
Interpretable and Parameter Efficient Graph Neural Additive Models with Random Fourier Features

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Abstract

Graph Neural Networks (GNNs) excel at jointly modeling node features and topology, yet their *black-box* nature limits their adoption in real-world applications where interpretability is desired. Inspired by the success of interpretable Neural Additive Models (NAM) for tabular data, Graph Neural Additive Network (GNAN) extends the additive modeling approach to graph data to overcome limitations of GNNs. While being interpretable, GNAN representation learning overlooks the importance of local aggregation and more importantly suffers from parameter complexity. To mitigate the above challenges, we introduce Graph Neural Additive Model with Random Fourier Features (G-NAMRFF), a lightweight, self-interpretable graph additive architecture. G-NAMRFF represents each node embedding as the sum of feature-wise contributions where contributions are modeled via a *Gaussian process* (GP) with a graph- and feature-aware kernel. Specifically, we construct a kernel using Radial Basis Function (RBF) with graph structure induced by Laplacian and learnable Finite Impulse Response (FIR) filter. We approximate the kernel using Random Fourier Features (RFFs) which transforms the GP prior to a Bayesian formulation, which are subsequently learnt using a single layer neural network with size equal to number of RFF features. G-NAMRFF is light weight with $168 \times$ fewer parameters compared to GNAN. Despite its compact size, G-NAMRFF matches or outperforms state-of-the-art GNNs and GNAN on node and graph classification tasks, delivering real-time interpretability without sacrificing accuracy¹.

1 Introduction

Graph Neural Networks (GNNs) are powerful and topology-aware deep representation learning architectures that leverage the structure of graphs as an inductive bias [12, 20, 32]. While GNNs have demonstrated impressive performance on various downstream machine learning tasks such as node and graph classification, they remain largely as a *black-box* models [5, 3]. As a result, the learned representations often lack *interpretability* which limits their adoption in regulated domains like healthcare, finance, and defense [31, 5]. Interpretability in machine learning focuses on designing models whose representations directly reveal how each feature contributes to the output [28]. This stands in contrast to *post hoc* explainable models which seeks to generate explanations for the model inference after the model has been trained [3, 13].

Additive models are the cornerstone for interpretable representation learning for tabular data. Notable examples of such models includes Neural Additive Model (NAM) [2], Neural Basis Model (NBM) [24] and Gaussian Process Additive Model (GPAM) [41]. The key innovation of this additive model lies in its ability to handle each feature independently by learning a separate univariate function for every feature and then summing these contributions to obtain the final prediction. Although all these models share a common trait i.e., additive structure, they differ in how each feature's

¹Code to reproduce the results is available at <https://github.com/FujitsuResearch/GNAM-RFF>

univariate function is represented and learned. For example, NAM approximates each feature's effect with a dedicated deep neural network (DNN), yielding high flexibility but also posing significant computational overhead. In contrast, NBM and GPAM represent each feature using a fixed dictionary of basis functions (e.g., splines, Fourier bases, or Gaussian process kernels) and learn only the linear combination of weights, thereby retaining interpretability while dramatically reducing training time.

Building on the success of additive models for tabular data, efforts have been made to extend it to graph data. GNAN is the first graph neural additive model that incorporates graph structure as an inductive bias into a neural additive models [5], thus making it a self-interpretable *glass-box* model by design, in contrast to the conventional and well-studied *post-hoc* models designed to explain *black-box* GNNs outputs [31, 3, 37, 22, 17]. GNAN disentangles feature effects and graph topology by learning separate univariate functions, one per each feature and one for neighborhood weighting via DNNs, respectively. The neighborhood weighting is done through a distance measure that spans the entire graph. However, this design has two key drawbacks. Firstly, modeling each feature and neighbourhood with separate neural networks with multiple layers leads to a large trainable parameters with a significant training time. Secondly, for a graph with N nodes and E -edges, GNAN aggregation over all nodes requires $\mathcal{O}(N + E)$ distance computations per node, leading to quadratic scaling of the neighbourhood weighting function with graph size. Additionally, distant, non-neighbouring nodes influence the embeddings through the weighting function in a non-trivial way, introducing opacity to the interpretation unlike localized aggregation.

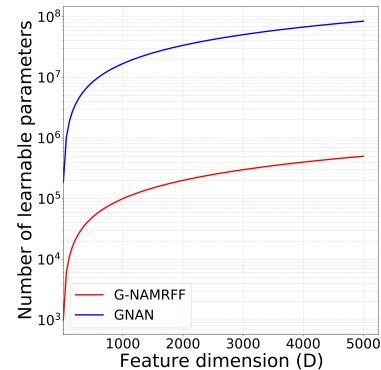


Figure 1: Parameter complexity.

In this work, we introduce the Graph-aware Neural Additive Model with Random Fourier Features (G-NAMRFF), a lightweight and inherently interpretable *glass-box model* designed for representation learning with graphs. Similar to NAM, G-NAMRFF represents each node prediction as the sum of individual feature contributions; however, it replaces deep neural networks with a Gaussian Process (GP) prior characterized by a kernel explicitly designed to be both graph- and feature-aware. Specifically, we propose a smoothness-promoting kernel that encourages neighboring nodes with similar attributes to yield similar outputs. In particular, the proposed kernel can be expressed as a Radial Basis Function (RBF) where inputs are projected features that capture one-hop neighbourhood in the graphs. Based on Bochner's theorem, we approximate the kernel effectively using RFFs, transforming the GP priors into a linear Bayesian formulation. To effectively capture multi-hop graph information, we embed the node features using Finite Impulse Response (FIR) filters with trainable coefficients. These coefficients, trained jointly with univariate functions help uncover critical graph structural information by highlighting which hops significantly influence the node predictions. With the equivalent Bayesian linear model established, we learn the model parameters using a single-layer network whose complexity depends solely on the number of RFFs, thereby ensuring G-NAMRFF's computational efficiency and lightweight nature. Figure 1, illustrates the parameter complexity comparison between our proposed model and existing method, clearly demonstrating the reduced parameter requirements of our approach. More importantly, by feeding RFFs with structure-aware features computed via learnable filter coefficients, our model seamlessly integrates graph topology and feature mapping into a single module unlike GNAN.

