

Qualifying Exam

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Introduction

- Overview of the problem area.
 - Graphs are an important data structure.
 - * GRAPHS provide an incredibly flexible structure for modeling complex data. Data can naturally appear as graphs, like molecules. We can reduce data to a graph, such as the key points of a image. We can even use graphs to add structure, such as grammatical relationships.
 - GNN models are good at prediction and inference on graph data.
 - * Graph Neural Networks (GNNs) have become a popular choice for prediction and inference on graph data. At their core, GNNs work by iteratively updating node embeddings based on information from neighboring nodes. The idea is to use the graph's structure to engineer better features. This message passing scheme allows GNNs to capture complex dependencies and patterns present within the graph structure. GNN architectures typically consist of multiple layers, each performing message passing and aggregation operations to refine the embeddings. These layers are often followed by pooling and dense prediction layers to produce the final output.
 - There are many important applications for graph classification models.
 - * Some important applications of graph classification include predicting chemical toxicity (Bai et al. 2019), classifying proteins (Gallicchio and Micheli 2019), and even detecting cancer from pathology slides (Xiao et al. 2023).
 - **Problem:** While GNNs achieve remarkable predictive power, their complexity prevents the exaction of the scientific rationale.
- Why is the problem important?
 - Explaining or interpreting GNN predictions would
 - * help with the adoption of such models for critical applications,
 - * prevent adversarial attacks,
 - * detect potential implicit discrimination,
 - * guide scientific as well as machine learning research.
- How does the problem relate to the fundamentals areas of Statistics?
 - Explain-ability vs Interpretability
 - * Yuan et al. (2022)
 - * A model is interpretable if the models decision process can be readily understood by humans. For example, a linear regression model is interpretable because the coefficient clearly define how any prediction get made.

- * A model is explainable if the models prediction can be reasoned post-hoc. Permuting each variable and measuring the variation in the predictions can be used to estimate each variables marginal effect [cite].
- One goal would be to create a GNN type model whose decision process is human interpretable. A straight translation from statistics would be a circuit type analysis [cite]. For graphs, this would mean some form of coefficients on subgraphs producing the prediction.
- Another goal might be to develop a method that determines if a feature is statistical significant to the GNN model. The challenge is that the graph features that matter to researchers aren't necessarily tabular.
- What is the impact of solving this problem?
 - In the application where GNNs have shown strong predictive power, we can exact a testable scientific hypothesis for the nature of the classification.
 - In the application where GNNs have weak predictive power, highlight the potential misunderstandings the model is having.

Notation

- Let G denote a graph.
- Any graph G can be describe by X, A, E . The node feature matrix, edge feature matrix, and adjacency matrix respectively
- Let $X = [X_c, X_d]$, where X_c is the subset of continuous node features and X_d is the subset of one-hot discrete node features.
- Let $E = [E_c, E_d]$, denoted in the same manner.
- Let n represent the number of nodes in the graph and v represent the number of edges.
- Let $\text{feat}_{(\cdot)}$ denote the number of features or columns in the the corresponding feature matrix.
- A is a binary $n \times n$ matrix where $A[i, j] = 1$ indicates that an edge exists between nodes labeled i and j .
- Let $\text{explaine}(G; \Omega) = h_G^{(1)}, \dots, h_G^{(L)}, \rho_G$ be an L layer GNN model with parameters Ω that we would like to explain.
- For any graph Let ν denote the set of node and \mathcal{E} denote the set of edges.

Analysis of Core Papers

GNNInterpreter

(Wang and Shen 2024)

