[RE] GNNBoundary: Finding Boundaries and Going Beyond Them

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Abstract

Graph classification models are becoming increasingly popular, while explainability methods face challenges due to the discrete nature of graphs and other factors. However, investigating model decision-making, such as through decision-boundary regions, helps prevent misclassification and improve model robustness. This study aims to reproduce the findings of *GNNBoundary: Towards Explaining Graph Neural Networks Through the Lens of Decision Boundaries* (Wang & Shen, 2024). Their work supports 3 main claims: (1) their proposed algorithm can identify adjacent class pairs reliably, (2) their GNNBoundary can effectively and consistently generate near-boundary graphs outperforming the cross entropy baseline and (3) the generated near-boundary graphs can be used to accurately assess key properties of the decision boundary; margin, thickness, and complexity. We reproduce the experiments on the same datasets and extended them to two additional real-world datasets. Beyond that, we test different boundary probability ranges and their effect on decision boundary metrics, develop an additional baseline, and conduct hyperparameter tuning. We confirm the first claim regarding the adjacency discovery as well as the second claim that GNNBoundary outperforms the cross-entropy baseline under the limitation that it requires intensive hyperparameter tuning for convergence. The third claim is partially accepted as we observe a high variance between reported and obtained results, disproving the reliability and precision of the boundary statistics.

1 Introduction

Reproducibility is the backbone of scientific progress, ensuring that findings are robust, reliable, and generalizable. In that, model explainability methods are often used by researchers to assess and improve the robustness of a model. This study focuses on GNNBoundary by Wang & Shen, a framework designed to analyze decision boundaries in graph neural networks (GNNs) (Scarselli et al., 2009), more specifically in GNN-based classifiers. Understanding decision boundaries is crucial for evaluating model robustness, as well as identifying and understaning modes of failure. This is especially important for real-world applications in domains such as social networks, biology, and recommender systems (Fan et al., 2023).

GNNs have shown remarkable performance in tasks involving graph data, such as node classification, link prediction, and graph classification (Errica et al., 2019). Despite their widespread utilization, the complexity of these models often leads to challenges in understanding their decision-making. GNNBoundary, as a post-hoc method, attempts to open this black-box by investigating decision boundaries with quantitative metrics and visualizing near-boundary graphs for adjacent class pairs. By doing so, the method offers insights into how GNNs distinguish between classes and the robustness of the classification.

The aim of this reproducibility study is to verify the results and claims made in the original GNNBoundary paper by Wang & Shen (2024). Specifically, this study attempts to determine whether the GNNBoundary framework can be used to consistently and reliably generate near-boundary graphs and collect boundary metrics for the discovered adjacent class pairs. This entails reproducing the authors' experiments, verifying the correctness of the implementation, and evaluating the robustness of the findings across four datasets:

Motif (Wang & Shen (2022)), Collab (Yanardag & Vishwanathan (2015)), Enzymes (Schomburg et al. (2004)), and IMDB (Yanardag & Vishwanathan (2015)).

Beyond reproducing the results from Wang & Shen (2024) using their instructions, we aim to enhance the applicability of GNNBoundary for practitioners and researchers by giving additional guidance. Moreover, we provide insights on the generalizability and robustness of the method through additional experiments and analyses.

2 Reproducibility Considerations

To guide our efforts, the claims and contributions defined in this section will carry through the following sections. The main claims made by the authors are as follows:

Main Claims:

1. Their proposed algorithm for identifying adjacent class pairs can reliably identify the degree of adjacency of a class pair.
2. GNNBoundary can effectively and consistently generate near-boundary graphs with faster convergence and a higher success rate than the cross-entropy baseline.
3. The generated near-boundary graphs can be used to accurately assess key properties of the decision boundary: margin, thickness, and complexity.

Our main contributions beyond the reproduction of the results from Wang & Shen (2024) are:

Contributions:

1. Performing hyperparameter optimization to systematically analyze the impact of different configurations on convergence behavior, leading to faster and more stable model training.
2. Developing an additional baseline by using over 500 GNNInterpreter graphs (Wang & Shen, 2022) per class in each dataset and connecting them via randomly assigned edges.
3. Extending experiments with two real-world datasets: posts from the forum site Reddit and a relational graph dataset IMDB, with actors and actresses connected by co-appearances in movies.
4. Investigating the trade-off between boundary metric approximation quality and target class probability ranges (e.g., $[0.49, 0.51]$, $[0.45, 0.55]$), offering practical insights into the training requirements for near-boundary graph sampling.

3 Background

3.1 Graph Neural networks

An increasing amount of graph structured data creates a need for a graph structure learning systems. Graph Neural Networks (GNNs) emerge from its predecessors in deep learning as models to operate on graph structures. Graphs have unique characteristics that differentiate them from other data types, such as a variable number of nodes and edges across graphs. This variability complicates the application of convolutions. Moreover, unlike images or text, where individual data instances are typically independent, graphs exhibit inherent dependencies, as nodes can be interconnected and therefore influence each other (Wu et al., 2020). GNNs are networks that aim to create a representation vector of a node or a whole graph given the features of the node and the graph structure (Xu et al., 2018). The higher need for graph analysis and the emergence of various GNNs such as Graph Convolutional Networks (Kipf & Welling, 2016) and Graph Attention Networks (Veličković et al., 2017), create the need for explainability and interpretability in the GNN domain.

3.2 Explainability of GNNs

In a review of explainability approaches to GNNs by Kakkad et al. the explanation is described to come from either self-interpretability or from post-hoc explainability methods. The former enables the model to justify its predictions during training and influence it, while the latter considers the training as a black-box process that is to be explained post-training. GNNBoundary is a post-hoc explainability method. It examines the decision boundaries of a trained GNN by learning to generate graphs near the boundary. The final distinction in the review is to instance-level and model-level explainability. Instance-level explainability aims to explain predictions of a certain instance, while the model-level method aims to justify the high-level decision-making process of the whole model. GNNBoundary is considered a model-level method as the generation of near-boundary graphs aims to explain global patterns in the decision process of a GNN classifier. In literature previous to GNNBoundary, generation-based methods do not yet explore the decision boundaries. However some methods explore the model-level behavior by generating graphs representative of a class, such as GNNInterpreter (Wang & Shen, 2022) and XGNN (Yuan et al., 2020).

3.3 Decision region and boundary

A classifier f partitions the d-dimensional space $\mathbb{R}^d$ into C decision regions $\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_C$, such that for any $G \in \mathcal{R}_c$, the predicted class is $c = argmax_k f_k(G)$ where $k \in [1, C]$ (Karimi et al., 2019). The decision boundary between class c_1 and class c_2 is defined as $\mathcal{B}_{c_1 \| c_2} = \{G : f_{c_1}(G) = f_{c_2}(G) > f_{c'}(G), \forall c' \neq c_1, c_2\}$, representing the set of graphs G where the classifier assigns equal probability to classes c_1 and c_2, while ranking them higher than all other classes. For the embedding space, Wang & Shen (GNNBoundary) define

$$\mathcal{B}^{(l)}_{c_1 \| c_2} = \{\mathbf{H}^{(l)} : \sigma(\eta_l(\mathbf{H}^{(l)}))_{c_1} = \sigma(\eta_l(\mathbf{H}^{(l)}))_{c_2} > \sigma(\eta_l(\mathbf{H}^{(l)}))_{c'}, \forall c' \neq c_1, c_2\} \tag{1}$$

where σ is the Softmax activation function and η_l are the last $L - l$ layers of the discriminator f that output the logits for graph embedding $\mathbf{H}^{(l)}$ after layer l. In other words, the decision boundary represents the points in $\mathbb{R}^d$ where the classifier is "uncertain" about assigning a label between classes c_1 and c_2.

4 GNNBoundary

Wang & Shen (2024) propose an adjacency finding algorithm, an objective function to generate near-boundary graphs for adjacent class pairs and a dynamic regularization scheduler to avoid local minima.

Notation. A graph, represented by $G = (\mathcal{V}, \mathcal{E})$, with $\mathcal{V} = \{v_1, v_2, \ldots, v_N\}$ and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ being the set of nodes and edges respectively. The total number of edges is denoted by M and total number of nodes is denoted by N. The adjacency relationships between nodes are captured by the adjacency matrix $\mathbf{A} \in \{0, 1\}^{N \times N}$, where an entry $a_{ij} = 1$ indicates an edge between node v_i and node v_j, and $a_{ij} = 0$ otherwise. Node features are stored in the feature matrix $\mathbf{Z} \in \mathbb{R}^{N \times d}$ where $\mathbf{z_i} \in \mathbb{R}^d$ corresponds to the feature vector of node v_i.