We summarize the main contributions of this paper as follows:

- We propose G-NAMRFF, a light-weight, interpretable graph neural additive model with RFFs and minimal parameter overhead. G-NAMRFF is a unified approach that seamlessly integrates topology and feature learning in one framework providing feature level interpretability through univariate functions and clear hop-level interpretability through the learned FIR coefficients.
- We provide theoretical guarantees that establish the robustness and permutation equivariance properties of G-NAMRFF.
- The proposed G-NAMRFF is parameter-efficient with $168\times$ fewer parameters compared to GNAN and consistently outperforms it on both node- and graph-classification tasks, and also

matches or outperforms state-of-the-art black-box GNNs, demonstrating its suitability for sensitive and performance critical applications.

Notation: Throughout this paper, we represent matrices and vectors as $\mathbf{X}$ (boldface capital letters) and $\mathbf{x}$ (boldface lowercase letters), respectively. The (i, j) -th element of a matrix is indexed by $x_{i,j}$. Identity matrix of dimension M is denoted by $\mathbf{I}_M$.

2 Preliminaries

In this section, we set up the mathematical background required for the development of the proposed model.

2.1 Graph Neural Additive Network

Consider a graph $\mathcal{G}$ with N nodes, with the feature vector associated with each node being $\mathbf{x} \in \mathbb{R}^D$; the feature matrix as $\mathbf{X} \in \mathbb{R}^{N \times D}$. The GNAN models each feature independently using a DNN and weights it with a learnable function that captures underlying graph topology. Formally, the embedding of k -th component of node i is given by,

$$z_{i,k} = \sum_{j=1}^N \frac{1}{\#\text{dist}_i(j, i)} \rho \left(\frac{1}{1 + \text{dist}(j, i)} \right) f_k(x_{j,k}), \quad (1)$$

Here $f(\cdot)$, $\rho(\cdot)$ are the learnable non-linear functions. $\text{dist}(i, j)$ captures the distance between the nodes and $\#\text{dist}_i(i, j)$ is the number of nodes at $\text{dist}(i, j)$ from node i . From (1), it is clear that embedding of the i -th node requires computing the distance of the i -th node to all the nodes of $\mathcal{G}$, which makes (1) ineffective to handle large graphs.

2.2 Gaussian Process

A Gaussian Process (GP) [26] is a probabilistic framework that defines a distribution over functions, where any finite set of function values follows a multivariate Gaussian distribution. It is completely specified by a mean function, $\mathbf{m}(\mathbf{x})$ and a covariance kernel $\mathbf{K}_\theta(\mathbf{x}, \mathbf{x}')$, where $\mathbf{x}$ and $\mathbf{x}'$ are data points on $\mathbb{R}^D$. We denote the GP prior as $f(\mathbf{x}) \sim \mathcal{GP}(\mathbf{m}(\mathbf{x}), \mathbf{K}_\theta(\mathbf{x}, \mathbf{x}'))$, where $\mathbf{K}_\theta(\mathbf{x}, \mathbf{x}') = \exp \left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\theta^2} \right)$ with θ being the bandwidth.

2.3 Kernel Approximation with Random Fourier Features

Random Fourier Features (RFFs) based kernel approximation is a popular technique for addressing the scalability of kernel-based methods such as Gaussian Processes [25]. The key idea behind RFFs is to approximate a shift-invariant kernel by expressing it as an inner product of low-dimensional feature mappings and is built on Bochner's theorem:

Theorem 2.1 (Bochner's Theorem and RFF Approximation [25]). *Let $\mathbf{K}_\theta \in \mathbb{R}^{N \times N}$ denote a bounded, shift-invariant and positive definite kernel (i.e., $\mathbf{K}_\theta$ is a Fourier transform of non negative measure). $\mathbf{K}_\theta$ when properly scaled can be approximated using RFF as*

$$\mathbf{K}_\theta(\mathbf{x}, \mathbf{x}') \approx \Phi_{\mathbf{a}}^T(\mathbf{x}) \Phi_{\mathbf{a}}(\mathbf{x}'), \quad \Phi_{\mathbf{a}}(\mathbf{x}) = \left\{ \sqrt{\frac{2}{M}} \cos(2\pi \mathbf{a}_m^T \mathbf{x} + b_m) \right\}_{m=1}^M, \quad (2)$$

where $\Phi_{\mathbf{a}}$ is a feature map termed as random Fourier features with M being the number of RFF features, $\mathbf{a}_m \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_D)$ and $b_m \in \text{Unif}(0, 2\pi)$ are drawn from normal and uniform distributions.

This approximation enables a scalable reformulation of the GP prior into linear Bayesian model. Specifically, prior can be modeled as $f(\mathbf{x}) = \Phi_{\mathbf{a}}^T(\mathbf{x}) \mathbf{w}$, where $\mathbf{w} \in \mathbb{R}^{M \times 1} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_M)$.

3 Graph-aware Neural Additive Model with Random Fourier Features

In this section, we present G-NAMRFF, a lightweight, self-interpretable graph neural additive model that integrates graph topology through GP priors and RFF.

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be weighted and undirected graph with N nodes and the associated graph Laplacian as $\mathbf{L}_{\mathcal{G}} \in \mathbb{R}^{N \times N}$. We assume that each node $i \in \mathcal{V}$ is associated with a D dimensional feature $\mathbf{x}_i \in \mathbb{R}^{D \times 1}$ and represent the feature matrix as $\mathbf{X} \in \mathbb{R}^{N \times D}$.

