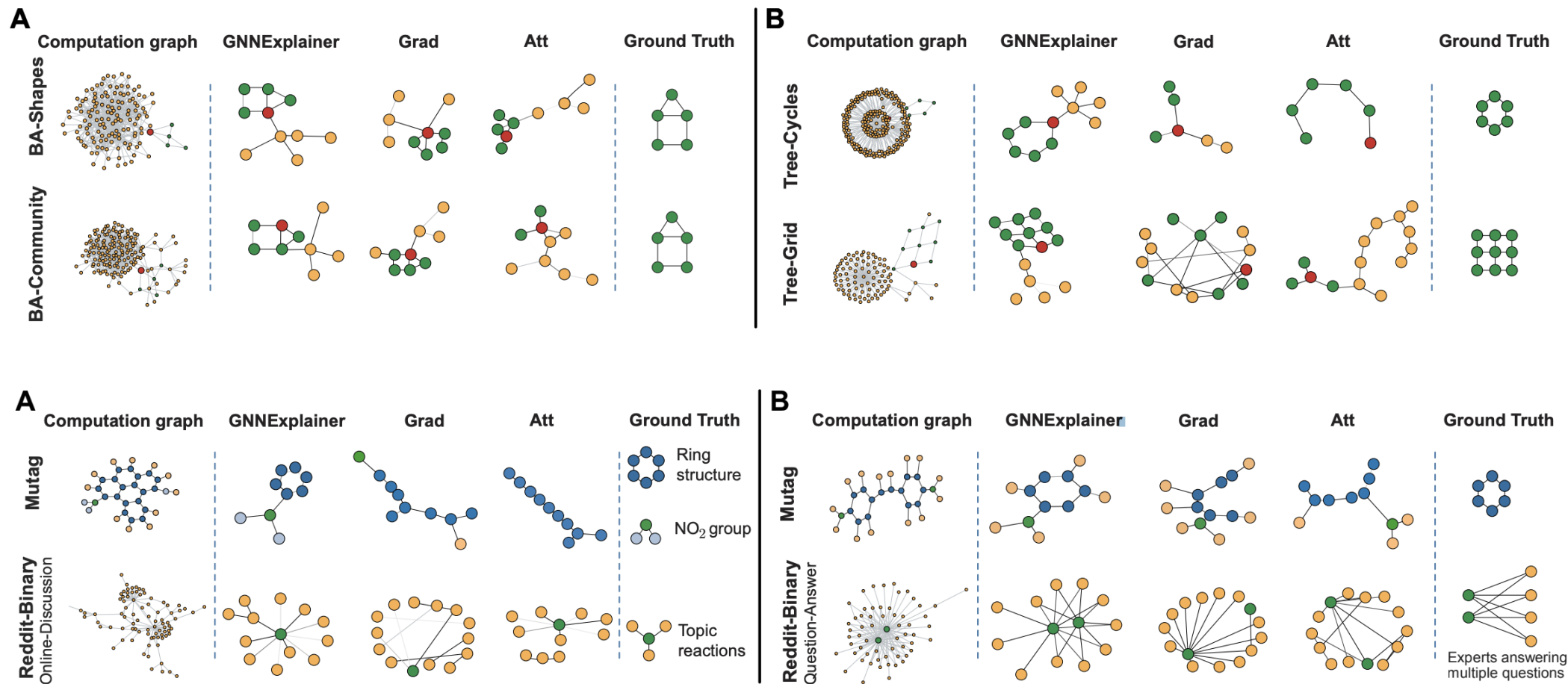
- Real-world tasks
 - Social networks (Reddit-binary dataset)
 - Reddit community prediction
 - Chemistry (Mutagenic molecule dataset)
 - Chemical property prediction
 - Graph classification

Results: Quantitative Analysis

- Node classification with ground-truth
- Measures accuracy of **explanation** with respect to **ground-truth**