4.1 Adjacency Discovery

Running the boundary analysis for all class pairs would be computationally prohibitive. Hence, Wang & Shen propose an adjacency discovery method that calculates adjacency rates based on the dataset and all but the last layer of discriminator model f denoted as embedding function η_{L-1}. This comes with the advantage that the embedding space after the last hidden layer has linear decision boundaries. The algorithm samples graphs $G_{c_1} \in \mathcal{R}_{c_1}$ and $G_{c_2} \in \mathcal{R}_{c_2}$, embeds them using η_{L-1} obtaining $\mathbf{H}^{(L-1)}_{c_1}$ and $\mathbf{H}^{(L-1)}_{c_2}$ respectively. They then interpolate between $\mathbf{H}^{(L-1)}_{c_1}$ and $\mathbf{H}^{(L-1)}_{c_2}$in the embedding space and use the remaining layer of the discriminator f to determine if the interpolated embedding is part of any intermediate decision region other than $\mathcal{R}_{c_1}$ or $\mathcal{R}_{c_2}$. The final adjacency score is the share of the K sampled graph pairs that do not cross any decision region other than $\mathcal{R}_{c_1}$ or $\mathcal{R}_{c_2}$.

4.2 Graph Generation

GNNBoundary Sampling. As discrete structures, graphs are not inherently differentiable. However, Wang & Shen propose a relaxation approach to mitigate this issue. The discrete graph structure is relaxed into a differentiable form allowing gradient-based optimization, using the reparameterization trick inspired by Jang et al. (2016), Wang & Shen (2022) and Luo et al. (2020). The boundary graphs are modeled as Gilbert random graphs (Gilbert, 1959), where the probability distribution of the graph $P(G)$ is formulated as the product of node feature probabilities $P(z_i)$ and edge probabilities $P(a_{ij})$. Edges are sampled from a Bernoulli distribution, while node features follow a Categorical distribution. To enable gradient-based learning, the categorical variables are relaxed using the Concrete distribution (Maddison et al., 2016), leading to a differentiable approximation. The concrete distribution is a continuous version of the Categorical distribution with closed-form density, $\tilde{z}_i \sim \text{Concrete}(\zeta_i, \tau_z)$ for the node features $\tilde{a}_{ij} \sim \text{BinaryConcrete}(\omega_{ij}, \tau_a)$ for edges, where τ_z and τ_a are hyperparameters to control the approximation of Categorical distribution, $\omega_{ij} \in \Omega$ and $\zeta_i \in \mathbb{Z}$. For sampling, the authors of GNNBoundary (Wang & Shen, 2024) utilize the Gumbel-Softmax trick (Jang et al., 2016), which ensures that both the edge variables and node feature variables remain differentiable. This is achieved by computing edge variables $\tilde{a}_{ij}$ and node feature variables $\tilde{z}_i$ using the transformations $\tilde{a}_{ij} = \text{Sigmoid}\left((\omega_{ij} + \log\epsilon - \log(1-\epsilon))/\tau_a\right)$ and $\tilde{z}_i = \text{Softmax}((\zeta_i - \log(-\log\epsilon))/\tau_z)$. Furthermore, the graph distribution is learned by minimizing the expected loss function through Monte Carlo sampling and gradient descent, making the boundary graph generation process efficient for discrete graph structures, and follows:

$$\min_{\mathbf{A},\mathbf{Z}} \mathcal{L}(G) = \min_{\mathbf{\Theta},\mathbf{P}} \mathbb{E}_{G\sim P(G)}\left[\mathcal{L}(\mathbf{A},\mathbf{Z})\right] \approx \min_{\mathbf{\Omega},\mathbf{Z}} \mathbb{E}_{\epsilon\sim U(0,1)}\left[\mathcal{L}(\tilde{\mathbf{A}},\tilde{\mathbf{Z}})\right] \approx \min_{\mathbf{\Omega},\mathbf{Z}} \frac{1}{K}\sum_{k=1}^{K} \mathcal{L}(\tilde{\mathbf{A}},\tilde{\mathbf{Z}}). \tag{2}$$

where $\mathbf{A}$ and $\mathbf{Z}$ denote the adjacency matrix and node feature matrix of the graph. We point out that this sampling framework builds on a strong independence assumption. Specifically, the probability distributions for the edges, nodes and node features are all independent of each other in this framework. While this assumption is needed to make the sampling computationally tractable, it yields a potentially inaccurate model of the graph sampling space. Future research could work on ways to mitigate this issue.

Boundary Criterion. To generate boundary graphs, the probability of a boundary graph belonging to both classes should be equal, i.e. $G_{c_1\|c_2} \in \mathcal{B}_{c_1\|c_2}$ with $\sigma(f(G))_{c_1} = \sigma(f(G))_{c_2} = 0.5$. As this is usually unattainable in practice, the authors propose a relaxed class probability range that the boundary graphs are permitted to belong to. Thus, the stopping criterion for the optimization that determines whether a graph G is close enough to the boundary $\mathcal{B}_{c_1\|c_2}$ is defined as:

$$\Psi(G) = \mathbb{I}_{p(c_1),p(c_2)\in[p_{\min},p_{\max}]}(G). \tag{3}$$

The authors suggest using $p_{min} = 0.45$ and $p_{max} = 0.55$. Due to this relaxation, the term "near-boundary graph" is more accurate than "boundary graph" and will be used in the following sections.

Optimization. To generate near-boundary graphs, the optimization objective must be designed to balance the trade-off between boundary classes while ensuring efficiency. A key limitation of using the cross-entropy loss as an objective function is its inability to fully satisfy the required constraints for near-boundary graph generation, as it still may lead to the minimization of one of the logit values of the boundary classes. This does not serve the goal of producing near-boundary graphs that have features of both adjacent classes. An improved objective function is proposed that encourages posterior probabilities for boundary classes, $p(c_1) = p(c_2) = 0.5$, while minimizing unwanted class probabilities, $b' \notin \{c_1, c_2\}$. Additionally, a squared penalty is introduced that penalizes logit values that differ from the target class probability vector. This optimization technique is essentially an "enhanced" cross-entropy that encourages higher probabilities for both adjacent classes and penalizes deviated logits. Formally,

$$\min_{G} \mathcal{L}(G) = \min_{G} \sum_{b'\notin\{c_1,c_2\}} \beta f(G)_{b'} \cdot p^*(b')^2 - \sum_{b\in\{c_1,c_2\}} \alpha f(G)_b \cdot (1-p^*(b))^2 \cdot \mathbb{I}_{p^*(b)<\max_{c\in[1,C]} p^*(c)}, \tag{4}$$

where $f(G)_{c_1}$ and $f(G)_{c_2}$ are logits of the function $f(G)$ of the two adjacent classes and α and β are constant hyperparameters.

Regularization. To control the graph size in terms of the number of nodes and edges, Wang & Shen propose the use of L_1 and L_2 regularization:

$$R_{\text{budget}} = \text{Softplus}\left(\|\text{Sigmoid}(\mathbf{\Omega})\|_1 - B\right)^2, \tag{5}$$

with B being the expected maximum number of nodes in a boundary graph G. Given that certain patterns require certain graph sizes, a size penalty is a potential problem for convergence. Hence, the authors propose a dynamic scheduling method within the training procedure that adapts the budget penalty. To not hinder convergence, a smaller penalty is applied on graphs further away from the decision boundary and bigger penalty on graphs closer to the decision boundary. The budget penalty weight is defined as,

$$w_{\text{budget}}^{(t)} = w_{\text{budget}}^{(t-1)} \cdot s_{\text{inc}}^{\mathbb{I}\{\Psi(G^{(t)})\}} \cdot s_{\text{dec}}^{\mathbb{I}\{\neg\Psi(G^{(t)})\wedge(s_{\text{dec}}\cdot w_{\text{budget}}^{(t-1)} \geq w_{\text{budget}}^{(0)})\}}, \tag{6}$$

where $w_{budget}^{(0)}$ is a hyperparameter for the initial weight, s_{inc} is for weight increment, s_{dec} is for weight decrement and $G^{(t)} = \mathbb{E}_{G\sim P(G)}[G]$ for an optimization iteration t. The dynamic regularization can help convergence by permitting the budget penalty to interfere with the main loss function.

4.3 Boundary Analysis

Margin. The boundary margin quantifies the minimum separation between decision regions in a graph classification model (Yang et al., 2020). Unlike classical margin definitions, which are based on worst-case distances, Wang & Shen (2024) use class representative graphs (also denoted as G_{c_1} in the following) generated using the GNNInterpreter framework (Wang & Shen, 2022). Given a dataset $\mathcal{D}$, a classification function f, and graph representations G_{c_1} and $G_{c_1\|c_2}$ belonging to different decision regions, the boundary margin is defined as:

$$\Phi(f, c_1, c_2) = \min_{(G_{c_1},\, G_{c_1\|c_2})} \|\phi_l(G_{c_1}) - \phi_l(G_{c_1\|c_2})\| \tag{7}$$

where $G_{c_1} \in \mathcal{R}_{c_1}$ and $G_{c_1\|c_2} \in \mathcal{B}_{c_1}$ represent graph samples from class c_1 and its nearest boundary region with class c_2, respectively. The function $\phi_l(G)$ denotes the graph embedding function extracted from classifier f, mapping the input graphs into a learned feature space. A larger margin implies better class separation, contributing to model robustness, while a smaller margin suggests higher decision boundary instability, increasing the risk of misclassification (Yang et al., 2020).