- Overview
 - Instance v. Model Level

- * In general, explanation methods serve to elucidate which features within the data influence disparate predictions. These methods typically fall into two categories: instance-level and model-level. Instance-level explanations aim to unveil the model’s rationale behind a particular prediction. In domains such as image and text analysis, a prevalent approach involves masking or perturbing the instance and assessing the impact on the model’s prediction. On the other hand, model-level explanations seek to understand how a model generally distinguishes between classes. In image and text analysis, for instance, one common technique involves treating the input as a trainable parameter and optimizing the model’s prediction towards a specific class. Consequently, the resulting optimized input comprises a set of features strongly associated with the targeted class.
- GNNInterpreter provides model level explanations for GNN in this manner.
- Formally, GNNInterpreter tries to learn the graph generating distribution for each class.
- GNNInterpreter works by optimizing the parameters of a generic graph generating distribution to produce samples that closely match the explaine’s understanding of the targeted class.
- Explanation of the graph generating distribution.
 - Graph generating distributions are hard to specify because there can be discrete and continuous elements of X , E and A . Furthermore, the interactions between these matrices can be complex.
 - The authors tackle these issues by making two simplify assumptions.
 1. Assume that G is a *Gilbert* random graph, every possible edge as an independent fixed probability of occurring.

$$\forall (i, j) \neq (k, l) \Pr(A[i, j] = 1) \perp \Pr(A[k, l] = 1) \quad (1)$$
 2. The features of every node and edge are independently distributed.
 - The author justify these assumptions by:
 1. The other graph distributions aren’t suitable.
 - a. Erdo-Renyi graphs have a fixed number of edges (and nodes, but nodes are also fixed for Gilbert).
 - b. Rado graphs are infinite in size.
 - c. The random dot-product graph model is just a generalization of Gilbert random graphs.
 2. Because the parameters of the independent distributions will be updated jointly using the *explaine* model, the *explaine*’s understanding of the latent correlation structure should be contained in the final estimates.
 - X_c and E_c can be sampled from any continuous distribution that can be expressed as a location-scale family. Separating the stochastic and systematic components is necessary for gradient based optimization. It is commonly known as the “re-parametrization trick”.
 - X_d , E_d as well as A need to be sampled from a continuous distribution for gradient based optimization, but the distribution has to have sampling properties close to a discrete distribution.

- The author assume that the true underlying distribution for every discrete node and edge feature is *categorical*. The categorical distribution is also know as the multi-bernoulli, where every sample has a fixed probability of being in one of the discrete categories.
- Suppose there are D categories with probabilities $\pi_\omega = \frac{\theta_\omega}{\sum_{i \in D} \theta_i}$. Then

$$I = \operatorname{argmax}_{i \in D} \log \theta_i + G^{(i)} \sim \operatorname{Cat}(\pi) \quad (2)$$

where $G^{(i)} \stackrel{i.i.d.}{\sim} \operatorname{Gumbel}(0, 1)$.

- The intuition is that the Gumbel or extreme value distribution is the density of the maximum order statistic of i.i.d. standard normals which makes it a good candidate for model the winning or maximum probability category. Adding Gumbel noise to the logits should maintain the true relative proportions, but enough skewness such that every category has some probability of having the maximum noised logit.
- **Proof 1:** In order for I to be a true categorical distribution, $\Pr[I = \omega] = \pi_\omega$. $I = \omega$ if and only if $\log \theta_\omega + G^{(\omega)} > \log \theta_i + G^i \forall i \in D \setminus \omega$. Let M_i denote a random variable that follows a $\operatorname{Gumbel}(\log \theta_i, 1)$ distribution.

$$\begin{aligned}
\Pr[I = \omega] &= \mathbb{E}_{M_\omega} \prod_{i \in D \setminus \omega} \Pr(M_i < m_\omega) \text{ i.i.d location shifted Gumbel distributions.} \\
&= \mathbb{E}_{M_\omega} \prod_{i \in D \setminus \omega} \exp(-e^{\log \theta_i - m_\omega}) \text{ Gumbel CDF.} \\
&= \mathbb{E}_{M_\omega} \exp\left(-\sum_{i \in D \setminus \omega} e^{\log \theta_i - m_\omega}\right) \\
&= \int_{-\infty}^{\infty} \exp(\log \theta_\omega - m_\omega) \exp(-e^{\log \theta_\omega - m_\omega}) \cdot \exp\left(-\sum_{i \in D \setminus \omega} e^{\log \theta_i - m_\omega}\right) dm \\
&\quad \text{Gumbel PDF.} \\
&= \int_{-\infty}^{\infty} \exp(\log \theta_\omega - m_\omega) \exp\left(-\sum_{i \in D} e^{\log \theta_i - m_\omega}\right) dm \\
&= \int_{-\infty}^{\infty} \theta_\omega \exp(-m_\omega) \exp\left(-e^{-m_\omega} \sum_{i \in D} \theta_i\right) dm \\
&= \pi_\omega \sum_{i \in D} \theta_i \int_{-\infty}^{\infty} \exp(-m_\omega) \exp\left(-e^{-m_\omega} \sum_{i \in D} \theta_i\right) dm \text{ From the above definition of } \pi_\omega \\
&= \pi_\omega \sum_{i \in D} \theta_i \frac{\exp\left(-e^{-m_\omega} \sum_{i \in D} \theta_i\right)}{\sum_{i \in D} \theta_i} \Big|_{-\infty}^{\infty} \\
&= \pi_\omega \sum_{i \in D} \theta_i \frac{1}{\sum_{i \in D} \theta_i} = \pi_\omega
\end{aligned}$$

