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 develope 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 $\text{feat}_{(.)}$ 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 $\text{explainee}(G;\ \Omega) = h_G^{(1)}, ...\, h_G^{(L)}, \rho_G$ be an L layer GNN model with parameters Ω that we would like to explain.
- Let $\hat{Y}_G$ be the predicted class label for graph G predicted from explainee().
- 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 explainee'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.

    $$\forall(i,\ j) \neq (k,l)\ Pr(A[i,\ j] = 1) \perp Pr(A[k,\ l] = 1) \tag{1}$$

    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 *explainee* model, the *explainee'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 $\pi_\omega = \dfrac{\theta_\omega}{\sum_{i \in D} \theta_i}$. Then

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

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

- 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.

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

  Reference: Huijben et al. (2022)

- Using inverse CDF sampling and 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).

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

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.

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

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:

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

- 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, $h^{(L)}_{G_{\text{gen}}}$. Normally $h^{(L)}_{G_{\text{gen}}}$ 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.

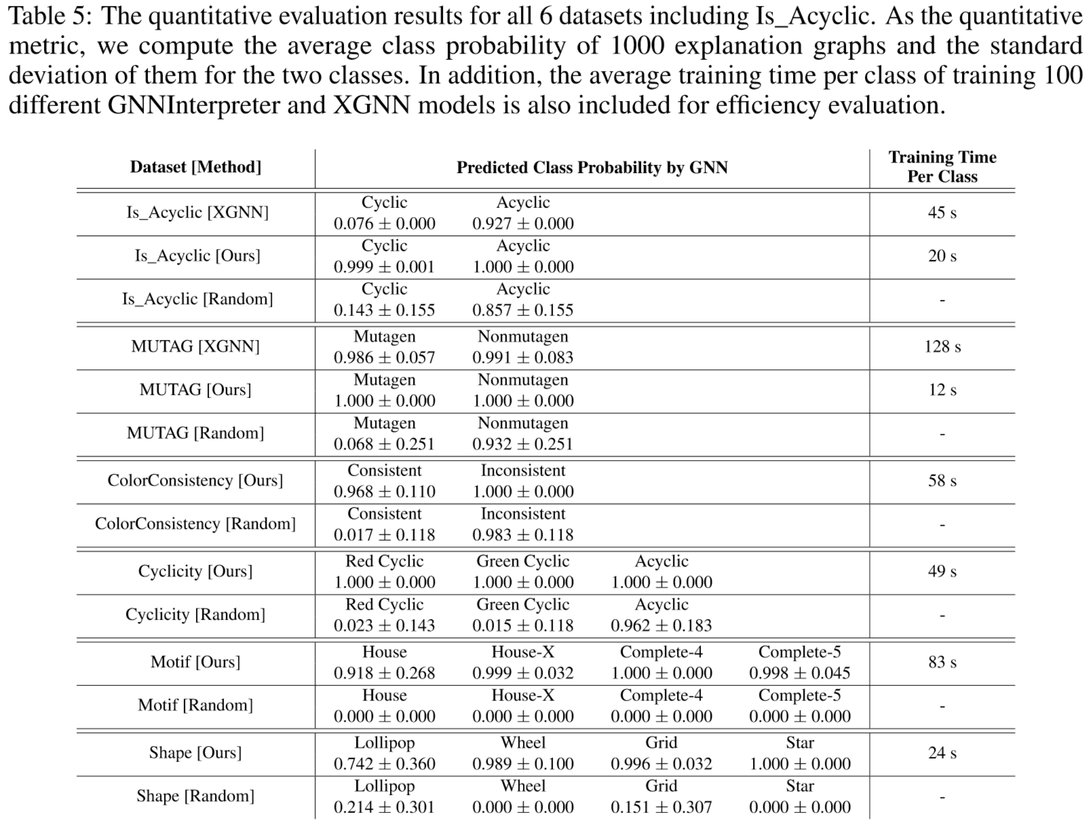


Table 5: The quantitative evaluation results for all 6 datasets including Is_Acyclic. As the quantitative metric, we compute the average class probability of 1000 explanation graphs and the standard deviation of them for the two classes. In addition, the average training time per class of training 100 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 0.076 ± 0.000	Acyclic 0.927 ± 0.000			45 s
Is_Acyclic [Ours]	Cyclic 0.999 ± 0.001	Acyclic 1.000 ± 0.000			20 s