Thickness. Boundary thickness is a metric that quantifies the width of a decision boundary. Given a classification function f, the asymmetric boundary thickness $\Theta(f, \gamma, c_1, c_2)$ is defined as the expected distance between pairs of graphs G_{c_1} and $G_{c_1\|c_2}$, sampled from a distribution P, weighted by the fraction of a continuous interpolation between these graphs where the posterior difference satisfies a margin condition. Formally, this is expressed as:

$$\Theta(f, \gamma, c_1, c_2) = \mathbb{E}_{(G_{c_1}, G_{c_1\|c_2})\sim P}\left[\left\|\phi_l(G_{c_1}) - \phi_l(G_{c_1\|c_2})\right\| \int_0^1 \mathbb{I}_{\gamma > \sigma(\eta_l(h(t)))_{c_1} - \sigma(\eta_l(h(t)))_{c_2}} dt\right] \tag{8}$$

where $h(t) = (1-t)\cdot\phi_l(G_{c_1}) + t\cdot\phi_l(G_{c_1\|c_2})$ defines an interpolation between the boundary graph embedding $\phi_l(G_{c_1\|c_2})$ and class graph embedding $\phi_l(G_{c_1})$. Boundary thickness captures the average width of the decision boundary. If the decision boundary has a low width and thus separates the data well, the integral in eq. (8) will become a small number. Hence, a low boundary thickness corresponds to a low graph density around the decision boundary and with that good separation of the data.

Complexity. The boundary complexity measure calculates the structural complexity of a classifier's decision boundary by analyzing the distribution of adversarial examples in feature space. Using Principal Component Analysis (PCA), the spread of adversarial examples is captured through the eigenvalues $\boldsymbol{\lambda}$ of

their covariance matrix (Guan & Loew (2020)). A simpler decision boundary results in adversarial examples aligning along a single eigenvector, whereas a more complex boundary distributes them across multiple eigenvectors. This complexity is computed as the Shannon entropy of the normalized eigenvalues:

$$\Gamma(f, c_1, c_2) = H\left(\frac{\boldsymbol{\lambda}}{\|\boldsymbol{\lambda}\|_1}\right) / \log D = \left(-\sum_i \frac{\lambda_i}{\|\boldsymbol{\lambda}\|_1} \log\left(\frac{\lambda_i}{\|\boldsymbol{\lambda}\|_1}\right)\right) / \log D. \tag{9}$$

Here, $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_n)$ represents the eigenvalues of the covariance matrix of the adversarial set, and $\|\boldsymbol{\lambda}\|_1$ is the sum of all eigenvalues, ensuring a normalized representation. The entropy function $H(\cdot)$ measures how evenly variance is distributed across eigenvectors, and D denotes the dimensionality of the feature space, normalizing the complexity measure to the range $[0, 1]$. A higher complexity indicates a more uneven decision boundary, implying greater sensitivity to perturbations and risk of over-fitting. On the other hand, a lower complexity score suggests a smoother boundary, which is more likely to generalize well to unseen data.

5 Experimental Setup

In addition to reproducing the results from Wang & Shen (2024), in order to confirm the validity and robustness of the described methods, we aim to convey an empirically-driven intuition behind the GNNBoundary and to make it more accessible to practitioners and researchers. To reproduce the results, we utilized the authors' publicly available code repository[1]. However, several critical components were absent in the original implementation, as detailed in Appendix H. We implement the missing parts and make it public as linked in the abstract.

5.1 Adjacency Discovery

To verify claim 1, we run the algorithm for identifying adjacent class pairs proposed by Wang & Shen for all datasets. To further verify the resulting adjacency scores, we analyze the measured success rates for near-boundary graph generation on the adjacent class pairs as well as on a selection of non-adjacent class pairs. High success rates would generally be expected on adjacent class pairs and low success rates would be expected on non-adjacent class pairs.

5.2 Datasets

The GNNBoundary method was originally evaluated on three datasets: Motif, Collab, and Enzymes, with the latter two being real-world graph datasets. The synthetic Motif dataset, introduced in Wang & Shen (2022), consists of graphs labeled with one of four predefined motifs: House, HouseX, Comp4, and Comp5. The Collab dataset comprises ego-networks of scientific collaboration, representing co-authorship networks in the fields of High Energy Physics (HE), Condensed Matter Physics (CM), and Astrophysics (Astro) Yanardag & Vishwanathan (2015). The Enzymes dataset Schomburg et al. (2004) consists tertiary-structured proteins classified into one of six enzyme classes.

Given that only 3 datasets are used in Wang & Shen (2024), we further assess the method's performance in real-world settings, using two additional real-world datasets: IMDB and Reddit-Mulitclass. The IMDB dataset consists of 1,500 graphs, where nodes represent actors and actresses. An edge is formed between two nodes if the corresponding individuals appeared in the same movie. Each graph is categorized into one of three genres: Comedy, Romance, or Sci-Fi. The Reddit dataset contains 232,965 posts collected from the social media platform Reddit. Each graph instance represents a subreddit community, where nodes correspond to posts, and edges indicate that a user commented on both posts. The dataset includes five class labels corresponding to different subreddits: *worldnews*, *videos* (general video-sharing), *AdviceAnimals* (humorous advice posts featuring animals), *Aww* (cute content), and *Mildlyinteresting*. This dataset contains larger graphs compared to the other datasets (cf. table 5) to test the scalability of the method.

[1]The authors' GitHub repository can be accessed at: https://github.com/yolandalalala/GNNBoundary

5.3 Hyperparameters

Wang & Shen report one set of hyperparameters for all datasets. Moreover, it is missing configurations for the dynamic regularization scheduler as well as the graph target size. Consequently, we ran Bayesian Optimization Shahriari et al. (2015) to find the optimal hyperparameter configuration for each dataset. The search space consists of the sample size K, the target size, the target probabilities, the learning rate, the temperature, and the weight budget increase for the dynamic regularization scheduler and the weight budget decrease. Details on the search space are given in appendix G. Moreover, we employed a simple custom loss for the hyperparameter tuning, being the average deviation of the class probabilities from the target 0.5:

$$\mathcal{L}(CP) = \frac{1}{N_{cp}} \sum_{cp} \frac{|p(c_1^{cp}) - 0.5| + |p(c_2^{cp}) - 0.5|}{2}$$

where N_{cp} is the number of class pairs in adjacent class-pair set CP and c_1^{cp} & c_2^{cp} are class one and two of a class pair respectively. We chose this simple criterion instead of GNNBoundaries' dynamic boundary criterion to be independent of the tested method as well as for simplicity and thus easier interpretability.

5.4 Baselines

Wang & Shen propose a random baseline that generates boundary graphs using a graph from c_1 and a graph from c_2 and combines them with a random edge.

Dataset-based Graph Sampling. In the absence of prior methods for analyzing the decision boundary of GNN-based classifiers, the authors proposed a simple baseline that samples a graph from the dataset for each class in the class pair and connects them with a randomly assigned edge to obtain a graph that is theoretically representative of both classes. Thus, it is expected to activate the classifier's probability distributions maximally for these two classes. Our reproduction of this baseline corroborates the authors' findings, demonstrating that this approach frequently fails to produce near-boundary graphs, as the randomly sampled graph structures often lack the properties needed to elicit near-boundary probability activations.

GNNInterpreter-based Graph Sampling. To address the limitations of the random sampling baseline, we devised a novel baseline leveraging GNNInterpreter (Wang & Shen, 2022). Specifically, we generate class-representative graphs with GNNInterpreter and connect them with a random edge. This aims at producing graph features more representative of each class. One limitation is that it introduces significant complexity due to the hyperparameter tuning required for GNNInterpreter (e.g., generating hundreds of graphs per class). These challenges render the GNNInterpreter-based baseline infeasible in settings where finding class-representative graphs (e.g. using GNNInterpreter) is not needed anyways. This reaffirms the need for better baselines for generating near-boundary graphs.

5.5 Boundary Embedding Discovery

In an attempt to shed light on the position of the near-boundary graphs in the discriminators embedding space (i.e., after applying the graph embedding function $\eta_{L-1}(G)$), we implement a method that randomly initializes an embedding and then optimizes it to a point in the embedding space where the discriminator assigns a probability in the [0.45, 0.55] target range for the corresponding class pair classes. This is to inspect the near-boundary regions in the embedding space after plotting it's UMAP (McInnes et al., 2020) and PCA (Jolliffe, 2002) 2D representation.
Formally, with η_L being the last layer of discriminator function f that assigns a probability to a given embedding, let $\mathbf{z}$ be an embedding, which does not necessarily have to correspond to an actual valid graph. We seek a near-boundary embedding $\mathbf{z}^*$ that satisfies:

$$\mathbf{z}^* = \arg\min_{\mathbf{z}} \mathcal{L}_{CE}(\eta_L(\mathbf{z}), \mathbf{y}^*)$$

where $\mathcal{L}_{CE}$ is the Cross-Entropy loss and $\mathbf{y}^*$ is the target vector of shape C. Suppose, we want to find a boundary embedding for class i and j, then $y_i^* = y_j^* = 0.5$ and $y_k^* = 0 \ \forall k \neq i, j$. The optimization is

performed over an initially random embedding $\mathbf{z}$ to cover most near-boundary regions in the embedding space. Note that this is only to find near-boundary points in the embedding space for the purpose of visualization and hence there is no need for $\mathbf{z}^*$ to be the embedding of a valid graph.

