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

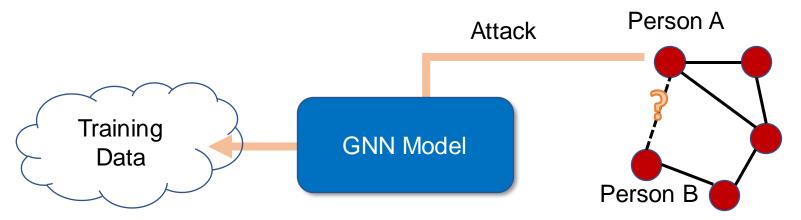
Aspects of Trustworthy GNNs

- Robustness (part 2)
- Explainability (part 3)
- Privacy
- Fairness
- 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

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

- 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

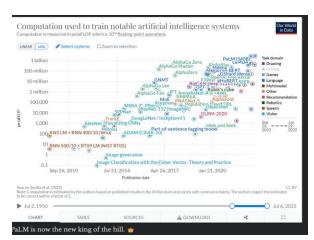
- Fair representation learning methods
 - Learn representations, from which one cannot infer sensitive attributes.
 - A common technique is adversarial training
- Fair prediction enhancement methods
 - Data augmentation
 - Perturbation of protected features
 - Fair graph
 - Modify graph structures (e.g. drop edges that may induce bias)
 - Regularisation
 - Ex) any two individuals who are similar should receive similar algorithmic outcome $\| \mathbf{Y}[i,:] \mathbf{Y}[j,:] \|_F^2 \mathbf{S}[i,j] \le \delta$ Predictions of node i Similarity between node i and j

Environmental Well-Being of GNNs

- GNNs should comform to the fundamential 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 \rightarrow specially designed software and hardware



Compute Clusters
Credit: Imaginima/E+/gettyimages



Large model training involves 10²⁴ 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 <u>Lecture 6</u>

Model compression

- Knowledge distillation
- Model pruning
- Reducing parameters
- Model quantisation

Efficient frameworks and accelerators

- Software: <u>PyTorch Geometric</u>, <u>Efficient AutoML</u>
- Hardware: <u>EnGN</u>, <u>HyGCN</u>

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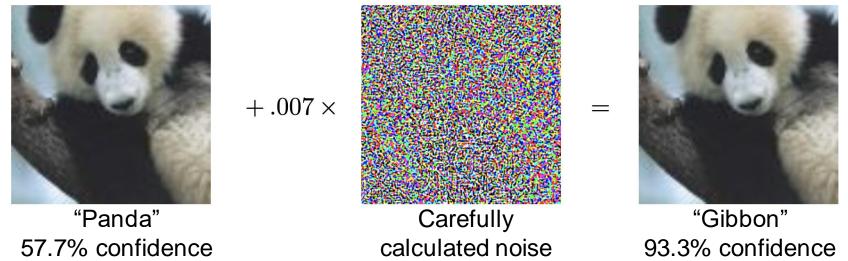
3. Explainability for GNNs

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.



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]

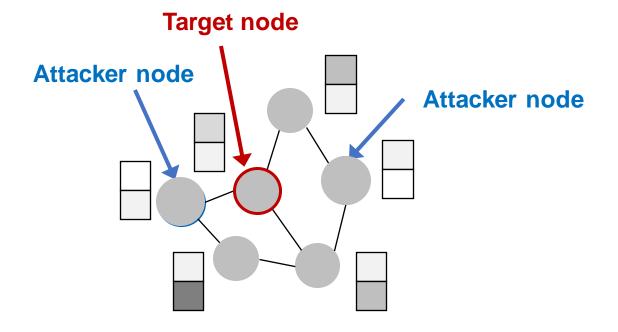
Predict labels of unlabeled nodes

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.