Is_Acyclic [Random]	Cyclic 0.143 ± 0.155	Acyclic 0.857 ± 0.155			-
MUTAG [XGNN]	Mutagen 0.986 ± 0.057	Nonmutagen 0.991 ± 0.083			128 s
MUTAG [Ours]	Mutagen 1.000 ± 0.000	Nonmutagen 1.000 ± 0.000			12 s
MUTAG [Random]	Mutagen 0.068 ± 0.251	Nonmutagen 0.932 ± 0.251			-
ColorConsistency [Ours]	Consistent 0.968 ± 0.110	Inconsistent 1.000 ± 0.000			58 s
ColorConsistency [Random]	Consistent 0.017 ± 0.118	Inconsistent 0.983 ± 0.118			-
Cyclicity [Ours]	Red Cyclic 1.000 ± 0.000	Green Cyclic 1.000 ± 0.000	Acyclic 1.000 ± 0.000		49 s
Cyclicity [Random]	Red Cyclic 0.023 ± 0.143	Green Cyclic 0.015 ± 0.118	Acyclic 0.962 ± 0.183		-
Motif [Ours]	House 0.918 ± 0.268	House-X 0.999 ± 0.032	Complete-4 1.000 ± 0.000	Complete-5 0.998 ± 0.045	83 s
Motif [Random]	House 0.000 ± 0.000	House-X 0.000 ± 0.000	Complete-4 0.000 ± 0.000	Complete-5 0.000 ± 0.000	-
Shape [Ours]	Lollipop 0.742 ± 0.360	Wheel 0.989 ± 0.100	Grid 0.996 ± 0.032	Star 1.000 ± 0.000	24 s
Shape [Random]	Lollipop 0.214 ± 0.301	Wheel 0.000 ± 0.000	Grid 0.151 ± 0.307	Star 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, $\bar{h}^{(L)}_{G_c}$, and the embedding of the generated explanation.

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

- 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.

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

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.

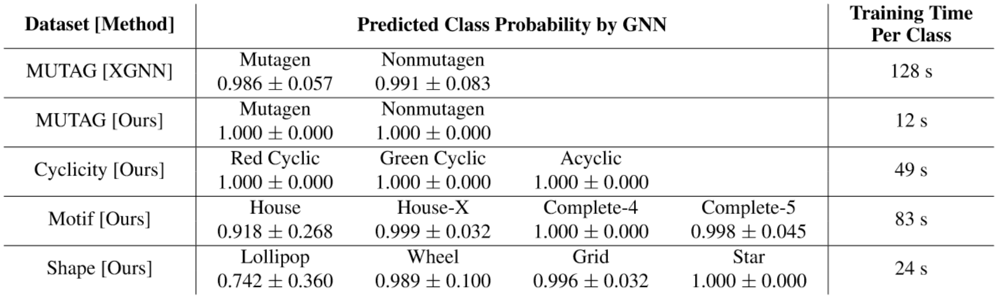
$$\mathcal{L}_{\text{Connect}}(\theta_A) = \sum_{i \in \nu} \sum_{j,k \in \mathcal{E}(i)} D_{KL}(\text{sigmoid}(\theta_A[i,\ j]) \mid\mid \text{sigmoid}(\theta_A[i,\ k])) \tag{8}$$

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:

$$\begin{aligned}\mathcal{L}_{\text{GNNInterpreter}}(\Theta \mid G_{\text{gen}}) =& \mathcal{L}_{\text{pred}}(\Theta \mid G_{\text{gen}}) + \mathcal{L}_{\text{embed}}(\Theta \mid G_{\text{gen}}) + \\ & \mathcal{L}_{\text{sparsity}}(\Theta \mid G_{\text{gen}}) + \mathcal{L}_{\text{connect}}(\Theta \mid G_{\text{gen}})\end{aligned} \tag{9}$$

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.



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  - 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.