5.6 Boundary Statistics under Different Target Probability Ranges

The accuracy of boundary metric approximations depends on both the quantity and quality of near-boundary graphs. The quality refers to how close these graphs are to the boundary (defined as having a probability of 0.5 for c_1 and c_2). To investigate this, we evaluate the boundary statistics (complexity, margin and thickness) for different target probability ranges and analyze the patterns.

6 Results & Discussion

To verify the stated claims 1, 2 and 3 we reproduce all experiments from Wang & Shen (2024) as well as the extensions described in section 5, report the results and discuss them in this section.

6.1 Reproduction of Results

Before contributing additional insights on the optimized hyperparameters, new real-world datasets, the new baseline and the boundary statistics, we attempt to reproduce the results from Wang & Shen (2024) as good as possible under their reported configurations (refer to table 8 in appendix G for an overview of the authors' hyperparameters). Since some hyperparameters are not explicitly stated in Wang & Shen (2024), we infer the values and ranges from the demo notebooks provided in the authors' code base: initial weight budget as 1, the weight increase as 1.15, the decrease as 0.95, and the target size as 30.

Finding Adjacent Class Pairs. We reproduce the results for the Collab, Motif and Enzymes datasets using their provided code and observe insignificant differences in adjacency scores (appendix A). As layed out in section 5.1, we also analyze the correlation between the adjacency score and the corresponding GNNBoundary success rate to verify the author's proposed adjacency discovery algorithm. Figure 1 depicts the measurements of the adjacency score and the GNNBoundary success rate for class pairs across datasets. Class pairs that were determined to be adjacent by Wang & Shen are depicted in blue, while a selection of non-adjacent class pairs is plotted in orange. The adjacency score used for fig. 1 is the one we obtained from the author's adjacency discovery algorithm.

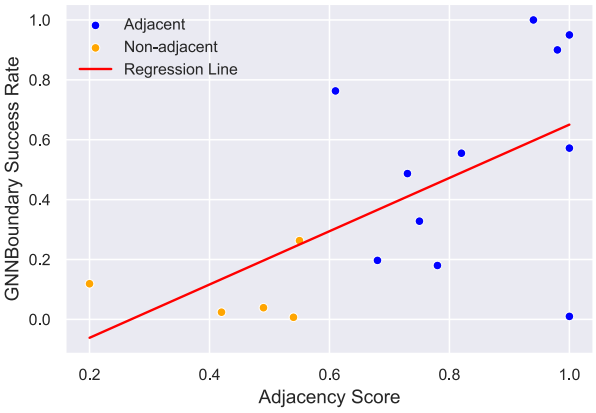

Figure 1: Comparison of success rate to adjacency score obtained using their adjacency finding algorithm. Success rates are measured under optimized hyperparameters we obtained from HPO (cf. section 6.2). Adjacent means that the GNNBoundary author's reported these as adjacent.

As expected, we can see a clear correlation between the adjacency score and success rate, indicating that the obtained adjacency score is a good proxy for adjacency. To further quantify these results, we find that the Pearson correlation coefficient is 0.6 and the p-value of the regression is 0.0139. Hence, there is a clear positive correlation and the regression is statistically significant under a 98% confidence level.

Given the clear positive correlation and statistical significance, we accept claim 1.

Boundary Graph Generation. When comparing our table 1 with table 1 in Wang & Shen (2024), we observe that we were mostly able to obtain very similar results when it comes to the ability of GNNBoundary

to generate near-boundary graphs with both class-probabilities being close to 0.5. An exception of this are the first four class-pairs of the Enzymes dataset which did not converge under the target probability range of $p_{min} = 0.45$ and $p_{max} = 0.55$. We hypothesize this discrepancy between our and the authors' results to be caused by subpar hyperparameter settings, slight differences in discriminator performance (cf. appendix D and figure 3 in Wang & Shen (2024)) and to some extend random variation. In terms of complexity, we mostly observe higher values, i.e. greater sensitivity to perturbations and overfitting, thus worse generalization to unseen graphs. As we reproduce their random baseline, we observe different values, but a similarly strong discrepancy between the class-probabilities and the targeted 0.5 probability as well as high standard deviations.
Despite the small discrepancy regarding the Enzymes dataset, we can mostly confirm the results from Wang & Shen regarding the class-pair probabilities of GNNBoundary boundary graphs. We confirm the superiority of GNNBoundary over the random baseline without limitations.

Table 1: Comparison of GNNBoundary and baseline near-boundary graph probabilities across datasets. We report the mean class probability among 500 boundary graphs and the corresponding standard deviation. No results were obtained for the Reddit dataset and convergence could not be reached for the "Romance-Sci-Fi" class pair (view section 6.3 for more details). **Probabilities closer to 0.5 are better**.

Dataset	c_1	c_2	**GNNBoundary**			**Random Baseline**	
			Complexity	$\mathbf{p(c_1)}$	$\mathbf{p(c_2)}$	$\mathbf{p(c_1)}$	$\mathbf{p(c_2)}$
Motif	House	HouseX	0.015	0.506 ± 0.030	0.494 ± 0.030	0.719 ± 0.264	0.064 ± 0.148
	House	Comp4	0.072	0.506 ± 0.029	0.493 ± 0.029	0.590 ± 0.308	0.382 ± 0.322
	HouseX	Comp5	0.230	0.506 ± 0.056	0.494 ± 0.056	0.886 ± 0.256	0.004 ± 0.018
Collab	HE	CM	0.313	0.481 ± 0.019	0.475 ± 0.018	0.314 ± 0.443	0.000 ± 0.000
	HE	Astro	0.253	0.495 ± 0.028	0.493 ± 0.027	0.046 ± 0.200	0.954 ± 0.200
Enzymes	EC1	EC4	0.198	0.436 ± 0.030	0.426 ± 0.022	0.190 ± 0.315	0.299 ± 0.434
	EC1	EC5	0.112	0.426 ± 0.021	0.510 ± 0.013	0.196 ± 0.304	0.203 ± 0.333
	EC1	EC6	0.206	0.435 ± 0.023	0.488 ± 0.037	0.227 ± 0.320	0.011 ± 0.070
	EC2	EC3	0.319	0.447 ± 0.040	0.463 ± 0.045	0.131 ± 0.286	0.371 ± 0.407
	EC4	EC5	0.126	0.490 ± 0.044	0.493 ± 0.044	0.302 ± 0.432	0.200 ± 0.330
	EC4	EC6	0.357	0.462 ± 0.042	0.450 ± 0.039	0.334 ± 0.380	0.053 ± 0.167
IMDB	Comedy	Romance	0.028	0.457 ± 0.006	0.463 ± 0.009	0.303 ± 0.136	0.112 ± 0.196
	Comedy	Sci-Fi	0.265	0.496 ± 0.028	0.496 ± 0.026	0.303 ± 0.132	0.622 ± 0.156
	Romance	Sci-Fi	–	–	–	–	–

Success Rate in Boundary Graph Generation. Under the authors' hyperparameter settings we cannot confirm the high reported success rates from Wang & Shen (2024) as well as we cannot confirm GNNBoundary consistently outperforming the cross-entropy baseline (cf. table 2) under their hyperparameter settings. When using our hyperparameter settings, we obtain success rates much closer to the authors' ones and consistent superiority over cross-entropy for the Motif and Collab dataset (cf. table 3). For Enzymes we again struggle to confirm their results even with optimized hyperparameters.

To summarize, we confirm the ability of GNNBoundary to find faithful near-boundary graphs and its superiority over the random baseline. However we cannot confirm their high convergence rates. Under this limitation, we still consider claim 2 to be valid.

Boundary Statistics Analysis. Based on the case study provided in section 5.3 of Wang & Shen (2024) we implement the boundary margin, boundary thickness and boundary complexity metrics and reproduce

the results for their three datasets and report them in appendix D. We generally observe significantly higher values for the boundary thickness, which corresponds to a comparatively high probability density of graphs on the boundary as opposed to the class regions. This can be interpreted as worse separability.
For Motif, the margins are comparable for about half of the class combinations and significantly higher for the remaining half. Given that higher margins indicate better class-separability and with that better robustness, our results for Motif are even better than the ones reported by Wang & Shen. For Collab, we observe mostly lower margins, i.e. worse separability and robustness when compared to the authors results and for Enzymes we also observe mostly mixed results compared to the authors reports, where some are higher and other are lower without a clear tendency. In general, there are significant discrepancies between our results and the author's results, which makes us question the reliability and precision of the employed boundary statistics. Based on our observations, we would rather see these statistics as an approximate low-precision indicator of the boundary structure. Beyond that, we hypothesize the worse separability exhibited by a lower margin and higher thickness to be connected to a slightly worse classification performance as compared to the authors (cf. the confusion matrix in appendix D to figure 3 in Wang & Shen (2024)). This is despite the fact that we used the authors' provided discriminator model checkpoints.

In the light of these findings, we accept claim 3 only under the strong limitation that the boundary statistics cannot be considered reliable or precise given their significant discrepancies under small changes of discriminator accuracy.