Reference: Huijben et al. (2022)

- Using inverse CDF sampling and relaxing the argmax to a Softmax, we can sample one-hot categorical vectors based on two parameters θ_{Cat} , a trainable parameter vector

of length equal to the number of categories, and τ , a hyperparameter that controls the degree of relaxation (smaller value approximate the discrete sampling better, but can result in numerical issues).

$$\text{Softmax}\left(\frac{\theta_{\text{Cat}} - \log(-\log \epsilon)}{\tau}\right), \quad \epsilon \sim U[0, 1] \quad (3)$$

This method, known as the concrete distribution (Maddison, Mnih, and Teh 2017), yields a reasonable smooth gradient w.r.t. to the probability parameters.

- The adjacency matrix can be sampled in a similar manner since the Bernoulli is just a special case of the categorical.

$$\text{sigmoid}\left(\frac{\theta_A + \log \epsilon - \log(1 - \log \epsilon)}{\tau}\right) \quad (4)$$

This is known as the binary concrete distribution (Maddison, Mnih, and Teh 2017).

- Notate the combined graph generating distribution as:

$$G_{\text{gen}} \sim \text{gen}(\Theta)$$

where Θ is the set of all parameters from the independently sampled distributions.

- Prediction objective.

- An obvious objective is to maximize the likelihood that the *explainee* model predicts a sampled graph to be a member of the target class.
- Let $\tilde{\rho}$ denote the desired predicted probability vector. Then the above objective can be expressed as:

$$\mathcal{L}_{\text{pred}}(\Theta \mid G_{\text{gen}}) = \mathbb{E}_{G_{\text{gen}}} \text{CrtEnt}(\text{explainee}(G_{\text{gen}}), \tilde{\rho}) \quad (5)$$

- Embedding objective.

- While the above objective enforces a desirable property, it isn't restrictive enough to make the generated graph realistic. This is because the final prediction, $\rho_{G_{\text{gen}}}$ is compute using only final embeddings, $h_{G_{\text{gen}}}^{(L)}$. Normally $h_{G_{\text{gen}}}^{(L)}$ contains all the needed information from the graphs structure; however, the generation scheme allows the feature distribution to be optimized directly. This means that explanation can ignore the graph structure and optimize towards the desired final embeddings.
- Another way of understanding the problems with the above objective is to consider the *out-of-distribution* (ood) issue. Since the above generation scheme is not restricted by the observed data distribution, the initial generated graphs may be very ood, but clearly on one side of the decision boundary.

- The author find that empirically GNN model exhibit a class preference.

Table 5: The quantitative evaluation results for all 6 datasets including Is_Acyclic. As the quantitative metric, we compute the average class probability of 1000 explanation graphs and the standard deviation of them for the two classes. In addition, the average training time per class of training 100 different GNNInterpreter and XGNN models is also included for efficiency evaluation.