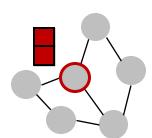
Attack Possibilities

- 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: $S = \{t\}$



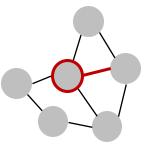
- Modify target node feature
 - Change website content

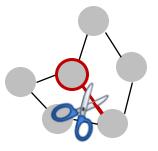


• Buy/likes/follows



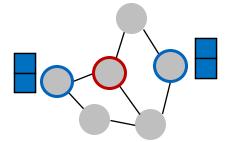
Unfollow users



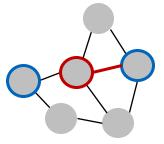


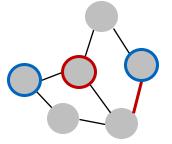
Attack Possibilities: Indirect Attack

 Indirect Attack: The target node is not in the attacker nodes: t ∉ 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



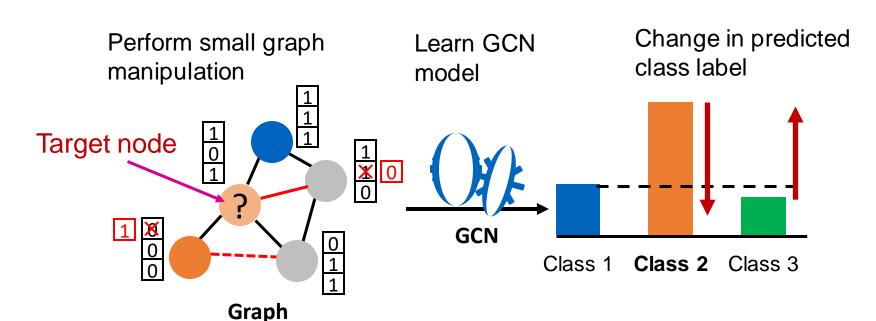


Formalizing Adversarial Attackers

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

$$\theta^* = \operatorname{argmin}_{\theta} \mathcal{L}_{train}(\theta; \widetilde{A}, \widetilde{X})$$
 What is \widetilde{A} and \widetilde{X} ?

GCN's original prediction on the target node:

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

• GCN's manipulated prediction on the target node

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

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

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

Predict the class c_v^* of vertex v

that has the highest predicted

probability

Mathematical Formulation (3)

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

Mathematical Formulation (4)

• Change of prediction on target node v:

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

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

Predicted (log) Predicted (log) probability of the newly-predicted class $c_{12}^{*\prime}$

probability of the originally-predicted class c_{ν}^*





Mathematical Formulation (5)

• Final optimization objective:

$$\operatorname{argmax}_{A',X'} \Delta(v;A',X')$$
subject to $(A',X') \approx (A,X)$

- 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

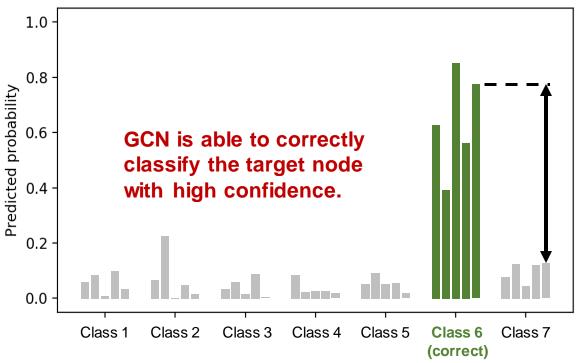
- Manipulation budget
- while $|A' A| + |X' X| < \delta$
 - Compute a candidate set for struct perturbations (all should be unnoticeable)
 - Pick the one which obtains the **highest** change of predictions
 - Compute a candidate set for node features perturbations (all should be unnoticeable)
 - Pick 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?

Netattack: Candidate Sets

- Efficiently compute candidate sets which make unnoticeable changes
- Main idea: use **siginificance 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).