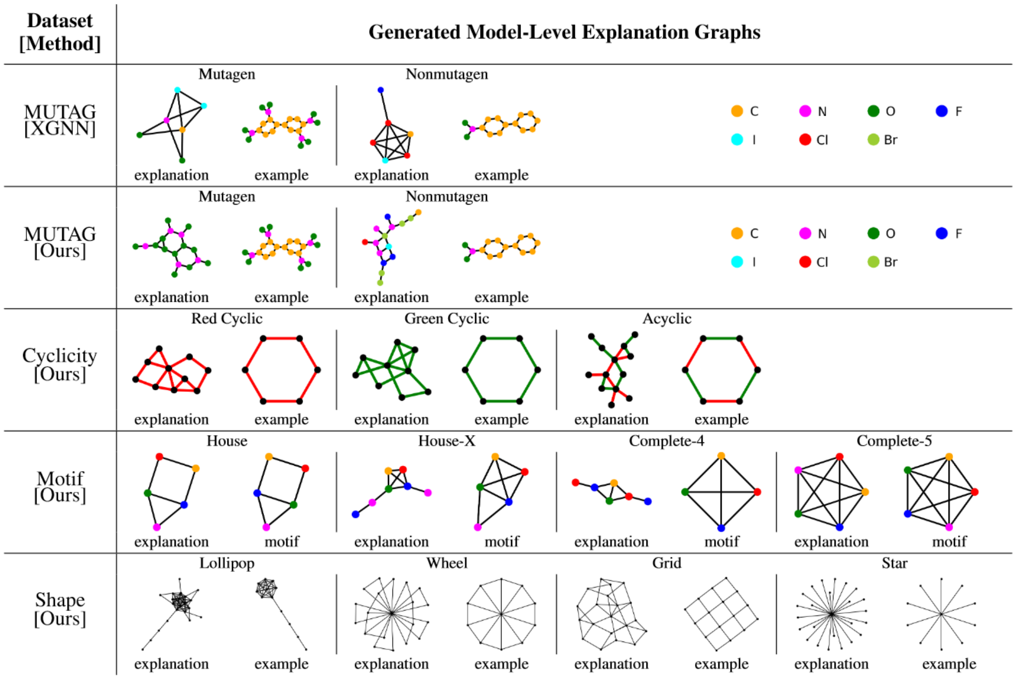


Figure 1: The qualitative results for 4 datasets. For each class in all datasets, the explanation graph with the class probability of 1 predicted by the GNNs is displayed on the left; as a reference, the example graph selected from the training data of the GNNs or the motif is displayed on the right. 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.
- Forward Diffusion
  - The authors here are focused on discrete structural diffusion. D4Explainer generate example graph by noising and de-nosing the adjacency matrices of observed graphs. The sampled graphs have the same features, but different structures.

  - The process of gradually adding noise to the input data is called forward diffusion.

During forward diffusion, random noise is added iteratively until the data becomes pure noise in the final iteration. This ensures that the denoising model can start with pure noise. Forward diffusion is usually a Markov process.

- If we assume that the observed graphs are Gilbert random graphs, like GNNInterpreter, pure noise would mean that $\forall\ (i,\ j)\ A[i,j] \sim \text{Bernoulli}(0.5)$.
- Let $t \in [0,T]$ denote the current iteration. Let β_t be the common probability that any edge changes state at time step t. $(\beta_1,\dots,\beta_T)$ is known as the variance schedule and is a set hyperparameter. Let A_t be a one-hot encoded version of the t^{th} noised adjacency, $[1,0]$ is the edge exists and $[0,1]$ otherwise. Then the forward diffusion process can be expressed as:

$$A_t[i,j] \sim q(A_t[i,\ j] \mid A_{t-1}[i,\ j]) = \text{Cat}(A_{t-1}[i,\ j] \cdot Q_t) \tag{10}$$

or

$$A_t[i,j] \sim q(A_t[i,\ j] \mid A_0[i,\ j]) = \text{Cat}\left(A_0[i,\ j]\prod_{i=1}^{t} Q_i\right) \tag{11}$$

where,

$$Q_t = \begin{bmatrix} 1-\beta_t & \beta_t \\ \beta_t & 1-\beta_t \end{bmatrix}$$

the t^{th} element-wise transition matrix.