Given $\mathbf{X}$ and $\mathbf{L}_{\mathcal{G}}$, G-NAMRFF models each feature contribution $f_k : \mathbb{R} \rightarrow \mathbb{R}$ through a Gaussian process whose covariance kernel enforces smoothness with respect to both the feature values and the underlying graph topology. In particular, G-NAMRFF obtains the contribution of each feature to node prediction y_i as

$$y_i = \sum_{k=1}^D f_k(x_{i,k}), \quad f_k \sim \mathcal{GP}(0, \mathbf{K}_{\mathcal{G}}(x_{i,k}, x_{j,k})) \quad (3)$$

where $\mathbf{K}_{\mathcal{G}}(\cdot, \cdot)$ is a graph covariance kernel. The embedding of node i i.e., $\mathbf{z}_i \in \mathbb{R}^D$ is obtained by stacking $[f_1(x_{i,1}), f_2(x_{i,2}), \dots, f_D(x_{i,D})]$. In what follows, we first define the graph covariance kernels that enforce smoothness assumption, which are shift invariant and can be approximated using RFFs. Then, leveraging this approximation we propose the light-weight model.

3.1 Gaussian Process Priors with Graph-aware Kernel

To encode the prior knowledge that adjacent nodes with similar feature values should output similar function values i.e., function should vary smoothly across the nodes, we impose the GP prior with the graph aware covariance kernel as

$$\mathbf{K}_{\mathcal{G}}(x_{i,k}, x_{j,k}) = \exp\left(\frac{-a_{i,j}(x_{i,k} - x_{j,k})^2}{2\Theta^2}\right), \quad (4)$$

where $\Theta > 0$ is the hyperparameter that controls the width of the function and $a_{i,j} > 0$ corresponds to i, j -element of weight matrix $\mathbf{A}$ with weights assigned based on the distance/similarity between the nodes. Observe that if the nodes are close in the graph and features are similar the kernel outputs high covariance, whereas for distant nodes with features being dissimilar $\mathbf{K}_{\mathcal{G}}$ yields low covariance. Thus, the proposed kernel $\mathbf{K}_{\mathcal{G}}$ is both feature and graph-aware. Imposing such a prior enforces $f_k(x_{i,k})$ to vary smoothly across the *connected* nodes. Note that for a fixed $a_{i,j}$, kernel defined in (4) is shift invariant with respect to nodes i, j locally, i.e., $\mathbf{K}_{\mathcal{G}}(x, y) = \mathbf{G}_{\mathcal{G}}(x - y)$, with $\mathbf{G}_{\mathcal{G}}(t) = \exp(-\frac{a_{i,j}t^2}{2\Theta^2})$. Shift invariance of the kernel (Stationarity is required for the approximation of kernels by Bochner's Theorem (see Theorem 2.1) which in turn aids in formulating the light-weight model.

Observe that Eq.(4) can be equivalently expressed as $\mathbf{K}_{\mathcal{G}}(x_{i,k}, x_{j,k}) = \exp\left(\frac{-(\sqrt{a_{i,j}}x_{i,k} - \sqrt{a_{i,j}}x_{j,k})^2}{2\Theta^2}\right)$. Let us call projected features as $\tilde{x}_{i,k} = \sqrt{a_{i,j}}x_{i,k}$ and $\tilde{x}_{j,k} = \sqrt{a_{i,j}}x_{j,k}$. By rewriting, we obtain kernel function with graph-aware inputs

$$\mathbf{K}_{\mathcal{G}}(x_{i,k}, x_{j,k}) = \exp\left(\frac{-(\tilde{x}_{i,k} - \tilde{x}_{j,k})^2}{2\Theta^2}\right), \quad (5)$$

In other words, the $\mathbf{K}_{\mathcal{G}}$ is modified RBF with inputs as filtered features based on one-hop neighbourhood since the projected variables use weighted graph adjacency.

Remarks:

- Although the proposed kernel function $\mathbf{K}_{\mathcal{G}}$ is *shift invariant* and *graph-aware*, it is apparent that it only captures the information from one hop and may fail to capture the information from larger depths (see the importance in section 6).
- More importantly, to study the interpretability, it is also important to analyze for a fixed node i which neighbors are influencing the predictions.

To address the aforementioned challenges, we reformulate the kernel to incorporate information from deeper neighborhoods. Specifically, we make the kernel inputs topology-aware by replacing the original features with graph-filtered representations. This yields an RBF kernel whose inputs are graph-aware feature embeddings. Notably, this formulation preserves both stationarity globally and positive definiteness, ensuring that the resulting covariance function remains valid under the Gaussian process framework and RFF approximation.

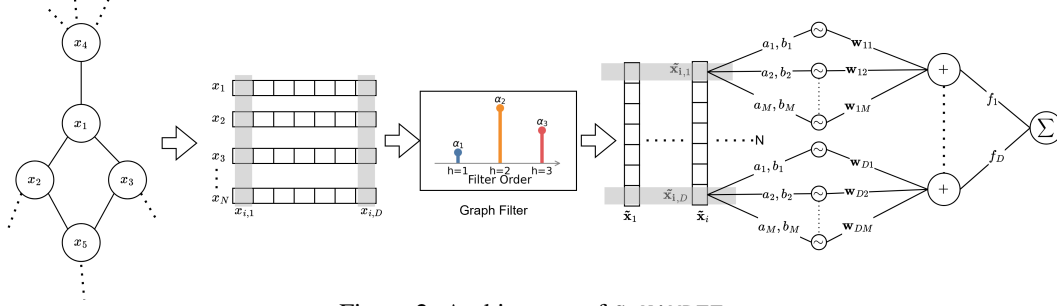


Figure 2: Architecture of G-NAMRFF.