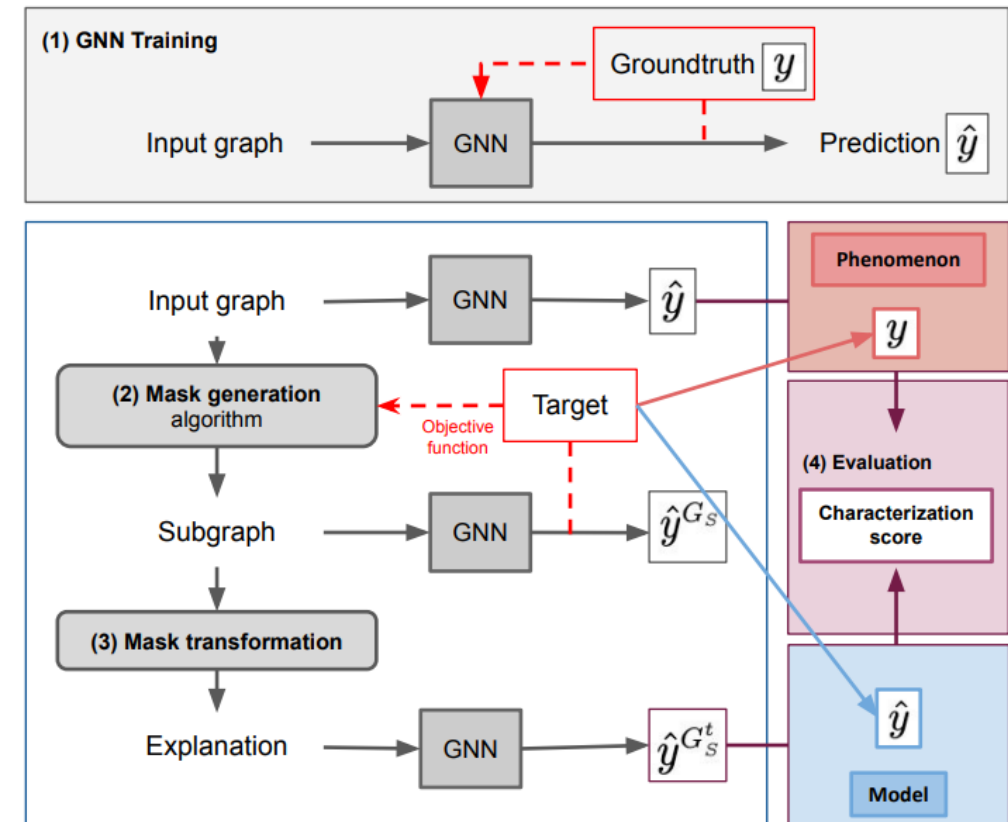
	BA-House	BA-Comm	Tree-Cycle	Tree-Grid
Grad	88.2	73.9	82.4	61.2
Att	81.5	75.0	90.5	66.7
GNN-Explainer	92.5	83.6	94.8	87.5

Results: Qualitative Analysis



Explainability Method Evaluation

- **Challenge: groundtruth might not always be available**
- Evaluation is **multi-dimensional**
- **Goal** (phenomenon vs. model)
- **Masking** strategy
- **Type** (sufficiency vs. necessity)
- **GraphFramEx**
- Benchmarks and evaluation criteria for graph explainability



Explanation Goal

- **Phenomenon** Explanation
 - Explain the underlying reasons for the ground truth phenomenon
- **Model** Explanation
 - Explain why model makes a particular prediction
- Adapt the **fidelity** measure for both cases

Phenomenon

$$fid_+ = \frac{1}{N} \sum_{i=1}^N \left| \mathbb{1}(\hat{y}_i = y_i) - \mathbb{1}(\hat{y}_i^{G_{C \setminus S}} = y_i) \right|$$
$$fid_- = \frac{1}{N} \sum_{i=1}^N \left| \mathbb{1}(\hat{y}_i = y_i) - \mathbb{1}(\hat{y}_i^{G_S} = y_i) \right|$$