- **Proof 2:** $\lim_{t\to\infty} q(A_t[i,\ j] \mid A_{t-1}[i,\ j]) \overset{D}{\to} \text{Bernoulli}(0.5)$ (converges in distribution).

$$\begin{aligned}
\lim_{t\to\infty} q(A_t[i,\ j] \mid A_{t-1}[i,\ j]) &= \lim_{t\to\infty} \text{Cat}\left(A_0[i,\ j]\prod_{i=1}^{t} Q_i\right) \\
&= \lim_{t\to\infty} \text{Cat}\left(A_0[i,\ j]\prod_{i=1}^{t} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1-2\beta_i \end{bmatrix} \begin{bmatrix} 0.5 & 0.5 \\ -0.5 & 0.5 \end{bmatrix}\right) \\
&\text{Eigen decomposition.} \\
&= \lim_{t\to\infty} \text{Cat}\left(A_0[i,\ j] \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \prod_{i=1}^{t} 1-2\beta_i \end{bmatrix} \begin{bmatrix} 0.5 & 0.5 \\ -0.5 & 0.5 \end{bmatrix}\right) \\
&= \text{Cat}\left(A_0[i,\ j] \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0.5 & 0.5 \\ -0.5 & 0.5 \end{bmatrix}\right) \\
&\text{Set } \beta < 0.5. \\
&= \text{Cat}([0.5, 0.5]) = \text{Bernoulli}(0.5)
\end{aligned}$$

- Backward Diffusion (Denoising Model)
  - A denoising model either predicts the error that was added or the value of the original observation. Even though only the adjacency matrix is being noised, we still want to include all available data. Thus the denoising model is parameterized as:

$$p(A_0 \mid A_t, t, X_0, E_0;\ \Omega) \tag{12}$$

where Ω is the set of trainable parameters.

  - The author employed a Provably Power Graph Network (PPGN) [cite] as their denoising model; however, they have added an additional neural network to learn the time or noise level effect.

- Loss Dist
  - Like most diffusion models, the primary objective is to minimize the distance between the predicted de-noised observation and the original. The author have added an additional weight term to focus the model on noisier or more difficult training examples.

$$\mathcal{L}_{dist}(\Omega \mid A_0) = \sum_{t=1}^{T} \left(1 - 2\bar{\beta}_t + \frac{1}{T}\right) \mathbb{E}_{\hat{A}_0} \text{CrtEnt}\left(A_0, \hat{A}_0\right) \tag{13}$$

where $\hat{A}_0 = p(A_0 \mid A_t, t, X_0, E_0;\ \hat{\Omega})$, $A_t[i,j] \sim q(A_t[i,\ j] \mid A_0[i,\ j])$, and

$$\bar{\beta}_t = \frac{1}{2} - \frac{1}{2}\prod_{i=1}^{t}(1 - 2\beta_i)$$

the cumulative transition probability.

- Model-level sampling algorithm
  - Use a set of observed graph features, D4Explainer generates model level explanations by sequentially denoising pure noise to generate an adjacency structure that has a high probability of being a member of the targeted class. At each step A_t is denoised to k candidates A_0, k. The candidate with the best predicted probability is then noised to a level of $t-1$ and the process is repeated. The pseudocode is reproduced below.

Algorithm 1 D4Explainer Model-level Explanation Reverse Sampling Algorithm

```
Require: $\hat{\Omega}$: trained denoising parameters; $q(A_t \mid A_0)$: forward diffusion process.
Input: N: maximum number of nodes; T: maximum noise level; K: number of candidates per
  iteration; $\tilde{\rho}$ targeted prediction vector; $(X, E)$: node and edge features.
Output: $\hat{A}$: adjacency matrix for model-level explanation.
  Sample $A_T[1:n, 1:n]$  Bernoulli(0.5)
  for t in T to 1 do
      Sample candidates $\{\hat{A}_{0,k} \sim p(A_t, t, X, E;\ \hat{\Omega}) : k \in 1, \ldots, K\}$
      Select the best candidate $\underset{j\ \in\ i,\ldots K}{\text{argmin}}$ CrtEnt(explainee($G = (X, A_{0,j}, E)$), $\tilde{\rho}$)
      Sample $A_{t-1}[1:n, 1:n] \sim q(A_{t-1}, A_{0,j})$
  end for
  return $A_0$
```

- In-Distribution metrics.
  - To access how well a sampled explanation matches the observed graph distribution, the author compute various maximum mean discrepancy (mmd) statistics.
  - MMD is a general technique to compute the distance between two distributions of data using only observed data. The distributions are estimated using a kernel an then the distance between there means are compared.