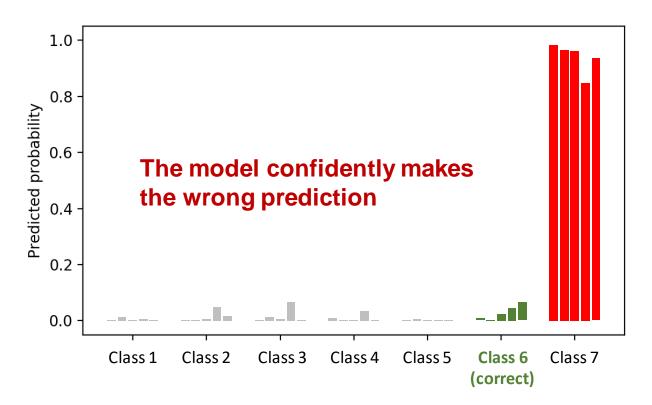
Predicted probabilities over 5 re-trainings (without graph manipulation, i.e., clean graph)

Classification margin

- > 0: Correct classification
- < 0: Incorrect classification

Experiments: Adversarial Attack (2)

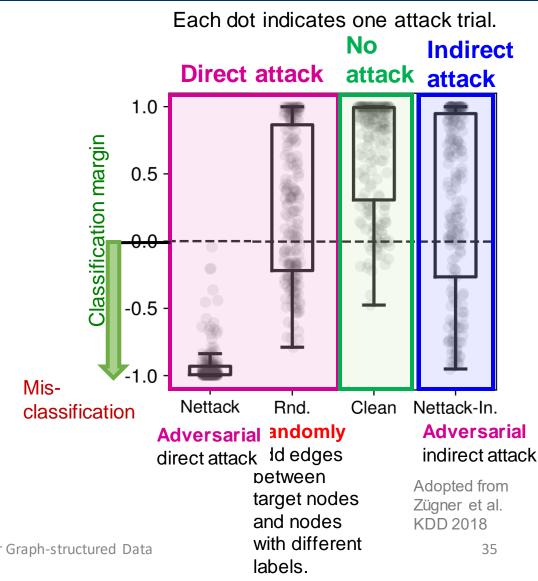
 GCN's prediction after carefully modifying just 5 edges attached to the target node (direct adversarial attack).



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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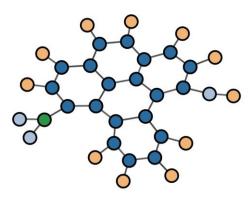
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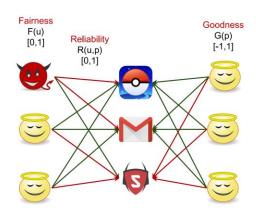
Explainability: Motivation (1)

- 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?





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

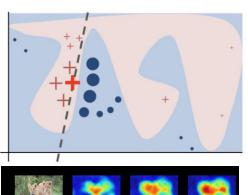
• Learn a inherently interpretable model locally approximating the original model (e.g. a linear model, interpret by weights).

Saliency Maps

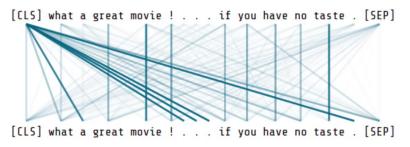
Compute gradients of outputs w.r.t. input pixels.

Attention Mechanisms

Visualize attention weights in a attention models.





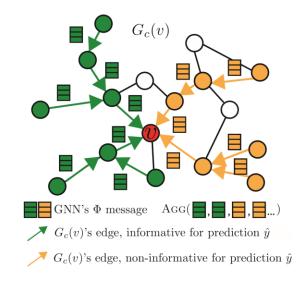


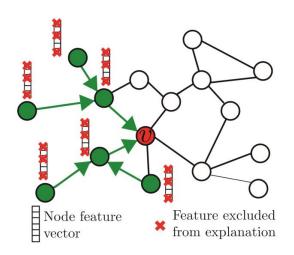
Challenges of Applying these Methods to Graphs

- 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





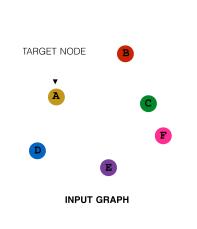
Structural explanation

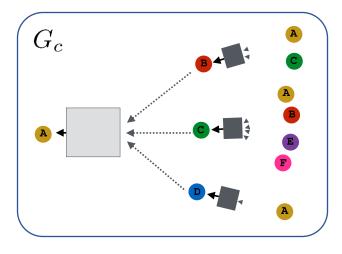
Feature explanation

GNNExplainer explain both aspects simultaneously

GNNExplainer Input

• Without loss of generality, consider node classification task:



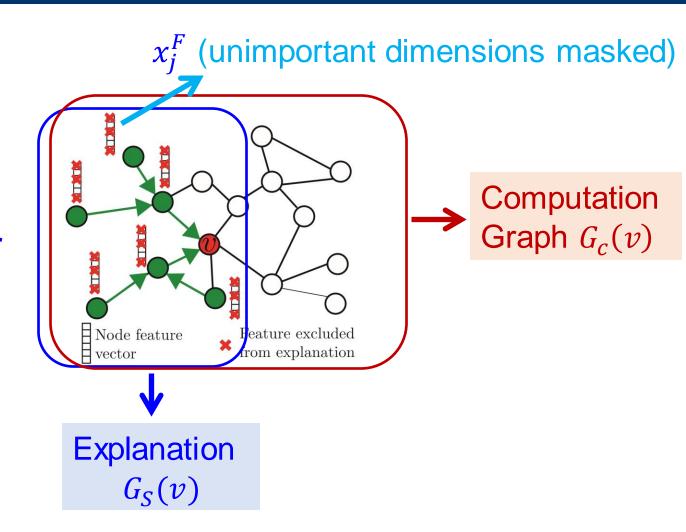


Suppose GNN predicts label \hat{y} for node v

- 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)
- $X_S^F = \{x_j^F | v_j \in G_S\}$ 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

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

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

- 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

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

- Optimize the expectation by masking Element-wise multiply
- Use A_C \odot 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).

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

$$P_{\mathcal{A}}(A_S) = \prod_{e=(j,k)\in G_C(v_i)} A_S[j,k]$$

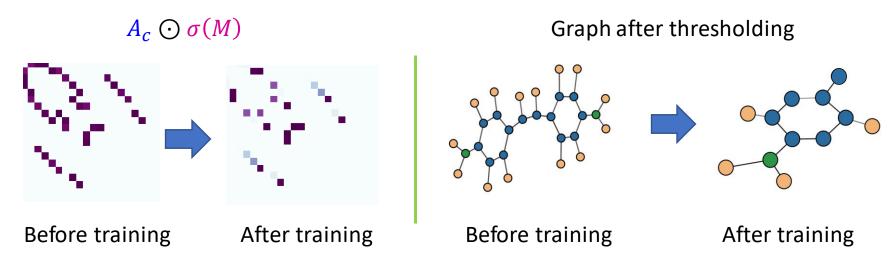
Objective:

$$\min_{M} -H(\log P_{\phi} (Y = y | G = A_{\mathcal{C}} \odot \sigma(M), X = X_{\mathcal{S}})$$

• 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

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

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

- 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: $Sum(\sigma(M))$
 - Feature size: $Sum(\sigma(F))$
- Final Objective

$$\min_{M} -H(\log P_{\phi}(Y=y|G=A_{c} \odot \sigma(M), X=X_{S}^{F}) + \lambda_{1} \operatorname{Sum}(\sigma(M)) + \lambda_{2} \operatorname{Sum}(\sigma(F))$$

Sum of entries in feature and adjacency masks

• Threshold $A_c \odot \sigma(M)$ to get the explanation G_s

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

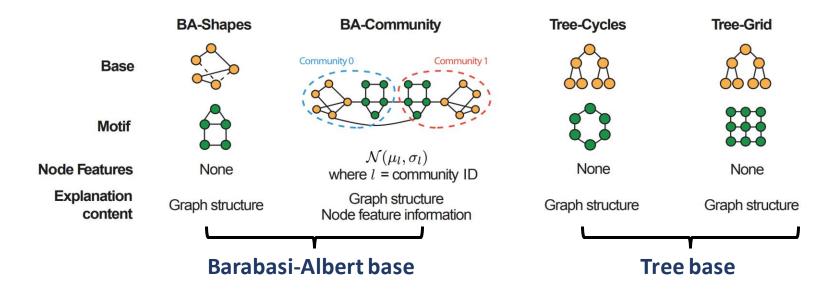
We use GNN general formulation

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)