While we are mostly able to confirm the results from Wang & Shen (2024) on the Motif and Collab datasets, we face challenges in reproducing the results for the Enzymes dataset throughout all experiments. Wang & Shen also observe class pair probabilities closer to the edges of the [0.45, 0.55] range, lower success rates and higher boundary thickness for the Enzymes dataset in comparison to the other datasets. However, we cannot reach their results, not even under optimized hyperparameters (cf. table 1, table 3, appendix D). We hypothesize this to be connected to the high complexity of the dataset given the higher number of classes and worse classifier performance. This highlights the methods dependency on classifier performance and its limitations when it comes to more complex datasets. Our attempts to improve the performance for the Enzymes classifier or to use a different model architecture to enhance classifier performance did not succeed.

6.2 Hyperparameters

Among the hyperparameters that were reported by the authors we tuned the target probability range, the learning rate and the temperature. As can be seen in table 8 in appendix G, the discovered optimal configurations are highly dependent on the dataset and mostly deviate significantly from the author's reported configuration. This highlights the need for dataset specific reporting of hyperparameters and offers an explanation for the large discrepancy in convergence between our table 2 and table 2 in Wang & Shen (2024). Notably, the optimal values for temperature and learning rate can mostly be found at the boundaries of our tuning ranges designed around the values provided by the authors, which highlights that the optimal configurations are far from the values reported by Wang & Shen. These results are expected given that different datasets come with different optimization landscapes that require appropriate hyperparameters. For instance, an optimization landscape with a higher number of local minima usually requires a higher learning rate to enable global convergence.

6.3 New Datasets

We find that GNNBoundary works mostly well for IMDB, while it is not possible to run it in a reasonable amount of time for the Reddit dataset.

IMDB Dataset. We obtain fast and stable convergence for boundary graphs in class pairs "Comedy-Romance" and "Comedy-SciFi", while we could not achieve convergence for class pair "Romance-SciFi". The same goes for GNNInterpreter training: we obtain good results for classes "Comedy" and "SciFi", but not for "Romance". We observe that the boundary graphs for "Romance-SciFi" are very sparsely connected (cf.

appendix E.1) and usually even contain several disconnected graphs. This is inherently problematic given that GNNs are based on message-passing and thus likely the reason for the described convergence issues.

Reddit Dataset. For training the boundary graph sampler, we increased the maximum number of nodes from 25 [2] to 550, which is slightly above the average graph size of 508 nodes (cf. table 5) to make convergence more likely. However, such a large graph has up to $\frac{n(n-1)}{2}$ undirected edges, which for 550 nodes would be up to 150.975 edges. This leads to training times of around 330 minutes for a single boundary graph sampler on an Apple M3 chip. HPO and generating 500 boundary graphs to compute the boundary statistics was hence not possible under the resource constraints of this work. Thus, we cannot report results for this dataset.

6.4 Random Baseline for Boundary Graph Class-Probabilities

Comparing table 1 and table 4, we cannot observe that the baseline based on dataset graphs has class probabilities closer to 0.5 than the one based on GNNInterpreter graphs: on average 35.7% for $p(c_1)$ and 23.1% for $p(c_2)$ when using dataset class graphs whereas the average probabilities for GNNInterpreter-based class graphs are 37.3% for $p(c_1)$ and 20.0% for $p(c_2)$. The variances of the class probabilities across the GNNInterpreter- and dataset-based baselines are also comparable. We also investigated using 2, 3 and 5 random edges but did not observe significant changes in the results and hence omit further details on this.

6.5 Robustness of Boundary Detection

As described in section 5.5, we attempt to inspect the classifier embedding space by plotting the 2D UMAP and PCA of each adjacent class pair, the corresponding GNNBoundary near-boundary graphs and the near-boundary embeddings discovered by our cross-entropy based method described in section 5.5. As can be seen in fig. 2 [3], the GNNBoundary graphs form a larger structure throughout the embedding space, while our boundary embeddings are concentrated in one location. This is due to the fact that our cross-entropy based method optimizes for probabilities under the use of a Softmax instead of the logits. Given that the logits are unbounded, our method always resorts to the same minimum for which the difference in magnitude of the logits enable the desired probability distribution. The GNNBoundary graph embeddings on the other hand, escape this issue and distribute along a larger structure in the latent space, highlighting GNNBoundary's robustness.

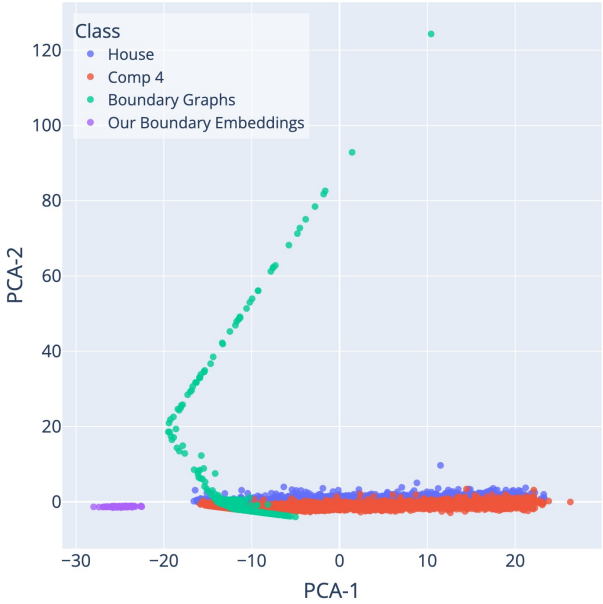

Figure 2: 2D PCA plot for showing the classifier embeddings for the dataset, the GNNBoundary embeddings and our boundary embeddings for the Motif class pair House-Comp 4.

We note that PCA is not locality-preserving. Hence, the fact that the boundary graphs do not appear in-between the classes on the plot does not necessarily corresponding to the actual proximity in high-dimensional latent space. Consequently, this empirical study might give an intuition for the existence of structures in latent space, but it cannot be used to argue about the precise location of the found boundary graphs in that latent space.

[2] We used a maximum number of nodes of 25 per graph for the other datasets.
[3] The corresponding UMAP plot can be found in appendix I

6.6 Boundary Statistics under Different Target Probability Ranges

To validate the $[0.45, 0.55]$ probability range $[p_{min}, p_{max}]$, we analyzed boundary statistics (thickness, margin, complexity) across several probability ranges, from $[0.42, 0.58]$ to $[0.495, 0.505]$ and present the full results in appendix J. This approach helps assess whether the range suggested by Wang & Shen (2024) reliably includes near-boundary graph properties.
Overall, $[0.45, 0.55]$ serves as a good baseline, but variations in some cases highlight the general instability of the graph generation process. This instability mainly comes from the stochastic nature of graph sampling, where small fluctuations in probability estimates can lead to different graph configurations. For example, in the Motif dataset, boundary thickness for the House-Comp4 class pair remains stable, while the Collab dataset shows larger deviations at $[0.495, 0.505]$. Similarly, the Enzymes dataset exhibits increasing margins for class pair EC4 and EC5 in narrower ranges.
Despite these fluctuations, the variance trend remains mostly stable, with occasional outliers. The $[0.45, 0.55]$ range balances precision and stability, though the observed variations reflect the inherent instability of the boundary graph generation approach.

7 Conclusion

GNNBoundary is a pioneering framework that enables finding near-boundary graphs in GNN classifiers that can be used to collect the boundary statistics margin, thickness and complexity for a quantitative assessment of a GNN classifiers robustness. It is the first work to offer explainability on the decision boundary of a GNN classifier. In this study, we reproduced the author's results and confirm the author's claims: (1) we observe similar results when using their adjacency discovery algorithm and report a high correlation between the obtained adjacency scores and near-boundary graph generation success rates. Further, (2) we find that GNNBoundary can consistently generate near-boundary graphs and is superior to the cross-entropy baseline. However, this was only possible after extensive hyperparameter optimization. Finally, (3) we observe high variations on the boundary statistics, which makes us question their reliability and precision. Nonetheless, they can still provide some orientation on the generalization capabilities of the classifier. As a result, we confirm only limited applicability of the boundary statistics. Throughout experiments, we observe performance issues with the Enzymes dataset and explain this with it's relatively high complexity and low classifier performance. To further assess GNNBoundary's general applicability, we test the method on two additional real-world datasets. In that, we observe fair results for one dataset (IMDB) and no results for the other (Reddit) due to a deficient scalability with larger graphs. Moreover, we conduct an empirical analysis of GNNBoundary's robustness in boundary detection and find it to be robust compared to a simple cross-entropy based baseline method for finding near-boundary embeddings that we introduce. Finally, we perform a study on the stability of the boundary statistics under different target class probability ranges and confirm the $[0.45, 0.55]$ range suggested by the authors.
In summary, we can commend the effort of the GNNBoundary authors as the interpretability of GNN classifiers is a valuable and underexplored topic, but issues around the usability of their method, including hurdles like the need for extensive hyperparameter optimization, confine future researchers ease to build upon this idea.

8 Next Steps

Future research could work on a more realistic graph sampling framework that overcomes the strong independence assumption being made by the independence of the distributions for edges, nodes and node features. Attempts to reduce the method's need for hyperparameter optimization or alternative approaches that are easier to apply could further contribute to GNN classifier explainability. Despite our extensive hyperparameter optimization efforts, we cannot confirm the author's consistently high convergence rates and observe significant discrepancies on the boundary statistics, highlighting the need for more robust methods.