Dataset [Method]	Predicted Class Probability by GNN				Training Time Per Class
Is_Acyclic [XGNN]	Cyclic	Acyclic			45 s
	0.076 ± 0.000	0.927 ± 0.000			
Is_Acyclic [Ours]	Cyclic	Acyclic			20 s
	0.999 ± 0.001	1.000 ± 0.000			
Is_Acyclic [Random]	Cyclic	Acyclic			-
	0.143 ± 0.155	0.857 ± 0.155			
MUTAG [XGNN]	Mutagen	Nonmutagen			128 s
	0.986 ± 0.057	0.991 ± 0.083			
MUTAG [Ours]	Mutagen	Nonmutagen			12 s
	1.000 ± 0.000	1.000 ± 0.000			
MUTAG [Random]	Mutagen	Nonmutagen			-
	0.068 ± 0.251	0.932 ± 0.251			
ColorConsistency [Ours]	Consistent	Inconsistent			58 s
	0.968 ± 0.110	1.000 ± 0.000			
ColorConsistency [Random]	Consistent	Inconsistent			-
	0.017 ± 0.118	0.983 ± 0.118			
Cyclicity [Ours]	Red Cyclic	Green Cyclic	Acyclic		49 s
	1.000 ± 0.000	1.000 ± 0.000	1.000 ± 0.000		
Cyclicity [Random]	Red Cyclic	Green Cyclic	Acyclic		-
	0.023 ± 0.143	0.015 ± 0.118	0.962 ± 0.183		
Motif [Ours]	House	House-X	Complete-4	Complete-5	83 s
	0.918 ± 0.268	0.999 ± 0.032	1.000 ± 0.000	0.998 ± 0.045	
Motif [Random]	House	House-X	Complete-4	Complete-5	-
	0.000 ± 0.000	0.000 ± 0.000	0.000 ± 0.000	0.000 ± 0.000	
Shape [Ours]	Lollipop	Wheel	Grid	Star	24 s
	0.742 ± 0.360	0.989 ± 0.100	0.996 ± 0.032	1.000 ± 0.000	
Shape [Random]	Lollipop	Wheel	Grid	Star	-
	0.214 ± 0.301	0.000 ± 0.000	0.151 ± 0.307	0.000 ± 0.000	

(Wang and Shen 2024)

For example, random graphs have an average predicted probability of being Non-mutagenic in the MUTAG dataset if 93.2%. This demonstrates why the above objective is insufficient to generate realistic or *in-distribution* (id) graph.

- In order to mitigate this issue, the author proposed additional minimizing the cosine distance between the average embedding of all the observed graph from the targeted class, $\bar{h}_{G_c}^{(L)}$, and the embedding of the generated explanation.

$$\mathcal{L}_{\text{embed}}(\Theta \mid G_{\text{gen}}) = \text{CosDist} \left(\bar{h}_{G_c}^{(L)}, h_{G_{\text{gen}}}^{(L)} \right) \quad (6)$$

- Regularization terms.

- Sparse graphs are easy for humans to interpret. To encourage sparsity the authors employed an L_1 , L_2 , and a budget penalty on the edge probabilities.

$$\mathcal{L}_{\text{Sparsity}}(\theta_A) = \|\theta_A\|_1 + \|\theta_A\|_2 + \text{softplus}(\text{sigmoid}\|\theta_A\|_1 - B)^2 \quad (7)$$

where B is the expected maximum number of edge for generated explanation graphs.

- Connectivity is another desirable property as it ensures a cohesive explanation. To encourage connectivity the author minimize the *KL-Divergence* between edge probabilities that share a common node.

$$\mathcal{L}_{\text{Connect}}(\theta_A) = \sum_{i \in \nu} \sum_{j, k \in \mathcal{E}(i)} D_{KL}(\text{sigmoid}(\theta_A[i, j]) \parallel \text{sigmoid}(\theta_A[i, k])) \quad (8)$$

where $\mathcal{E}(i)$ is the set of edges that connect to node i .