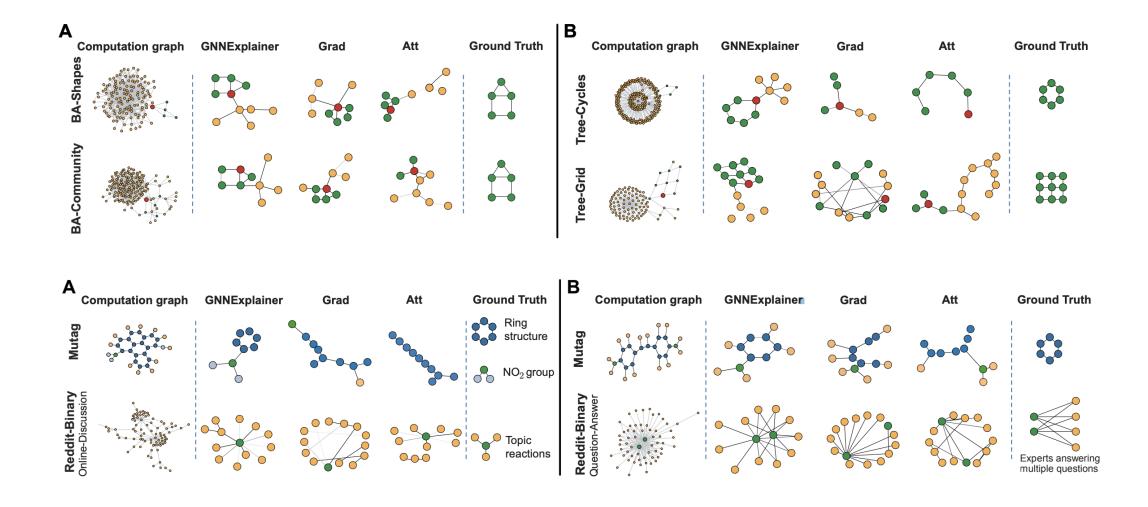
- Real-world tasks
 - Social networks (Reddit-binary dataset)
 - Reddit community prediction
 - Chemistry (Mutagenic molecule dataset)
 - Chemical property prediction
 - Graph classification

Results: Quantiative Analysis

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

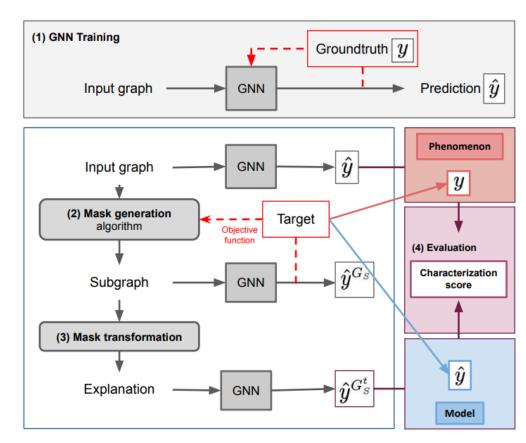
	BA-House	BA-Comm	Tree-Cycle	Tree-Grid
Grad	88.2	73.9	82.4	61.2
Att	81.5	75.0	90.5	66.7
GNN-Explainer	92.5	83.6	94.8	87.5

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

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

$$fid_{-} = \frac{1}{N} \sum_{i=1}^{N} \left| \mathbb{1}(\hat{y}_{i} = y_{i}) - \mathbb{1}(\hat{y}_{i}^{G_{S}} = y_{i}) \right| \qquad fid_{-} = 1 - \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}(\hat{y}_{i}^{G_{S}} = \hat{y}_{i})$$