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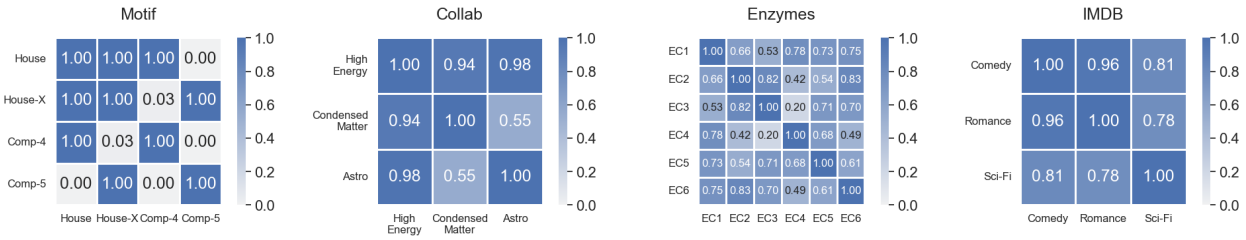
A Adjacency Finding

Adjacency rates reported in the original work differ slightly from the values obtained when reproducing adjacency tables, using the checkpoints provided and the seed noted in the open source code. As the differences are minimal, we decide upon accepting the adjacent pairs stated by the authors and proceed further with the research using them.

Figure 3: Adjacency matrices for each dataset. Small adjacency values indicate that no decision boundary between the two classes is present in the classifier. A threshold of 0.8 is applied to explore the *adjacent class-pairs*, while the class-pairs below this threshold are considered *non-adjacent*.



B Success Rates of Boundary Graph Generation

Given that the reported success rates were not achieved using the authors' implementation, HPO was used to find improved configurations. Given the discrepancy between the success rates using the author's hyper-parameters and our optimized ones with the reported results, we consider their report of experimental setup insufficient for reproducing their work.

Table 2: Convergence success rates **under the author's hyperparameters** across class pairs comparing GNNBoundary to the baseline cross-entropy criterion for success rate and average convergence iteration. **Higher success rate is better**.

Dataset	c_1	c_2	**Success Rate**		**Avg. Convergence Iteration**	
			GNN-Boundary	**Cross Entropy**	**GNN-Boundary**	**Cross Entropy**
Motif	House	HouseX	**0.072**	0.055	**125.24**	273.40
	House	Comp4	**0.681**	0.653	79.86	**64.59**
	HouseX	Comp5	0.000	**0.002**	–	**429.50**
Collab	HE	CM	0.793	**0.998**	118.00	**65.30**
	HE	Astro	**0.998**	0.923	**12.38**	109.27
Enzymes	EC1	EC4	**0.120**	0.004	216.62	**103.25**
	EC1	EC5	0.054	**0.631**	222.30	**174.01**
	EC1	EC6	0.184	**0.853**	241.34	**51.63**
	EC2	EC3	0.242	**0.776**	158.28	**103.92**
	EC4	EC5	0.102	**0.720**	**103.84**	157.04
	EC5	EC6	0.440	**0.972**	**59.08**	72.80

No results were obtained for the Reddit dataset (cf. section 6.3 for more details) and convergence could not be reached for the "Romance-SciFi" class pair (cf. section 6.3).

Table 3: Convergence success rates **under optimized hyperparameters** across class pairs comparing GNNBoundary to the baseline cross-entropy criterion for success rate and average convergence iteration. **Higher success rate is better**.

Dataset	c_1	c_2	**Success Rate**		**Avg. Convergence Iteration**	
			GNN-Boundary	**Cross Entropy**	**GNN-Boundary**	**Cross Entropy**
Motif	House	HouseX	**0.527**	0.055	**201.65**	273.40
	House	Comp4	**0.950**	0.653	**41.45**	64.59
	HouseX	Comp5	**0.010**	0.002	**343.23**	429.50
Collab	HE	CM	**1.000**	0.998	77.75	**65.30**
	HE	Astro	**0.900**	0.923	**19.71**	109.27
Enzymes	EC1	EC4	**0.180**	0.004	216.62	**103.25**
	EC1	EC5	0.487	**0.631**	222.30	**174.01**
	EC1	EC6	0.328	**0.853**	241.34	**51.63**
	EC2	EC3	0.555	**0.776**	158.28	**103.92**
	EC4	EC5	0.197	**0.720**	**103.84**	157.04
	EC5	EC6	0.763	**0.972**	**59.08**	72.80
IMDB	Comedy	Romance	**0.750**	0.0720	**86.11**	182.92
	Comedy	Sci-Fi	**0.770**	0.5080	**228.52**	243.43
	Romance	Sci-Fi	–	–	–	–

C Baseline using GNNInterpreter

Given some ambiguities in Wang & Shen (2024) and the fact that GNNInterpreter graphs are used for the boundary statistics, we also compute the random baseline using GNNInterpreter graphs. It works the same way as the standard random baseline with the only difference being that it samples class-graphs from previously trained GNNInterpreter samplers instead of the labeled training datasets themselves.

Table 4: Baseline probabilities for datasets and class tuples sampling using **GNNInterpreter class graphs** connected using a random edge to obtain boundary graphs.

Dataset	**Class Pairs**		**Baseline**	
	c_1	c_2	$p(c_1)$	$p(c_2)$
Motif	House	HouseX	0.3799 ± 0.4140	0.0742 ± 0.2260
	House	Comp4	0.3171 ± 0.3784	0.4397 ± 0.4307
	HouseX	Comp5	0.2394 ± 0.3648	0.4669 ± 0.4934
Collab	HE	CM	0.9607 ± 0.0008	0.0000 ± 0.0000
	HE	Astro	0.9607 ± 0.0008	0.0393 ± 0.0008
Enzymes	EC1	EC4	0.0360 ± 0.1575	0.0272 ± 0.1551
	EC1	EC5	0.0736 ± 0.2442	0.0250 ± 0.1501
	EC1	EC6	0.4461 ± 0.4790	0.0010 ± 0.0160
	EC2	EC3	0.0748 ± 0.2462	0.6005 ± 0.4589
	EC4	EC5	0.3377 ± 0.4299	0.5146 ± 0.4564
	EC5	EC6	0.2760 ± 0.4256	0.0211 ± 0.1212

D Boundary Statistics

We run the boundary complexity, margin and thickness as well as a confusion matrix for all three datasets from Wang & Shen (2024) and report on all of them except for the boundary complexity (which can be found in table 1) in the following fig. 4. These results are discussed in section 6.1.

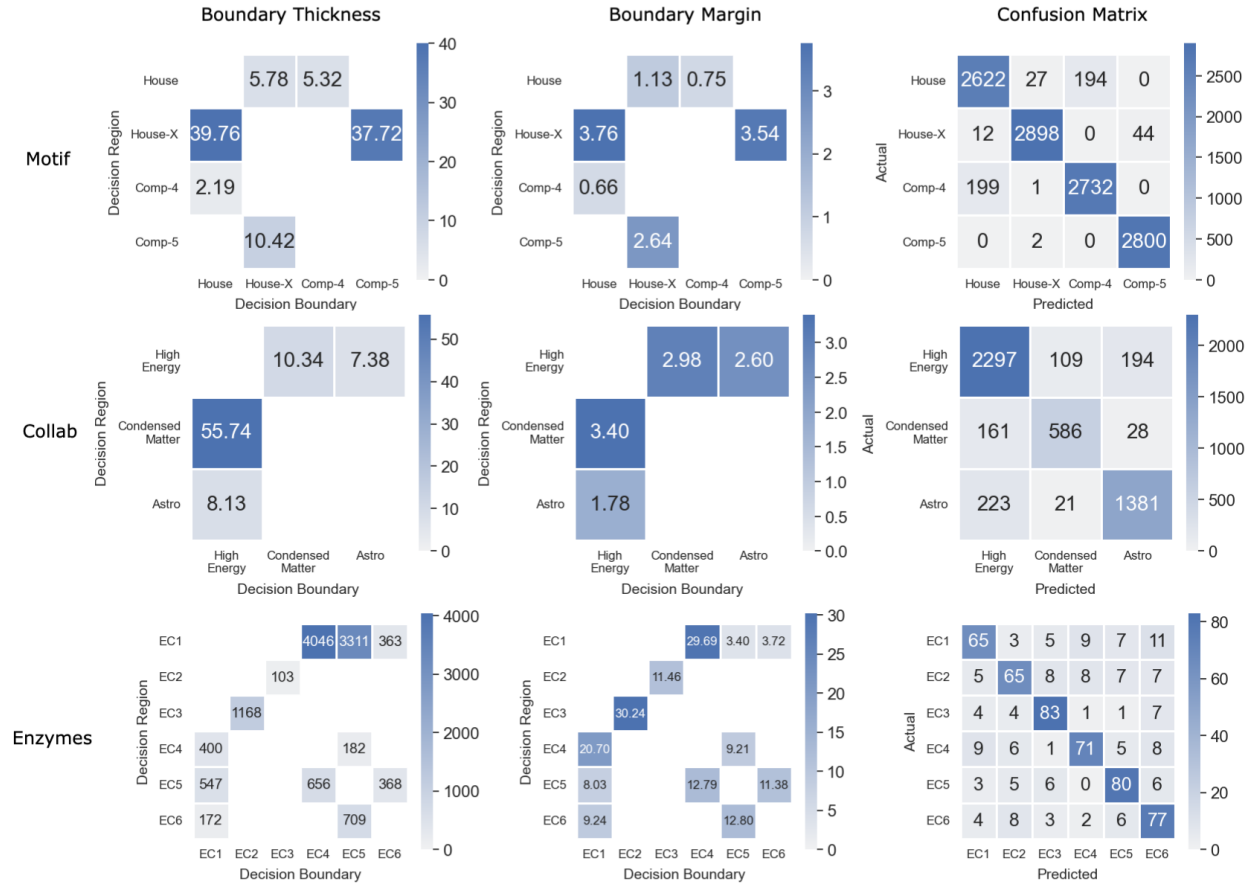


Figure 4: Boundary metric analyses and confusion matrices.