Model

$$fid_+ = 1 - \frac{1}{N} \sum_{i=1}^N \mathbb{1}(\hat{y}_i^{G_{C \setminus S}} = \hat{y}_i)$$
$$fid_- = 1 - \frac{1}{N} \sum_{i=1}^N \mathbb{1}(\hat{y}_i^{G_S} = \hat{y}_i)$$

Masking Strategy

- **Hard mask**
 - Produce a subgraph as an explanation for the prediction
- **Soft mask**
 - A number between 0 to 1 on edges and features to indicate their importance

Types of Explanations

- **Sufficiency**

- An explanation is sufficient if it leads by its own to the initial prediction of the model explanation. ($fid_- \rightarrow 0$)

- **Necessity**

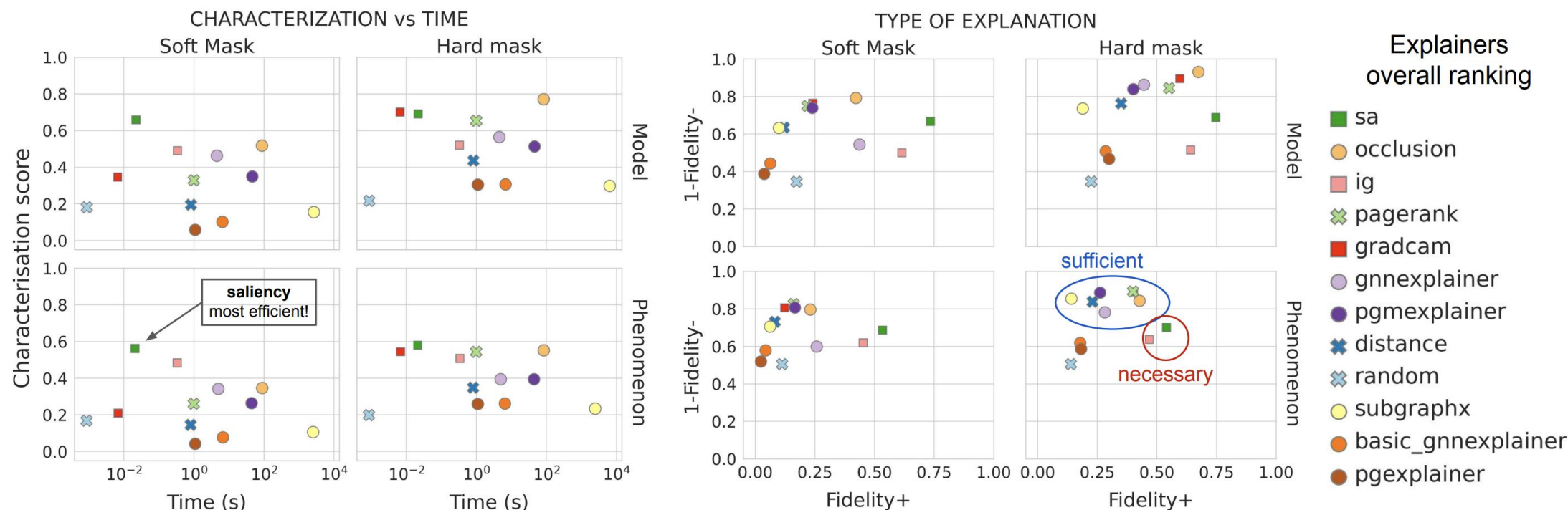
- An explanation is necessary if the model prediction changes when removing it from the initial graph. ($fid_+ \rightarrow 1$)

- **Characterization** score to summarize the explanation quality

$$character = \frac{w_+ + w_-}{\frac{w_+}{fid_+} + \frac{w_-}{1 - fid_-}} = \frac{(w_+ + w_-) \times fid_+ \times (1 - fid_-)}{w_+ \cdot (1 - fid_-) + w_- \cdot fid_+}$$