- A common way to approximate a density is to use the average of Gaussian distributions centered at each observation:

$$\begin{aligned} f(x)_X &\approx \frac{1}{n}\frac{1}{\sqrt{2\pi}\sigma}\sum_{i=1}^{n} e^{\dfrac{-(x-x_i)^2}{2\sigma^2}} \\ &\approx \frac{1}{n}\frac{1}{\sqrt{2\pi}\sigma}\sum_{i=1}^{n} \phi(x)^T\phi(x_i) \end{aligned}$$

  where, $k(x_i, x_j) = \phi^T(x_i)^T\phi(x_j)$ is the Gaussian kernel function. As long as the chosen kernel is *characteristic* the kernel mean embedding

$$\frac{1}{n}\sum_{i=1}^{n}\phi(x_i)^T = \frac{1}{n}\phi(\vec{x})\mathbb{1}$$

  is representative of the distribution. Here $\vec{x}$ is the vector of observations and $\mathbb{1}$ is the appropriate dimensional vector of 1s.

- MMD statistics are then simple the l2 distance between the kernel mean embeddings:

$$\begin{aligned} MMD(\vec{x},\vec{y}) &= ||\frac{1}{n}\phi(\vec{x})\mathbb{1} - \frac{1}{m}\phi(\vec{y})\mathbb{1}||_2^2 \\ &= \left(\frac{1}{n}\phi(\vec{x})\mathbb{1} - \frac{1}{m}\phi(\vec{y})\mathbb{1}\right)^T \left((\frac{1}{n}\phi(\vec{x})\mathbb{1} - \frac{1}{m}\phi(\vec{y})\mathbb{1}\right)^T \\ &= \frac{1}{n^2}\phi(\vec{x})^T\phi(\vec{x}) + \frac{1}{m^2}\phi(\vec{y})^T\phi(\vec{y}) - \frac{2}{nm}\phi(\vec{x})^T\phi(\vec{y}) \end{aligned}$$

- Intuitively $\phi(\vec{x})^T\phi(\vec{x})$ and $\phi(\vec{y})^T\phi(\vec{y})$ can be thought of as the distance within the observations of x and y and $\phi(\vec{x})^T\phi(\vec{y})$ as the distance between. Therefore an MMD statistic close to zero means that the distribution are approximately the same.

- The author use MMD statistics to compare the degree, clustering, and spectrum distributions of the generated explanation against the observed data. The degree distribution of a graph indicates how frequently nodes have different numbers of connections, reflecting the overall connectivity pattern. The clustering coefficient of a node measures the proportion of the node's neighbors that are also connected to each other, representing local clustering. The spectrum distribution, which is the distribution of eigenvalues of the adjacency matrix or Laplacian matrix, provides insights into the graph's structural characteristics and dynamic properties.

- Like GNNInterpreter, the author of D4Explainer also value the sparsity of their generate example. They measure the density of a graph as the number of present edges divided by the number of possible edges or

$$\text{Density} = |\mathcal{E}|/|\nu|^2 \tag{14}$$

- Loss CF
  - In additional to model-level explanations, D4Explainer can provide *counterfactual explanation* be include an additional term in the loss function. The authors define a counterfactual explanation for a particular observed graph to be G^c such that $\hat{Y}_{G^c} \neq \hat{Y}_G$, but the difference between G^c and G is minimal.

- $\mathcal{L}_{dist}$ ensures that the G^c generated won't deviate too far from the observed graph distribution.
- Adding $\mathcal{L}_{CF}$ minimize the probability that the generated graph is classified the same as the input graph.

$$\mathcal{L}_{CF}(\Omega \mid A_0) = \mathbb{E}_{\hat{A}_0} - \log(1 - \rho_{G^c}[\hat{Y}_G]) \tag{15}$$

  where $G = (X, A, E)$ is an observed graph and $G^c = (X, \hat{A}_0, E)$.
- To quantify the quality of generated counterfactual explanations, the author report *Counterfactual Accuracy*, *Fidelity*, and modification ratio.
  - CF-ACC measure the proportion of G^cs that have different predicted labels than there associated observed graph.