E Datasets

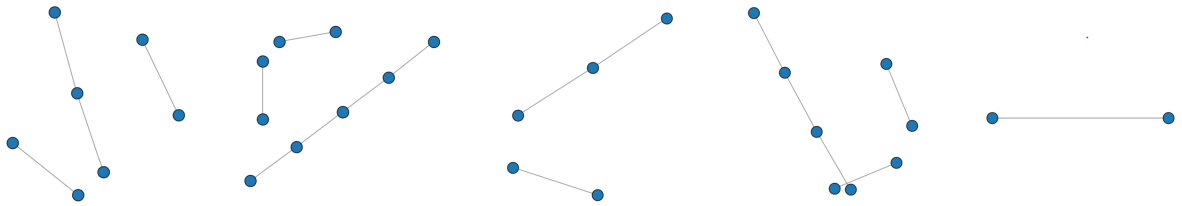
Apart from the datasets we added, Wang & Shen (2024) employ the Motif, Collab and Enzymes datasets described in the following. For a better understanding of the employed datasets, we provide table 5.

Table 5: Dataset statistics. Size refers to the number of nodes in a graph.

Statistic	Size (Nodes)	Mean Graph Size	Median Graph Size	Min Graph Size	Max Graph Size	Std Graph Size
Motif	11,531	57.07	51.00	14	112	25.65
Collab	5,000	74.49	52.00	32	492	62.30
Enzymes	600	32.46	32.00	2	125	14.87
Reddit	4,999	508.51	374.00	22	3,648	452.57
IMDB	1,500	13.0	10.0	7	89	8.52

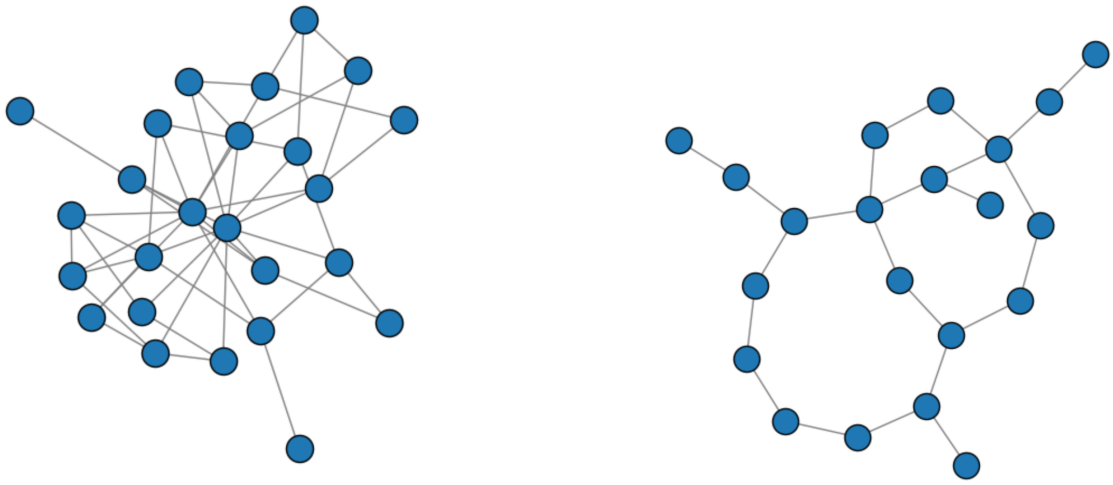
E.1 Details on the IMDB Dataset

Following the challenges on generating boundary graphs for the "Romance-SciFi" class pair and GNNInterpreter graphs for the "Romance" class, we provide examples of "Romance"-graphs and "Romance-SciFi"-graphs to identify potential root causes.



(a) (b) (c) (d) (e)

Figure 5: Examples of Romance-SciFi near-boundary graphs.



(a) Near-boundary graph for Romance-Comedy.

(b) Near-boundary graph for Comedy-SciFi.

Figure 6: Comparison of near-boundary graphs for Romance-Comedy and Comedy-SciFi class pairs.

F GCN Classifier

Table 6: Classifier accuracies, class-wise F1-scores, and GNN architecture hyperparameters for each dataset, using pre-trained checkpoints from the authors' work. For IMDB, the classifier was trained with architecture parameters informed by the dataset's graph properties.

Dataset	**Test Accuracy**	**Class**	**F1 Score**	**Architecture**	
				Hidden Channels	**Num Layers**
Motif	0.961	House	0.923	6	3
		House X	0.984		
		Comp 4	0.946		
		Comp 5	0.994		
Collab	0.782	High Energy	0.802	64	5
		Condensed Matter	0.617		
		Astro	0.823		
Enzymes	0.483	EC1	0.273	32	3
		EC2	0.526		
		EC3	0.750		
		EC4	0.348		
		EC5	0.500		
		EC6	0.500		
IMDB	0.453	Comedy	0.156	64	5
		Romance	0.491		
		Sci-Fi	0.573		

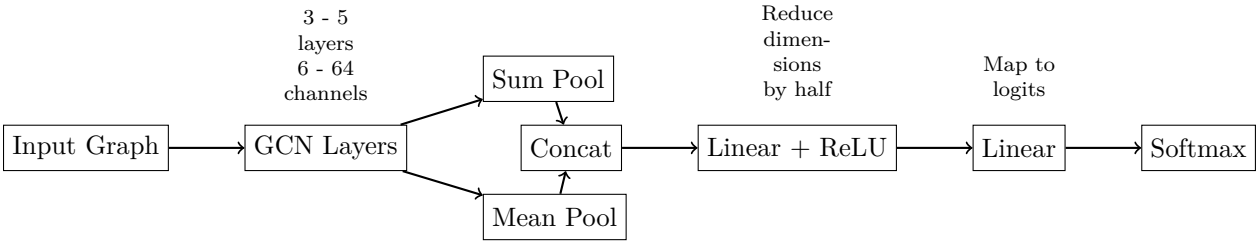


Figure 7: Architecture overview of the GCN classifier. The model processes input graphs through multiple GCN layers with LeakyReLU and Dropout, performs global weighted pooling operations, and uses linear layers for the final classification.

G Hyperparameter Optimization

The following table shows the search space employed for automatic hyperparameter optimization using Bayesian Optimization. We worked with 8 random starts, 200 tuning iterations and 3 runs per iteration. We found that the results within those 3 runs were mostly consistent and we took the mean performance across those 3 runs as the performance of the entire tuning iteration. Each run had 1000 training iterations. Hyperparameter optimization was done separately for each of the datasets.

Table 7: Search Space for Hyperparameters

Hyperparameter	Data Type	Range / Values	Prior Distribution
Target Size	Integer	[20, 60]	Uniform
Target Probabilities	Categorical	{"0.45-0.55", "0.4-0.6", "0.35-0.65"}	Uniform
Learning Rate	Real	[0.01, 1]	Uniform
Temperature	Real	[0.05, 0.5]	Log-Uniform
Weight Budget inc.	Real	[1.05, 1.2]	Uniform
Weight Budget dec.	Real	[0.94, 0.99]	Uniform

Table 8: Hyperparameter optimization results. The search space includes the sample size K, the target size, the target probabilities, the learning rate, the temperature, the weight budget increase for the dynamic regularization scheduler and the weight budget decrease. HPO for the Reddit dataset was not possible under the given configurations due to the high graph size (cf. section 6.3).

Hyperparameter	Collab	Motif	Enzymes	IMDB	Reddit	Authors
Iterations	1000	1000	1000	1000	1000	1000
Sample Size K	32	32	32	32	32	32
Init. Weight Budget	1	1	1	1	-	-
Target Size	60	50	46	60	-	-
Target Probabilities	[0.45, 0.55]	(0.4, 0.6)	(0.35, 0.65)	(0.4, 0.6)	-	[0.45, 0.55]
Learning Rate	0.01	1.0	0.02	0.9	-	1.0
Temperature	0.05	0.05	0.5	0.49	-	0.15
Weight Budget Inc.	1.20	1.05	1.10	1.12	-	-
Weight Budget Dec.	0.99	0.99	0.95	0.94	-	-
Custom Loss	0.038	0.118	0.170	0.10	-	-

H Remarks on Implementation

We commend the authors for their efforts to ensure the reproducibility of their work by releasing their code, pre-trained model checkpoints, and providing detailed Readme instructions. In the spirit of transparency, we offer additional context on the implementation process and suggestions for improvement, with the hope of contributing to future learning opportunities in the field.