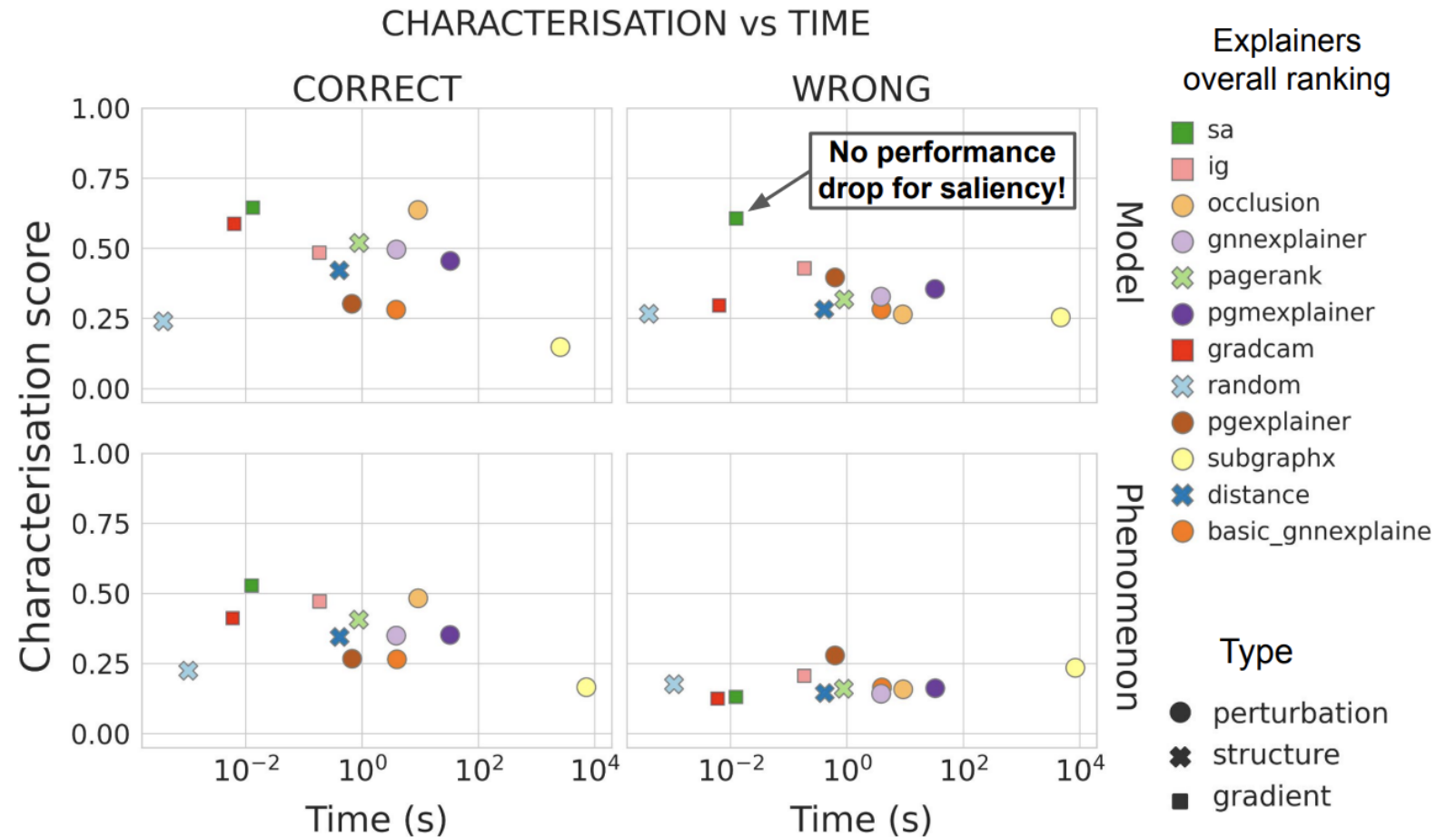
Results: Explain Efficiency vs. Characterization Score

- Saliency has the highest overall characterization score and efficiency.
- Occlusion has the best overall score in the setting of hard mask.