$$\text{CF-ACC} = \mathbb{E}_{A_t} I(\hat{Y}_{G^c} \neq \hat{Y}_G) \tag{16}$$

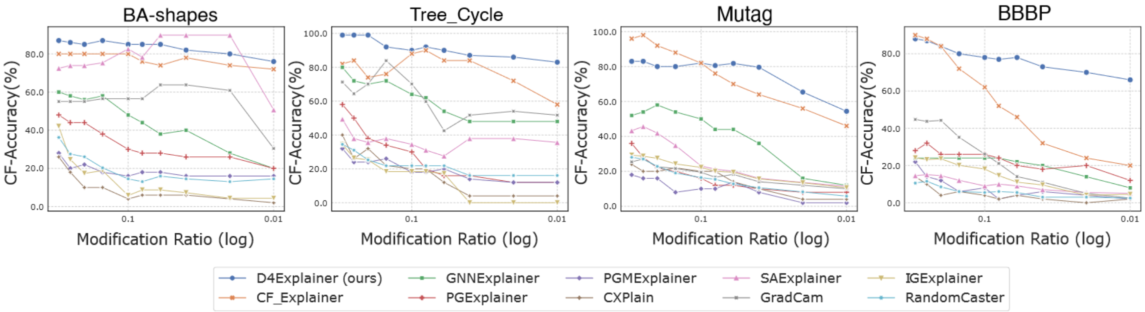
  - Fidelity measures the difference in the predicted probability of G and G^c with respected to the original class label.

$$\text{Fidelity} = \mathbb{E}_{\hat{A}_0} \rho_G[\hat{Y}_G] - \rho_{G^c}[\hat{Y}_G] \tag{17}$$

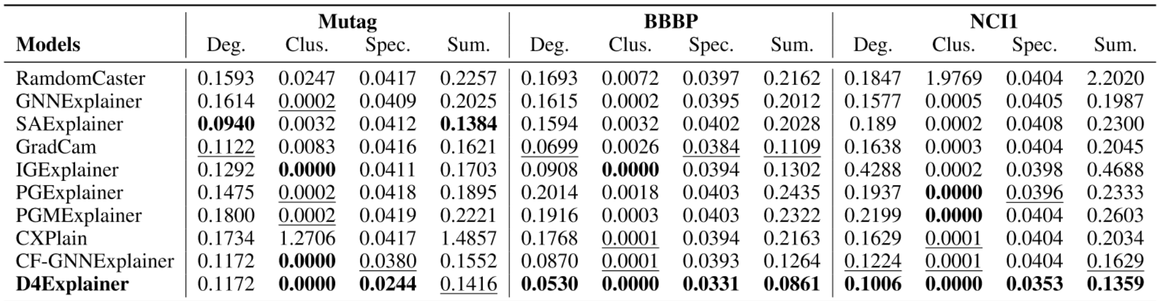
  - Modification ratio measures difference in edges between G^c and G relative to the size of the original graph.

$$\text{MR} = \frac{|\sum_{i,j} A[i,j] - \hat{A}_0(i,j)|}{\sum_{i,j} A[i,j]} \tag{18}$$

- Summary of Results + Figures
  - Similar to GNNInterpreter, the author report the mean predicted probability for the targeted class. Using a maximum of 6 nodes, the author were able to achieve a mean of 0.832 on the MUTAG dataset.
  - Since the counterfactual explanation are generated on a per observation basis, the author's compared their method to other popular instance-level explanation methods.



The above plot displays that D4Explainer can flip the prediction on ~80% of observed graphs at most modification levels. Missing from the plot is a variance measure. It is possible that the counterfactual accuracy varies more between different data splits or hyperparameter than the other methods.



	Mutag				BBBP				NCI1			
Models	Deg.	Clus.	Spec.	Sum.	Deg.	Clus.	Spec.	Sum.	Deg.	Clus.	Spec.	Sum.
RamdomCaster	0.1593	0.0247	0.0417	0.2257	0.1693	0.0072	0.0397	0.2162	0.1847	1.9769	0.0404	2.2020
GNNExplainer	0.1614	0.0002	0.0409	0.2025	0.1615	0.0002	0.0395	0.2012	0.1577	0.0005	0.0405	0.1987
SAExplainer	**0.0940**	0.0032	0.0412	**0.1384**	0.1594	0.0032	0.0402	0.2028	0.189	0.0002	0.0408	0.2300
GradCam	0.1122	0.0083	0.0416	0.1621	0.0699	0.0026	0.0384	0.1109	0.1638	0.0003	0.0404	0.2045
IGExplainer	0.1292	**0.0000**	0.0411	0.1703	0.0908	**0.0000**	0.0394	0.1302	0.4288	0.0002	0.0398	0.4688
PGExplainer	0.1475	0.0002	0.0418	0.1895	0.2014	0.0018	0.0403	0.2435	0.1937	**0.0000**	0.0396	0.2333
PGMExplainer	0.1800	0.0002	0.0419	0.2221	0.1916	0.0003	0.0403	0.2322	0.2199	**0.0000**	0.0404	0.2603
CXPlain	0.1734	1.2706	0.0417	1.4857	0.1768	0.0001	0.0394	0.2163	0.1629	0.0001	0.0404	0.2034
CF-GNNExplainer	0.1172	**0.0000**	0.0380	0.1552	0.0870	0.0001	0.0393	0.1264	0.1224	0.0001	0.0404	0.1629
D4Explainer	0.1172	**0.0000**	**0.0244**	0.1416	**0.0530**	**0.0000**	**0.0331**	**0.0861**	**0.1006**	**0.0000**	**0.0353**	**0.1359**