Reproducing the main results of the study required a significant investment of both time and computational resources. While the provided notebooks served as helpful examples, we encountered issues with hyperparameter configurations as they led to convergence problems and were incomplete. Since no dedicated

training script was included to replicate the results in the original paper, we implemented our own training runs using the parameters specified in the paper or inferred from the notebooks. As shown in table 2, this configuration often failed to generate sufficient near-boundary graphs, making the reproduction of the results significantly harder. To address this, we conducted hyperparameter optimization (HPO) to derive class-pair-specific configurations that improved convergence. However, even with the optimized parameters, the success rates remained lower than the authors reported ones.

An implementation for the boundary complexity, thickness and margin was also a not included in the code publicized by the authors.

The environment setup was facilitated by both an environment.yml and a pyproject.toml file. The latter included a Git dependency from a common XAI library[4] used by both the GNNInterpreter (Wang & Shen (2022)) and GNNBoundary (Wang & Shen (2024)) repositories. This common library contains several crucial components, but its inheritance structure introduced implementation challenges. Specifically, overlapping versions of key components within the shared repository led to confusion. Notably, the absence of a clear training script, the lack of well-defined boundary metric calculations, and the presence of multiple versions of graph sampling implementations required significant effort to understand and resolve the intended design.

I Embedding Space Inspection

In fig. 8, we can see a very similar phenomenon as in fig. 2. The GNNBoundary near-boundary graph embeddings are spread across a larger area in a specific structure while the near-boundary embeddings are collapsed to the same location in the embedding space during optimization. This supports the findings that the GNNBoundary dynamic boundary criterion allows for a more robust optimization process than our cross-entropy based method. More details on our reasoning are provided in section 6.5.

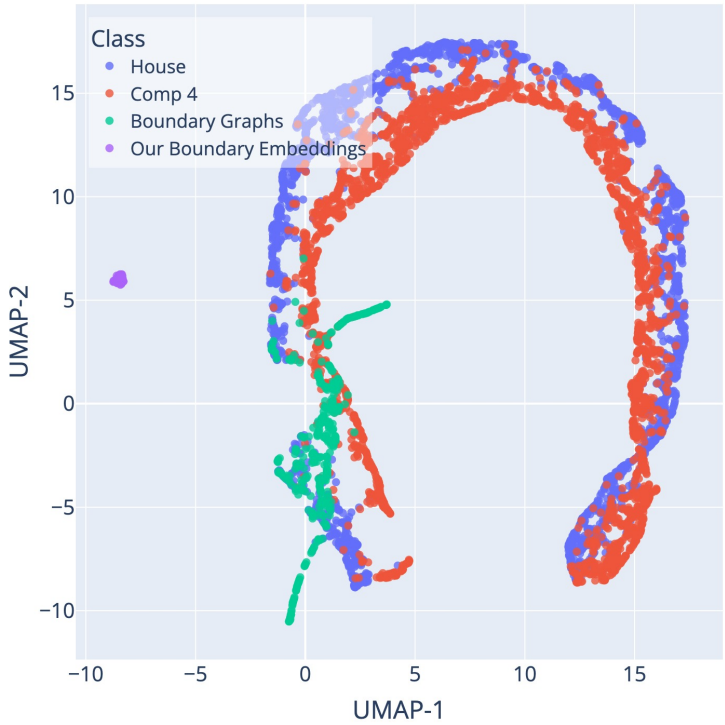


Figure 8: 2D UMAP plot for showing the classifier embeddings for the dataset, the GNNBoundary embeddings and our boundary embeddings for the Motif class pair House-Comp 4.

[4]The gnn-common-xai repository can be found at: https://github.com/yolandalalala/gnn-xai-common

J Relationship Between Boundary Metrics and Target Ranges

Table 9: Relationship between boundary thickness and target range

Dataset	**Class**	**(0.43,0.57)**	**(0.44,0.56)**	**(0.45,0.55)**	**(0.47,0.53)**	**(0.48,0.52)**	**(0.49,0.51)**	**(0.495,0.505)**
Motif								
	House	21.860	21.860	21.860	21.039	20.657	22.296	24.124
	Comp-4	23.006	23.006	23.006	22.959	22.366	23.980	24.727
	HouseX	94.832	94.108	92.528	89.067	87.809	95.975	95.114
	Comp-5	49.071	48.010	46.773	46.545	46.309	48.020	49.969
	House	36.431	36.431	36.431	34.393	35.824	35.774	37.607
	HouseX	65.062	65.062	65.062	64.079	62.873	68.698	64.628
Collab								
	High Energy	69.331	69.331	69.331	73.337	69.895	93.291	44.445
	Astro	2047.92	2047.92	2047.92	1605.01	1741.06	2198.34	3204.41
	High Energy	222.807	222.807	222.807	209.575	160.713	-	-
	Condensed Matter	36.111	36.111	36.111	25.734	22.746	-	-
Enzymes								
	EC4	205.928	206.793	210.382	220.714	219.387	230.614	229.475
	EC5	286.960	282.358	292.259	308.021	300.307	363.206	298.949
	EC5	207.833	209.161	204.640	180.781	162.449	163.469	-
	EC6	115.654	110.911	114.174	75.252	77.022	84.510	-
	EC1	272.131	272.131	303.868	327.851	-	-	-
	EC5	255.304	255.304	333.342	272.701	-	-	-
	EC1	374.599	315.357	143.406	-	-	-	-
	EC4	174.381	105.329	75.279	-	-	-	-
	EC1	216.613	209.391	227.606	151.933	-	-	-
	EC6	100.109	77.762	74.587	48.068	-	-	-
	EC2	91.520	96.992	86.903	77.186	81.010	113.270	98.641
	EC3	1192.97	1192.71	1052.94	277.830	453.337	67.647	43.763

Table 10: Relationship between boundary margin and target range

Dataset	Class	(0.43,0.57)	(0.44,0.56)	(0.45,0.55)	(0.47,0.53)	(0.48,0.52)	(0.49,0.51)	(0.495,0.505)
Motif								
	House	0.337	0.337	0.337	0.337	0.123	0.123	0.915
	Comp-4	0.416	0.416	0.416	0.416	0.220	0.347	0.744
	HouseX	0.492	0.755	0.755	0.755	0.909	3.046	3.046
	Comp-5	1.626	3.797	3.797	3.797	4.480	4.480	7.069
	House	1.236	1.236	1.236	1.503	1.430	1.430	1.922
	HouseX	0.972	0.972	0.972	0.972	1.456	2.011	2.996
Collab								
	High Energy	3.023	3.023	3.023	2.598	3.333	3.318	4.097
	Astro	2.796	2.796	2.796	2.689	2.979	12.058	9.505
	High Energy	1.997	1.997	1.997	1.997	2.497	-	-
	Condensed Matter	1.645	1.645	1.645	1.645	1.982	-	-
Enzymes								
	EC4	17.748	17.748	17.748	32.503	32.503	32.300	34.783
	EC5	4.815	4.815	4.815	33.999	33.999	33.633	33.633
	EC5	3.045	3.045	3.045	17.337	24.270	16.537	-
	EC6	11.425	11.425	11.425	10.411	14.968	6.294	-
	EC1	17.251	17.251	18.542	18.542	-	-	-
	EC5	12.642	12.642	24.377	24.377	-	-	-
	EC1	5.919	4.399	28.629	-	-	-	-
	EC4	13.383	12.763	28.059	-	-	-	-
	EC1	20.664	20.677	9.465	25.900	-	-	-
	EC6	13.949	15.315	10.926	36.139	-	-	-
	EC2	12.138	3.154	3.154	18.348	18.348	27.913	37.612
	EC3	9.944	10.469	14.045	18.061	18.061	27.764	34.422

Table 11: Relationship between boundary complexity and target range

Dataset	Class	(0.43,0.57)	(0.44,0.56)	(0.45,0.55)	(0.47,0.53)	(0.48,0.52)	(0.49,0.51)	(0.495,0.505)
Motif								
	House and Comp4	0.072	0.072	0.072	0.064	0.062	0.064	0.060
	HouseX and Comp-5	0.182	0.135	0.114	0.080	0.057	0.058	0.066
	House and HouseX	0.015	0.015	0.015	0.012	0.010	0.008	0.007
Collab								
	High Energy and Astro	0.253	0.253	0.253	0.229	0.217	0.240	0.253
	High Energy and Condensed Matter	0.313	0.313	0.313	0.298	0.343	-	-
Enzymes								
	EC4 and EC5	0.138	0.168	0.166	0.187	0.189	0.182	0.247
	EC5 and EC6	0.349	0.326	0.335	0.403	0.413	0.374	-
	EC1 and EC5	0.0455	0.0455	0.021	0.000	-	-	-
	EC1 and EC4	0.199	0.122	0.189	-	-	-	-
	EC1 and EC6	0.168	0.171	0.167	0.099	-	-	-
	EC2 and EC3	0.306	0.289	0.296	0.313	0.348	0.596	0.000