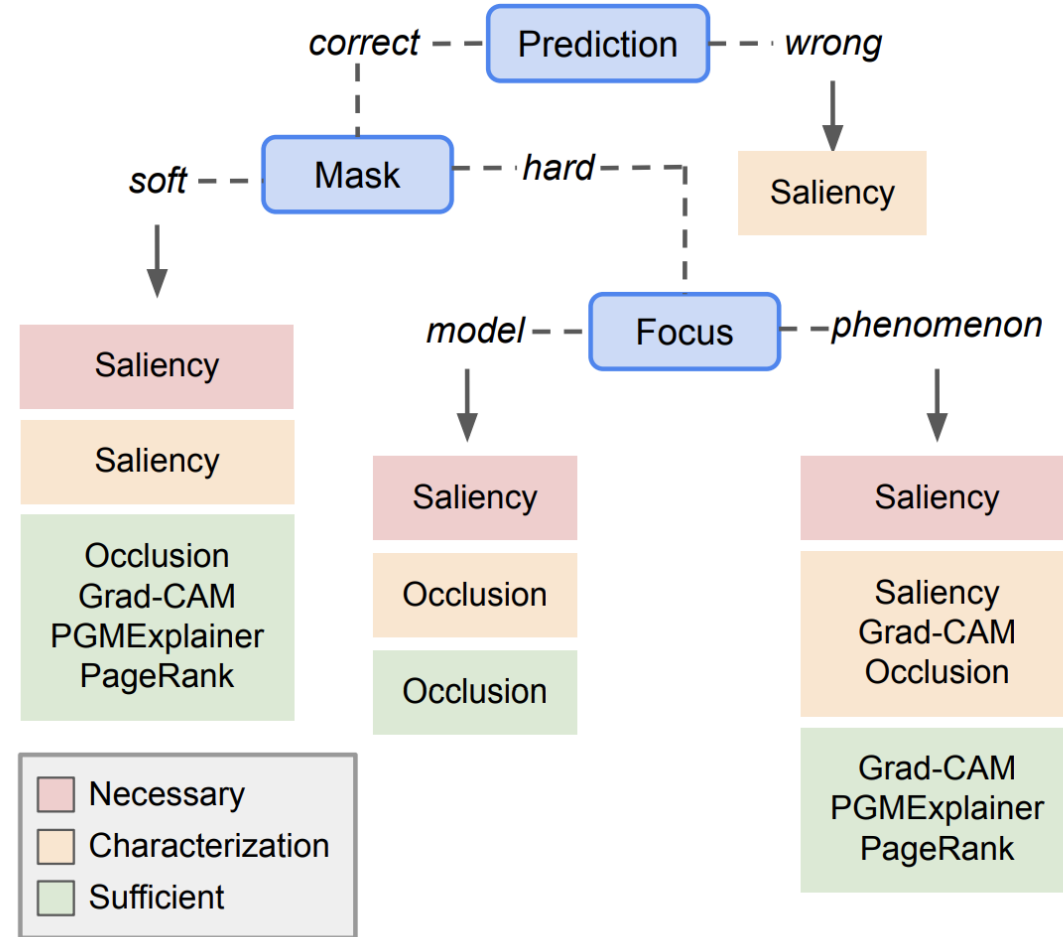
Results: Correct & Wrong Predictions

- Correct predictions → phenomenon & model
- Wrong predictions → model



Results: How to Select an Explainability Method

- Decision Tree which guides users to select the optimal method



Summary of the Lecture

- Trustworthy GNN
 - Robustness, explainability, privacy, fairness, accountability, environmental well-being,...
- Adversarial Attacks and Robustness of GNNs
 - Adversarial examples
 - Attack possibilities: direct attack, indirect attack
 - Mathematical formulation
- Explainability of GNN
 - GNNExplainer
 - GraphFramEx