3.1.1 Topology-Aware Random Fourier Features with Learnable FIR Filters

We aggregate multi-hop information through learnable FIR filters, represented as polynomial functions of the graph shift operator—either the adjacency matrix or the graph Laplacian. Specifically, employing the graph Laplacian as the shift operator, the filter is implemented as:

$$\mathbf{H} = \sum_{h=0}^R \alpha_h \tilde{\mathbf{L}}_G^h, \quad (6)$$

where $\tilde{\mathbf{L}}_G = \mathbf{I} - \mathbf{D}^{-1/2} \mathbf{A} \mathbf{D}^{-1/2}$ is the normalized graph Laplacian and R is the filter order which is a hyperparameter that controls how multi-hop information is aggregated. In our framework, we set the filter parameters as learnable. We emphasize that instead of fixing the filter parameters, making them learnable enhances the interpretability (see Section 6). In particular, one can inspect the filter coefficients and infer information such as the hops that are contributing to the node embedding. Using Eq.(6), the filtered response is given by $\tilde{\mathbf{X}} = \mathbf{H} \mathbf{X} \in \mathbb{R}^{N \times D}$, with $\tilde{\mathbf{X}}$ is now the smoothed graph features encoding much richer neighborhood beyond one-hop. Note that modifying the kernel input by the filtered response transforms $\mathbf{K}_G$ to be structure aware RBF that is shift invariant and also non negative. Following Bochner's theorem, it can be expressed as $\mathbf{K}_G(x_{i,k}, x_{j,k}) = \Phi_{\mathbf{a}}^T(\tilde{x}_{i,k}) \Phi_{\mathbf{a}}(\tilde{x}_{j,k})$, where $\tilde{x}_{i,k}$ corresponds to (i, k) -th element of $\tilde{\mathbf{X}}$.

Leveraging the kernel approximation technique (Bochner's theorem), the GP prior defined in 3 can be equivalently expressed in linear Bayesian formulation as

$$f_k(x_{i,k}) = \Phi_{\mathbf{a}}^T(\tilde{x}_{i,k}) \mathbf{w}_k, \quad \mathbf{w}_k \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_M) \quad (7)$$

where $\Phi_{\mathbf{a}}(\tilde{x}_{i,k}) = \left\{ \sqrt{\frac{2}{M}} \cos(2\pi a_m \tilde{x}_{i,k} + b_m) \right\}_{m=1}^M$ with $\Phi_{\mathbf{a}}(\cdot)$ is a feature map, which we refer to as graph-aware Random Fourier Features (G-RFFs), $a_m \sim \mathcal{N}(0, 1)$ and $b_m \in \text{Unif}(0, 2\pi)$ are drawn from normal and uniform distributions. To summarize, G-NAMRFF, learns contribution of features to node- i prediction as

$$y_i = \sum_{k=1}^D \Phi_{\mathbf{a}}^T(\tilde{x}_{i,k}) \mathbf{w}_k, \quad \mathbf{w}_k \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_M). \quad (8)$$

RFF Linear Layer

Note that under modified prior, each f_k is a linear transformation whose weights can be obtained by *single-layer neural network* with exactly M learnable parameters per feature. Also, embedding the structural information into features and representing the univariate function using graph-aware RFFs results in a light-weight model with number of trainable parameters dependent on number of RFFs and filter order (more discussion in section 4). We conclude this section with some important observations: (a) for $R = 1$ and $\alpha_0 = 0$, the present approach resembles the first approach where features are transformed based on one-hop neighbourhood. (b) The filter order and number of RFF features required are less compared to hidden units for all the graph datasets (more details in Appendix C.3).

3.2 Implementation Details

In Fig. 2, we present end to end architecture of G-NAMRFF for obtaining the prediction of i -th node as a summation of univariate function outputs. Considering $\mathbf{X} \in \mathbb{R}^{N \times D}$, we pass each feature

Algorithm 1 Algorithm for G-NAMRFF

- 1: **Inputs:** Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times D}$, normalized Laplacian $\tilde{\mathbf{L}}_G$, RFF dimension M , bandwidth Θ , filter order R .
 - 2: **Trainable parameters:** $\{\alpha_h\}_{h=0}^R$, weight vectors $\{\mathbf{w}_k \in \mathbb{R}^M\}_{k=1}^D$.
 - 3: **Output:** Node predictions $\{y_i\}_{i=1}^N$.
 - 4: **Filtering:** Compute filtered features $\tilde{\mathbf{X}} = \sum_{h=0}^R \alpha_h \tilde{\mathbf{L}}_G^h \mathbf{X}$.
 - 5: **RFF computation:** Sample frequencies $\{a_{k,m}\}_{m=1}^M \sim \mathcal{N}(0, 1)$ and phases $\{b_{k,m}\}_{m=1}^M \sim \text{Uniform}(0, 2\pi)$ for each k . RFF map: $\Phi_{\mathbf{a}}(x) = \sqrt{\frac{2}{M}} [\cos(a_{k,1}x + b_{k,1}), \dots, \cos(a_{k,M}x + b_{k,M})]^\top$
 - 6: **for** each node $i = 1, \dots, N$ **do**
 - 7: **for** each feature $k = 1, \dots, D$ **do**
 - 8: Obtain feature embedding: $f_k(x_{i,k}) = \Phi_{\mathbf{a}}^\top(\tilde{x}_{i,k}) \mathbf{w}_k$.
 - 9: **Prediction:** $y_i \leftarrow \sum_{k=1}^D f_k(x_{i,k})$.
 - 10: **return** $\{y_i\}_{i=1}^N$.
-

column through the graph filter parameterized by shared filter coefficients. The magnitude of the filter coefficients reflects the importance of the neighbourhood. In other words, they explain which hop information plays a key role in the prediction. We also emphasize that sharing filter parameters reduces the complexity without compromising the accuracy (more details in Section 6). In the following step, for the target node i , we extract D -features and feed them to RFF layer where it undergoes the cosine transformation with the sampling parameters $\{a_m, b_m\}_{m=1}^M$ shared across the features. The output of the RFF layer is the M -dimension RFF vector ($\Phi_{\mathbf{a}}$) for each feature. Each of these undergoes a linear transformation using a single layer NN with size as number of RFF features. The final predictions are obtained depending on the downstream tasks:

For node classification: For node classification task, the predictions obtained following (8) are passed through activation function (for ex., sigmoid or softmax).

For graph classification: We obtain the representation for the complete graph by sum pooling as $\mathbf{z}_G = \sum_{i=1}^N \mathbf{z}_i$. Then the prediction follows by passing representation through an activation function.

Handling multi-class datasets: If the dataset contains C -classes, we project the weights of a single layer RFF to the number of classes thereby enabling class-wise interpretability (more details in Section 6). We present detailed step by step process in Algorithm 1.

4 Theoretical Characterization and Learnable Parameters Computation

In this section, we discuss some important properties of G-NAMRFF *i.e.*, permutation equivariance and robustness to the perturbations, and then discuss parameter complexity.