Model

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

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. $(fid_- \rightarrow 0)$

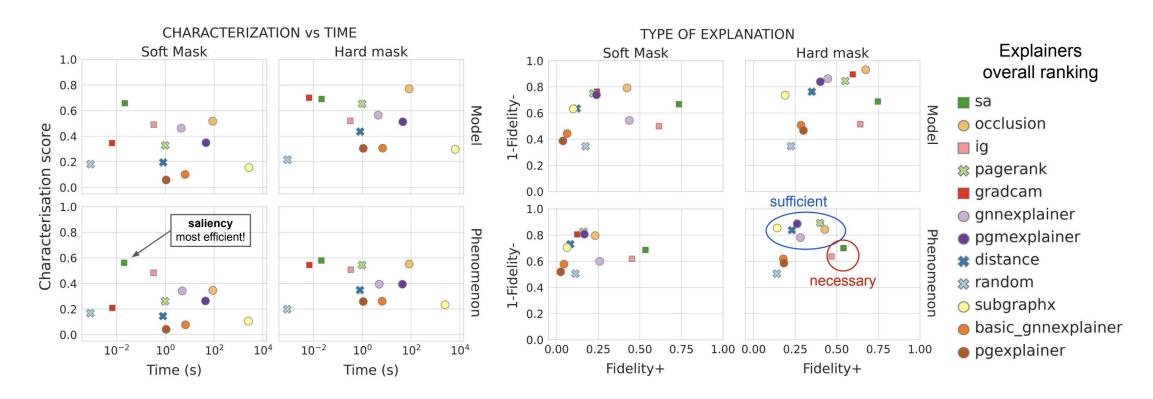
Necessity

- 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

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

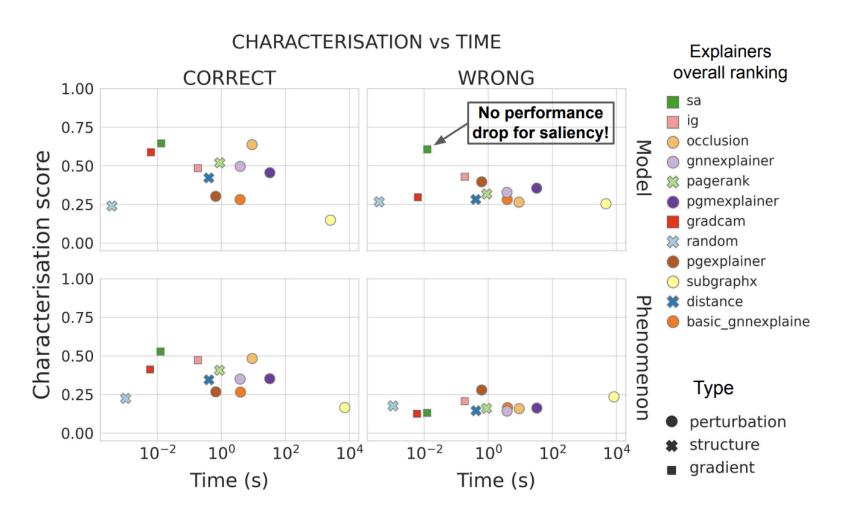
Results: Explain Efficiency vs. Characterization Score

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



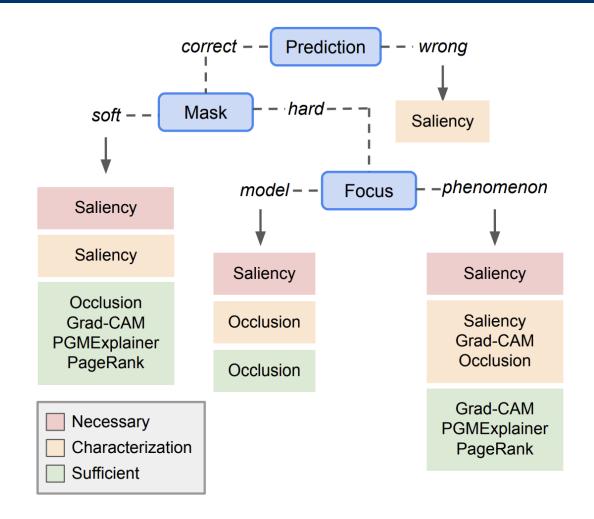
Results: Correct & Wrong Predictions

- 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 wellbeing,...
- Adversarial Attacks and Robustness of GNNs
 - Adversarial examples
 - Attack possibilities: direct attack, indirect attack
 - Mathematical formulation
- Explainability of GNN
 - GNNExplainer
 - GraphFramEx