- Summary of Results + Figures

- The final generator model is trained by sampling $G_{\text{gen}} \sim \text{gen}(\Theta)$ and then iterative updated Θ via gradient descent on the full loss:

$$\mathcal{L}_{\text{GNNInterpreter}}(\Theta \mid G_{\text{gen}}) = \mathcal{L}_{\text{pred}}(\Theta \mid G_{\text{gen}}) + \mathcal{L}_{\text{embed}}(\Theta \mid G_{\text{gen}}) + \mathcal{L}_{\text{sparsity}}(\Theta \mid G_{\text{gen}}) + \mathcal{L}_{\text{connect}}(\Theta \mid G_{\text{gen}}) \quad (9)$$

Table 2: The quantitative results for 4 datasets. As the quantitative metric, we compute the average class probability of 1000 explanation graphs and the standard deviation of them for every class in all 4 datasets. In addition, the average training time per class of training 100 different GNNInterpreter and XGNN models, is also included for efficiency evaluation.

Dataset [Method]	Predicted Class Probability by GNN				Training Time Per Class
MUTAG [XGNN]	Mutagen	Nonmutagen			128 s
	0.986 ± 0.057	0.991 ± 0.083			
MUTAG [Ours]	Mutagen	Nonmutagen			12 s
	1.000 ± 0.000	1.000 ± 0.000			
Cyclicity [Ours]	Red Cyclic	Green Cyclic	Acyclic		49 s
	1.000 ± 0.000	1.000 ± 0.000	1.000 ± 0.000		
Motif [Ours]	House	House-X	Complete-4	Complete-5	83 s
	0.918 ± 0.268	0.999 ± 0.032	1.000 ± 0.000	0.998 ± 0.045	
Shape [Ours]	Lollipop	Wheel	Grid	Star	24 s
	0.742 ± 0.360	0.989 ± 0.100	0.996 ± 0.032	1.000 ± 0.000	

- GNNInterpreter achieve remarkable accuracy on most target classes. Many of the interval are tight and very close to 1, which implies that the examples generated are almost always classified as the targeted class. The explanations for the house motif and the lollipop shape are worse in terms of predictions. Although the author critique the use of predictions as the sole objective, they do not use any other quantitative metric to evaluate the validity of their explanations.
- Qualitatively we can see some limitation in terms of realism.
- For example, for the mutagen class, the explanation correctly identifies the importance of the N02 group; however, the generated graph isn’t realistic and might not even be chemically possible. Furthermore, the non-mutagen example doesn’t display any clear patterns or identifiable structures.
- The explanations for the Cyclicity dataset as well as the Wheel class do not appear to be members of the underlying data distribution.
- GNNInterpreter provides a way of generating example graph that would be classified as a target class by a GNN model, without needing to specify domain specific rules. On the other hand, optimizing predictions and even embeddings does not appear to be a sufficient objective for producing in-distribution graphs. The author correctly point out that optimizing predictions can lead to unrealistic graphs, but they have also inadvertently demonstrated that optimizing embeddings is not necessarily sufficient either.