The above table indicates that the generated graph tend to have feature distribution that are close to the original dataset; however, there might be a hidden class bias. The distributions might only be close for the majority class, skewing the averages.

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

Methodology

- Since GNNInterpreter only makes qualitative assessments of generated structures, we applied the metrics describe in D4Explainer to quantify the properties of the generating distribution.

- We reimplemented GNNInterpreter using an identical generation scheme and loss function.

- We trained the reimplemented model on the MUTAG dataset which consists of nitroaromatic compounds, with the goal being to predict their mutagenicity on Salmonella typhimurium [cite]. Each observation is a graphs representing a chemical structure, where vertices denote atoms and edges represent bonds [cite]. MUTAG is a standard benchmark graph classification dataset.

- For our explainee model, we also implemented a 3-layer GCN model. There are slight variations between the architectures and training hyperparameter, but the accuracies are comparable, 86% (ours) and 92% (theirs).

- We additionally reimplement D4Explainer's counterfactual generator. Although not discussed in the original paper, this model can also be used to produce model level explanations. We simply randomly sample a graph from the opposite class and take the generated counter factual graph as our explanation.

Results

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
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

- We were unable to achieve 0 variance predictive accuracy, but again the values are comparable (see table ?) given the lack of extensive hyperparameter tuning. The prediction are similarity superior to that of D4Explainer (see table ?).
- As noted by the authors, the explainee model has a bias towards the mutagenic class (class 0), which can explain the greater deviation between the class 0 models.
- Another limiting factor is a lower set maximum number of nodes. We set it to 8 to make the results more comparable to the model-level explanation reported by D4Explainer.
- Surprisingly D4Explainer produces sparser graphs, in terms of density, than GNNInterpreter, despite no explicit penalty in the loss function.
- Based on the MMD statistics, the D4Explainer produces graph with better in-distribution properties. This might be the result of the explicit regularization in GNNInterpreter. Penalize the edge probabilities should result in a different degree distribution. The clustering coefficient might also be effect since fewer edges result in fewer triangle clusters.
- The spectrum distributions are close for both model, since both model enforce similarity in the explainee embedding space which is similar to the nature of the spectrum distribution.
- On the other hand, an argument could be made that a similar degree distribution and clustering coefficient isn't actually desirable. For larger or more densely connected graphs, lower MMD statistics might results in explanations that are too complex to be useful.
- The reimplement D4Explainer produces the least dense graphs, but has the least discriminative predictions. The latter makes sense, since the goal of the counterfactual loss is to flip the prediction, not necessarily maximize it. One the other hand, this model demonstrates that it is possible to generate sparse predictions and maintain a similar degree distribution and clustering.