Theorem 4.1 (Permutation Equivariance). Let $\mathcal{P} = \{\mathbf{P} \in \{0, 1\}^{N \times N} : \mathbf{P}^\top \mathbf{P} = \mathbf{P} \mathbf{P}^\top = \mathbf{I}_N\}$ be the set of all $N \times N$ permutation matrices. Then under the permutation of the graph Laplacian $\mathbf{L}_G$ and node-feature matrix $\mathbf{X}$ by any $\mathbf{P} \in \mathcal{P}$, the outputs from G-NAMRFF also modifies as $\mathbf{y}_{\text{perm}} = \mathbf{P} \mathbf{y}$, where $\mathbf{y} \in \mathbb{R}^N$ is the predictions across all the nodes.

The proof for Theorem 4.1 is relegated to Appendix A. Observe that Theorem 4.1 guarantees any simultaneous permutation of node indices in the Laplacian and feature matrix results in the same permutation of the learned embeddings. This symmetry is essential for ensuring that the model's predictions depend only on the graph's structure, not on an arbitrary ordering of its nodes.

Theorem 4.2 (Robustness to perturbation of graph Laplacian). Let $\hat{\mathbf{L}}_G = \mathbf{L}_G + \Delta \mathbf{L}_G$ be the Laplacian of the perturbed graph, with $\|\Delta \mathbf{L}_G\|_2 \leq \epsilon$, and assume that the RFF map $\Phi_{\mathbf{a}}(\cdot)$ is C_{RFF} -Lipschitz continuous. Then each node prediction satisfies $|\hat{y}_i - y_i| \leq C K \epsilon D \|\mathbf{X}\|_2$, where $C = C_{\text{RFF}} (\max_k \|\mathbf{w}_k\|_2)$, $K = \frac{1}{4} \|\alpha\|_1 (R^2 - 1) \left(\frac{R-1}{R+1}\right)^R$ are constants.

The proof for Theorem 4.2 is relegated to Appendix A. It emphasizes the error *i.e.*, difference between the predictions from G-NAMRFF is bounded linearly with the norm of the error term $\Delta \mathbf{L}_G$. Hence, the

node predictions are robust to small changes in the graph structure. The proof follows by leveraging the perturbation bounds on FIR filters and then invoking the Lipschitz continuity of RFF features.

4.1 Parameter Complexity

Recall, GNAN employs a deep network f_k for each of D features plus an additional DNN for ρ to encode the graph structure. If each of these $D + 1$ is an L layer feed forward neural network with H_u hidden units, the total number of parameters to be learnt are $(D + 1) \times (H_u^2 \times (L - 1) + (L + 2) \times H_u + 1)$.

For G-NAMRFF, the only learnable parameters are filter coefficients and weights of dimension M . Therefore, total number of learnable parameters are $D \times M + R + 1$, where R is the filter order. For numerical comparison, considering the values given in GNAN [5] with $H_u = 64$, $L = 5$ and $D = 100$, for the proposed method with $M = 100$ and $R = 5$, the number of parameters are approximately $168\times$ fewer. This reduction in model size, translates to arguably smaller run times of G-NAMRFF (see discussion on run times in Appendix C.2).

5 Related Works

The existing works that are closely related to ours can be broadly classified into 3 categories as follows:

Black-box GNN Architectures: Graph representation learning with GNNs has become ubiquitous across a wide range of applications. Broadly speaking, existing *black-box* GNNs can be categorized into two types: (a): Message-passing models, which iteratively aggregate and update node features via learned message functions [12, 35, 11]. (b): Spectral-convolutional architectures, which perform graph filtering in the Fourier domain to capture global structure [40, 6, 20, 42, 34]. Additionally, to better weigh the influence of individual neighbors while aggregating messages, attention-based extensions such as Graph Attention Networks (GAT) [32], and more recently, graph transformer variants [39, 33] have been proposed. [33, 39, 32]. Finally, several works employ Gaussian processes over graphs to capture predictive uncertainty directly [7, 10]. [7, 10]. Despite these advances, all these approaches model a *black-box* function, and their learned embeddings must be supplemented by separate interpretability techniques.

Interpretable Additive Models: Additive modeling is the workhorse principle of interpretable architectures for tabular data since the inception of Generalized Additive Models (GAMs) [14] to recent methods such as GPAM [41] [15, 2, 24, 8]. However, these methods were developed primarily for tabular inputs, and naive application of them to graph-structured data fails to exploit the relational inductive biases inherent in the graph topology. To address this gap, [5] extends generalized additive modeling to graphs by learning node-wise contributions aggregated across neighborhoods. As discussed earlier, this approach suffers with high parameter complexity and employs aggregation schemes that do not fully capture the influence of local graph structure.

Post-hoc GNN Explainers: Explainable models for graph data are mostly *post-hoc* methods that interpret pretrained GNNs by identifying critical substructures or features after model training. For instance, models like GNN-Explainer [37], PG-Explainer [22] uncover the important subgraphs and corresponding node features for explaining the feature predictions, whereas Graph-LIME [17] extends LIME [27] to GNN architectures to quantify each feature contribution to a node-level decision. Recently, GRAPHTRAIL[4] enhances GNN interpretability by translating learned representations into concise, human-readable Boolean formulas. A comprehensive study of post-hoc explainable models are detailed in [31, 38].

6 Numerical Experiments and Discussion on Interpretability

In this section, we evaluate G-NAMRFF performance and demonstrate its ability to learn interpretable representations on node and graph classification tasks.

6.1 Interpretability on Node Classification Task

To begin with, we analyze the univariate functions learnt on PubMed [29] dataset with node-classification task. PubMed is a multiclass citation-network dataset where nodes are research articles

categorized into three diabetes classes: Type 1, Type 2 and gestational [5]. To reveal how individual features influence the model’s predictions, we plot each learned function against its corresponding raw input values. In particular, as G-NAMRFF produces three outputs per feature (one score for each class), we plot three separate curves for each feature as shown in Fig. 3. At any given feature value, the curve with the highest output indicates the class that the feature most strongly supports.