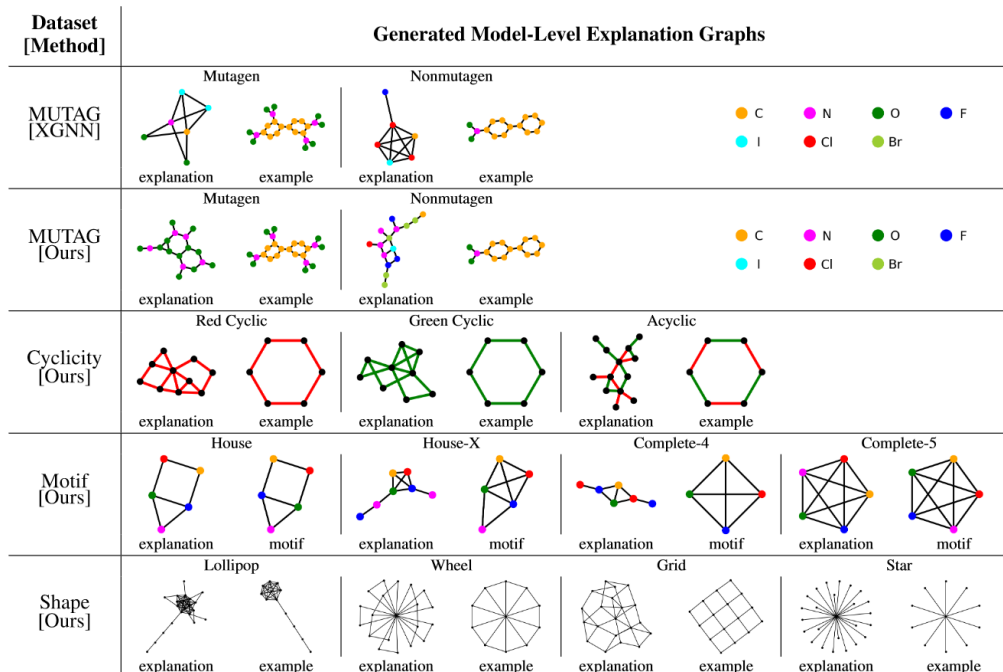


Figure 1: The qualitative results for 4 datasets. For each class in all datasets, the explanation graph with the class probability of 1 predicted by the GNNs is displayed on the left; as a reference, the example graph selected from the training data of the GNNs or the motif is displayed on the right. The different colors in the nodes and edges represent different values in the node feature and edge feature.

D4Explainer

(Chen et al. 2023)

- Overview
 - D4Explainer or in-Distribution GNN explanations via Discrete Denoising Diffusion attempt to directly address the realism of generated graphs in model-level explanation by using the observed data to train a Diffusion model.
 - In the image domain, diffusion model have been shown to produce the most realistic images when compared to other generative AI methods such as Generative Adversarial Networks (GANs).
 - Diffusion model work by iteratively noising an observation until it is pure noise. Then a denoising model is trained to predict the noise added at any given time step. Then new observations can be generated by passing pure noise through the diffusion model in a process known as reverse sampling.
 - Additional label information can be passed to generate observations with similar a label.
- Generation Scheme
 - The authors of D4Explainer generate example graph by noising and de-nosing the adjacency matrices of observed graphs.
 - The process of iteratively adding noise is known as forward diffusion.
 - Let $t \in [0, T]$ denote the iterative steps.
 - A_t denote

- Loss Dist
- Loss CF
- Model-level sampling algorithm
- CF-ACC
- Fidelity
- Density
- MMD
- Summary of Results + Figures
- Forward Diffusion
 - The process of iteratively adding noise is known as forward diffusion.
 - Let X_0 be a noise free observation.
 - If X_0 is continuous, Gaussian noise is most common.
 - Noise is added based on fixed hyperparameter known as the variance schedule and is denoted by $(\beta_1, \dots, \beta_T)$ where T is the total number of noising steps (theoretical X_T need to be pure noise).
 - Using Gaussian noise, continuous forward diffusion is defined as
- Note on counter-factual explanations.

ProtGNN

(Zhang et al. 2021)

Synthesis of Core Papers

- Comparison of generation methods.
 - GNNInterpreter uses continuously relaxed discrete distributions.
 - D4Explainer uses diffusion.
 - Diffusion is slower, but can be more realistic. Probably because diffusion is less subject to the **out-of-distribution (OOD) problem**.
 - Prototype projection are like generative methods. Restricted to in distribution, but realism is all but guaranteed.

Technical Details

Table 1

	Predictions	Density	Deg.	CLus.	Spec.
GNNInterpreter Original					
Class 0	1.0 +/- 0.0	NA	NA	NA	NA
Class 1	1.0 +/- 0.0	NA	NA	NA	NA

GNNInterpreter Reimplemented

Class 0	0.93 +/- 0.01	0.38 +/- 0.002	1.77	1.53	0.07
Class 1	0.98 +/- 0.01	0.32 +/- 0.003	1.41	1.43	0.04

D4Explainer Original

Aggregated	0.92	0.315	0.12	0.00	0.02
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D4Explainer Reimplemented

Class 0	0.63 +/- 0.23	0.13 +/- 0.03	0.27	0.57	0.05
Class 1	0.66 +/- 0.20	0.13 +/- 0.03	0.08	0.25	0.04

¹ +/- 1 standard deviation; 1000 graphs.

* Empty

Future Directions

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