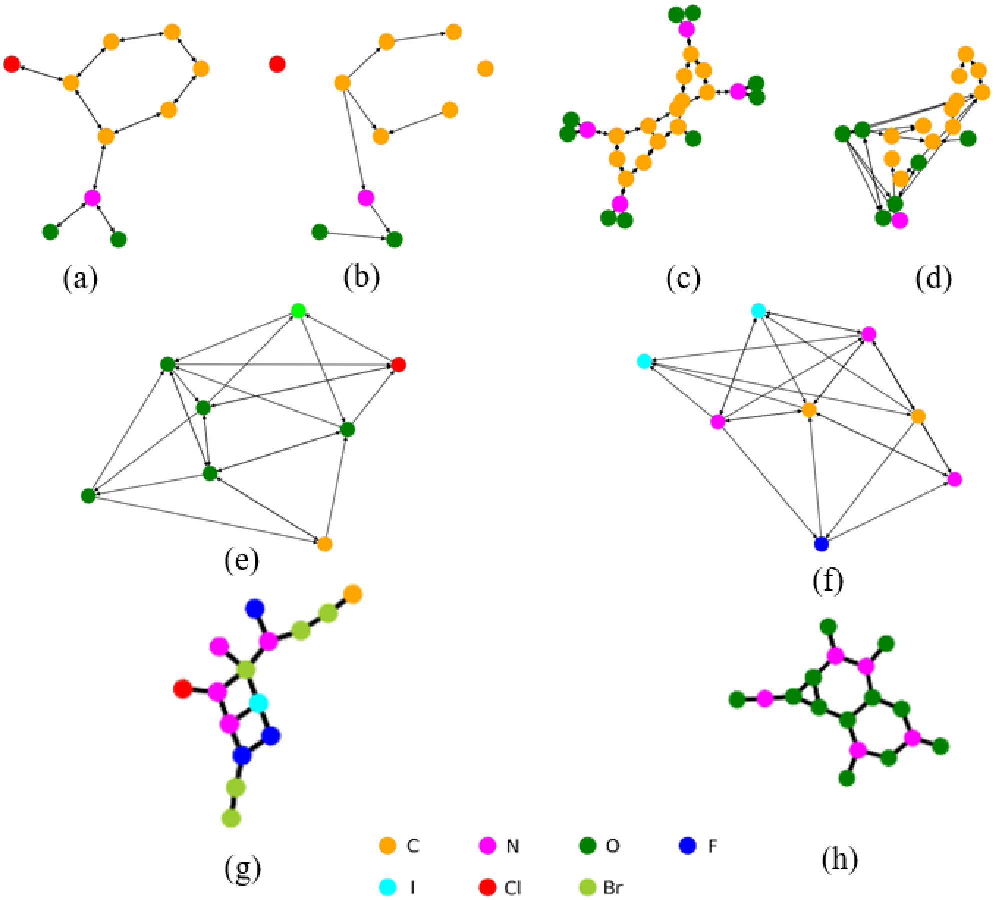


Figure 1: (a) Observed graph from class 0, Pr = 0.92; (b) Generated counterfactual explanation of (a) from D4Explainer reimplemented, Pr = 0.67; (c) Observed graph from class 1, Pr = 0.96; (d) Generated counterfactual explanation of (b) from D4Explainer reimplemented, Pr = 0.96; (e) Generated explanation for class 0 from GNNInterpreter reimplemented, Pr = 0.94; (f) Generated explanation for class 1 from GNNInterpreter reimplemented, Pr = 1.0; (g) Generated explanation for class 0 from GNNInterpreter (Wang and Shen 2024, fig. 1, pg.7), Pr = 1.0; (h) Generated explanation for class 1 from GNNInterpreter (Wang and Shen 2024, fig. 1, pg.7), Pr = 1.0.

- This results lead to two main conclusions.
    - First, the generator model should make use of the graph level observations. GNNInterpreter only use information about the graph structure through the explainee, never on the raw scale.
        - This lack of graph level information result can result in unrealistic distributional properties.
        - This could be done by using the observed graphs to predict the distributional parameters.
        - Alternatively, the generator could be replaced with a diffusion model without any need to modify the loss.
    - Second, the generator model should use class or prediction information.
        - D4Explainer's model-level sampling algorithm is less efficient and less accuracy than GNNInterpreter's direct optimization during training.
        - The reimplemented sampling algorithm demonstrates that direct denoising can still maintain low MMD statistics.
        - A possible modification would be to add the $\mathscr{L}_{\text{pred}}$ and $\mathscr{L}_{\text{embed}}$ from GNNInterpreter to the loss.
        - Alternatively, one could embedding the class label, similar to the way time is embedded, in order to establish a conditional diffusion model, which has worked extremely well in other applications.
        - Additionally, it would be easy to explore diffusing the node and edge features as well as like *DiGress* [cite].

Future Directions

Graph Edit Distance

- Class lean problem.
- GED as QAP.
- Simulation

Graph Prototype Masking Network

- Theory
- Diagram

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