In Fig 3(a), we show the influence of feature “children” on model output. It can be observed that model learnt a stronger contribution toward Type 1 diabetes, indicating that the presence of this term in an article increases the likelihood of it being classified under this category. This observation aligns with clinical understanding, as Type 1 diabetes is autoimmune in nature with children being susceptible[30], leading to increased mention of pediatric-related terms in relevant literature. Similarly, in Fig. 3(c), we show the influence of BMI (Body Mass Index), where it is clear that model associates predominantly with Type 2 diabetes. This clearly aligns with the clinical findings that elevated BMI is a major risk factor for Type 2 diabetes [1]. In Fig. 3(b), we show the influence of “sex (gender),” where model shows relatively lower contributions to both Type 1 and Type 2 diabetes, which is consistent with the fact that sex plays a mere role for diagnosis of Type 1 and Type 2 diabetes. However, in the case of gestational diabetes, which by definition is diagnosed during pregnancy, the model attributes higher importance.

Although these explanations merely match model prediction and interpretation with ground truth, for more challenging and high-stakes scenarios, a subject matter expert would better assess the correctness of such plots. Doing so, we can truly utilize the transparency of the model to increase the belief in such predictions and also use the feedback to improve the model further.

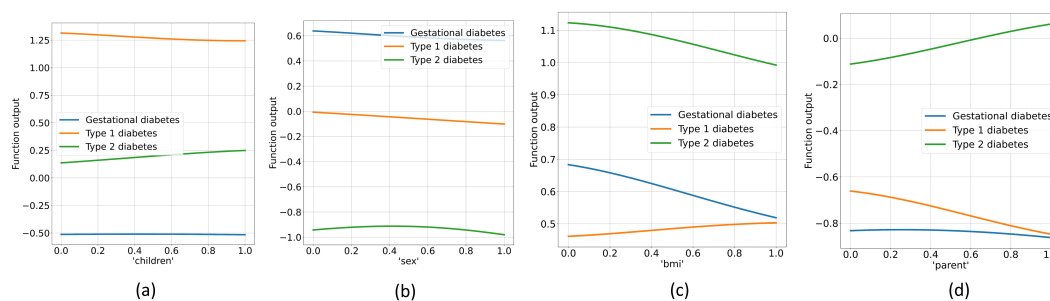


Figure 3: PubMed dataset: Univariate function outputs on different features.

6.2 Empirical Results on Node Classification Task

Having demonstrated G-NAMRFF’s ability to learn interpretable representations, we empirically evaluate its performance on medium-scale and large scale datasets namely Cora, Citeseer, PubMed [36], Cornell[23], ogbn-arxiv and ogbn-products [16]. In Table 1, we report mean classification accuracy along with the standard deviation over five independent runs with different random seeds. Hyperparameter details (e.g., number of RFFs (M), scale (Θ), filter order (R), and optimizer settings) are provided in the Appendix C.1.

Across all six datasets, G-NAMRFF matches or exceeds the performance of state-of-the-art *black-box* GNNs, confirming that interpretability need not come at the cost of accuracy. We also observe that incorporating information from multiple hops (G-NAMRFF) outperforms the one-hop variant (G-NAMRFF ($R = 1$)), highlighting the value of deeper neighborhood aggregation. Finally, among interpretable models, G-NAMRFF outperforms the state-of-the-art models in addition to scaling effectively. In particular, on ogbn-products, both NAM and GNAN encounter out-of-memory errors, whereas G-NAMRFF trains successfully. A comprehensive study on hyperparameters is presented in the Appendix C.3.

6.3 Interpretability on Graph Classification Task

In this section, we discuss the interpretability on the graph classification task with the widely studied Mutagenicity dataset [18, 9]. The dataset includes 4,337 molecules represented as graphs and each graph is associated with binary labels. In contrast to node classification, here we present both global level and local level interpretations. Recall that we obtain the graph-level embeddings by sum pooling node embeddings. To begin with, we discuss the feature level importance.

Table 1: Performance comparison on node classification task.

Model	Cora	Citeseer	Pubmed	Cornell	ogbn-arxiv	ogbn-products
GCN [20]	81.23 $\pm$ 1.1	71.20 $\pm$ 1.7	78.50 $\pm$ 1.3	65.90 $\pm$ 0.5	71.74 $\pm$ 0.3	75.64 $\pm$ 0.3
GAT [32]	80.32 $\pm$ 2.3	70.26 $\pm$ 2.3	77.12 $\pm$ 2.4	72.50 $\pm$ 0.7	71.95 $\pm$ 0.6	79.45 $\pm$ 0.5
GraphSAGE [12]	79.94 $\pm$ 3.4	65.12 $\pm$ 1.9	78.25 $\pm$ 1.2	75.90 $\pm$ 5.0	71.49 $\pm$ 0.2	75.63 $\pm$ 0.3
Graph Transformer [39]	80.70 $\pm$ 0.5	76.00 $\pm$ 0.9	78.80 $\pm$ 1.4	70.50 $\pm$ 1.7	70.13 $\pm$ 0.5	74.74 $\pm$ 0.5
NAM [2]	51.35 $\pm$ 2.3	55.40 $\pm$ 1.9	58.16 $\pm$ 2.3	59.15 $\pm$ 2.6	56.12 $\pm$ 3.4	OOM
GPAM [41]	59.96 $\pm$ 3.2	60.30 $\pm$ 3.9	62.30 $\pm$ 3.7	60.12 $\pm$ 3.6	62.35 $\pm$ 4.2	60.13 $\pm$ 3.9
GNAN [5]	77.89 $\pm$ 5.1	65.23 $\pm$ 3.7	75.13 $\pm$ 2.4	71.76 $\pm$ 4.2	69.56 $\pm$ 0.9	OOM
G-NAMRFF ($R = 1$)	75.32 $\pm$ 1.8	67.12 $\pm$ 1.1	75.12 $\pm$ 3.8	64.12 $\pm$ 2.9	66.94 $\pm$ 1.6	55.73 $\pm$ 1.8
G-NAMRFF	79.84 $\pm$ 1.7	69.45 $\pm$ 2.5	77.30 $\pm$ 1.4	73.54 $\pm$ 4.9	70.02 $\pm$ 3.9	72.13 $\pm$ 0.4

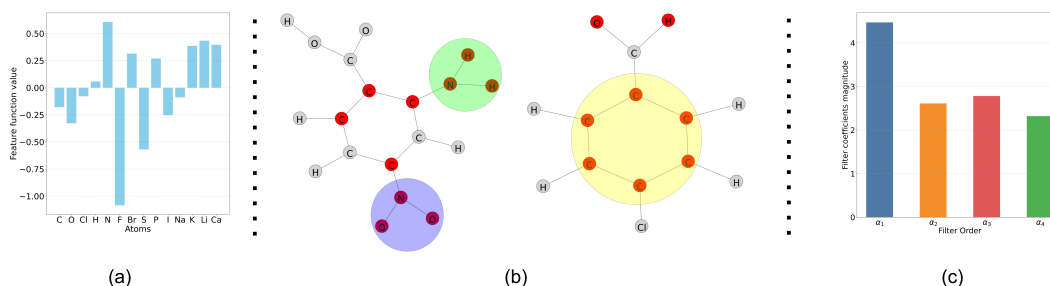


Figure 4: (a). Feature level explanation on Mutagenicity dataset. (b). Local structure level explanation on Mutagenicity dataset. (c). Learnt FIR filter coefficients.

Focusing on mutagenic class, we obtain the feature level scores globally by taking the sum of each atom’s contribution across the graphs. In Fig. 4(a), we present per-atom importance for the mutagenic class. Notably, Nitrogen, Oxygen, and Lithium atoms exhibit the highest positive contributions towards predicting mutagenicity. This interpretability not only helps us understand *why* the model makes a given prediction, but also directs domain experts to inspect and, if necessary, adjust the features or model. For example, if the model misclassifies a molecule, one can review the atom importance scores to assess which atomic features drove the error and representation learning can be modified accordingly.

Although feature-level importance gives insight into individual atom contributions, understanding which substructures are responsible for mutagenicity is crucial for molecular datasets. Using our model, we obtain *local explanations* by aggregating the feature-level attributions along the neighborhood to highlight the subgraph responsible for a prediction.

In Fig. 4(b), we visualize these extracted substructures for two representative molecules classified as mutagenic. In the first molecule, the nitro (NO_2) and amino (NH_2) groups emerge as the dominant substructures each exhibiting strong positive attribution toward the mutagenic label. In the second, the aromatic carbon ring itself drives the mutagenicity score. These findings align closely with prior toxicology studies [9, 37], which identify NH_2 , NO_2 , and polycyclic aromatic rings as key mutagenic motifs. Importantly, our model reveals that hydrogen and oxygen atoms directly bonded to nitrogen also carry a significant contribution towards a mutagenic class, whereas isolated hydrogens on carbon rings do not play that significant role. This observation supports the global atom-importance ranking in Fig. 4(a), where nitrogen outranks hydrogen. The study presented again emphasizes the G-NAMRFF ability in global-level and local-level attributions. Recall that each FIR filter coefficient α_h quantifies how much the model weights information from its h -hop neighborhood. To demonstrate this on the Mutagenicity dataset, in Fig. 4(c), we plot the filter coefficients for a fixed filter order. It can be observed that there is a clear decay in magnitude as h increases, confirming that our model naturally prioritizes close neighbors and progressively down-weights more distant nodes. As explained earlier, these learned coefficients thus offer direct, interpretable insight into the receptive field of each atom.

6.4 Empirical Evaluation on Graph Classification Task

In this section, we report G-NAMRFF performance on several standard graph-classification benchmarks: Proteins, NCI1, Mutagenicity, MUTAG, and PTC [16]. We compare the proposed model against both *black-box* GNNs and interpretable models. In Table 2, we present the mean graph classifica-

Table 2: Performance comparison on graph classification task.

Model	Proteins	Mutag	Mutagenicity	NCI1	PTC
GCN [20]	70.97±4.6	68.07±6.3	75.69±0.9	66.35±1.3	56.98±5.8
GAT [32]	69.92±4.0	67.20±3.4	69.40±1.2	66.12±2.1	55.60±11.1
GraphSAGE [12]	67.35±2.3	64.12±2.4	69.25±3.9	65.56±3.9	57.12±4.9
Graph Transformer [39]	69.76±3.2	66.30±5.3	73.10±0.9	68.24±3.4	55.90±3.5
NAM [2]	62.45±4.2	63.12±9.1	67.35±2.5	57.15±1.2	54.97±7.5
GPAM [41]	65.68±4.1	64.30±8.4	65.46±2.2	53.80±2.7	52.65±8.1
GNAN [5]	59.64±2.4	67.35±3.9	66.64±4.7	50.87±1.4	55.07±5.2
G-NAMRFF ($R=1$)	67.83±4.4	71.20±6.7	68.98±3.4	63.65±2.8	55.65±5.6
G-NAMRFF	69.94±3.7	79.81±5.3	71.70±2.0	66.10±1.7	61.91±3.4

tion accuracies from 10-fold cross-validation, each repeated over three random seeds. The results highlights the strength of proposed model in obtaining the interpretable graph embeddings without compromising the accuracy. Detailed hyperparameter settings and ablation studies are provided in Appendix C.1 and C.3.

7 Limitations and Future Directions

While G-NAMRFF models the prediction output as a sum of independent feature-wise contributions, this formulation overlooks potential correlations among features. A straightforward extension that explicitly models both individual and pairwise feature interactions would substantially increase the parameter count, compromising the model efficiency. Hence designing a parameter-efficient formulation that can capture feature dependencies and higher-order correlations without sacrificing interpretability remains an important direction for future research. Further, recall that the smoothness prior imposed on the function limits its effectiveness on heterophilic graphs, where connected nodes often have dissimilar labels. Therefore, extending the current approach to better handle heterophilic data presents an interesting and promising direction for future research.

8 Conclusions

In this work, we introduced G-NAMRFF, a self-interpretable, lightweight additive model for graphs. We proposed a unified interpretable architecture that integrates both graph topology and node features into univariate functions via Random Fourier Features. Further, we provided theoretical guarantees showing that G-NAMRFF is robust to graph perturbations and permutational equivariant. Our analysis on parameter complexity revealed that G-NAMRFF requires $168\times$ fewer parameters than GNAN. Finally, through experiments on node and graph classification benchmarks, we demonstrated that although being light-weight and interpretable, G-NAMRFF does not compromise predictive performance.

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Appendix

We organize the content in the Appendix as follows: In section A, we present proofs that supports permutation equivariance and robustness properties of G-NAMRFF. In section B, we include an additional discussion on interpretability with node and graph classification tasks. In section C, we present an ablation studies with respect to the hyperparameters.

A Proofs for the Theoretical Characterization of G-NAMRFF

In this section, we present the proofs for the permutation equivariance and robustness properties of G-NAMRFF.

Theorem. 4.1. (Permutation Equivariance) *Let $\mathcal{P} = \{\mathbf{P} \in \{0, 1\}^{N \times N} : \mathbf{P}^\top \mathbf{P} = \mathbf{P} \mathbf{P}^\top = \mathbf{I}_N\}$ be the set of all $N \times N$ permutation matrices. Then under the permutation of the graph Laplacian $\mathbf{L}_G$ and node-feature matrix $\mathbf{X}$ by any $\mathbf{P} \in \mathcal{P}$, the output from G-NAMRFF also modifies as $\mathbf{y}_{\text{perm}} = \mathbf{P} \mathbf{y}$, where $\mathbf{y} \in \mathbb{R}^N$ is the predictions across all the nodes.*

Proof. Let $\mathbf{P} \in \mathcal{P}$ be the permutation matrix acting on the graph $\mathcal{G}$. Under this permutation, the graph Laplacian and feature matrix transforms as $\tilde{\mathbf{L}}_{G, \text{perm}} = \mathbf{P} \tilde{\mathbf{L}}_G \mathbf{P}^\top$ and $\mathbf{X}_{\text{perm}} = \mathbf{P} \mathbf{X}$. Let us call the prediction of the node i under the permutation as $y_{i, \text{perm}}$, whereas $\mathbf{y}_{\text{perm}}$ is obtained by stacking $y_{i, \text{perm}}$.

Under the permutations, filter output modifies as

$$\begin{aligned} \tilde{\mathbf{X}}_{\text{perm}} &= \sum_{h=0}^R \alpha_h \tilde{\mathbf{L}}_{G, \text{perm}}^h \mathbf{X}_{\text{perm}} = \sum_{h=0}^R \alpha_h \mathbf{P} \tilde{\mathbf{L}}_G^h \mathbf{P}^\top \mathbf{P} \mathbf{X} \\ &\stackrel{(a)}{=} \sum_{h=0}^R \alpha_h \mathbf{P} \tilde{\mathbf{L}}_G^h \mathbf{X}, \\ &\stackrel{(b)}{=} \mathbf{P} \tilde{\mathbf{X}}, \end{aligned} \tag{9}$$

where (9)(a), follows from the property of permutation matrix i.e., $\mathbf{P}^\top \mathbf{P} = \mathbf{I}$. Observe that from (9)(b) under the permutation, filtered outputs also gets permuted. Leveraging this, we now evaluate the prediction of G-NAMRFF under permutation as

$$\begin{aligned} \mathbf{y}_{\text{perm}} &= [y_{1, \text{perm}}; \dots; y_{N, \text{perm}}], \\ &= \sum_{k=1}^D \underbrace{[\Phi_{\mathbf{a}}^\top(\tilde{x}_{1, k, \text{perm}}); \dots; \Phi_{\mathbf{a}}^\top(\tilde{x}_{N, k, \text{perm}})]}_{\Psi_{k, \text{perm}}} \mathbf{w}_k, \\ &\stackrel{(a)}{=} \mathbf{P} \sum_{k=1}^D [\Phi_{\mathbf{a}}^\top(\tilde{x}_{1, k}); \dots; \Phi_{\mathbf{a}}^\top(\tilde{x}_{N, k})] \mathbf{w}_k, \\ &= \mathbf{P} \mathbf{y}, \end{aligned} \tag{10}$$

where (10)(a), follows from (9)(b) where it can be observed that for a fixed feature k i.e., $\tilde{\mathbf{x}}_{k, \text{perm}} \in \mathbb{R}^{N \times 1} = \mathbf{P} \tilde{\mathbf{x}}_k$, therefore mappings gets reordered with $\Psi_{k, \text{perm}} \in \mathbb{R}^{N \times M} = \mathbf{P} \Psi_k$. Also it can be observed that $\mathbf{z}_{k, \text{perm}} = [f_k(x_{1, k}), f_k(x_{2, k}), \dots, f_k(x_{N, k})] \in \mathbb{R}^{N \times 1} = \mathbf{P} \mathbf{z}_k$ from the permutational equivariance of Ψ_k . $\square$

Theorem. 4.2. (Robustness to perturbation of graph Laplacian) *Let $\hat{\mathbf{L}}_G = \mathbf{L}_G + \Delta \mathbf{L}_G$ be the Laplacian of the perturbed graph, with $\|\Delta \mathbf{L}_G\|_2 \leq \epsilon$, and assume that the RFF map $\Phi_{\mathbf{a}}(\cdot)$ is C_{RFF} -Lipschitz continuous. Then each node prediction satisfies $|\hat{y}_i - y_i| \leq C K \epsilon D \|\mathbf{X}\|_2$, where $C = C_{\text{RFF}} (\max_k \|\mathbf{w}_k\|_2)$, $K = \frac{1}{4} \|\alpha\|_1 (R^2 - 1) \left(\frac{R-1}{R+1}\right)^R$ are constants.*

Proof. Before proceeding to the proof, we state the following Lemma that bounds the error between the FIR filters built with $\mathbf{L}_G$ and $\hat{\mathbf{L}}_G$. With slight abuse of notation from here on we represent normalized Laplacian with $\mathbf{L}_G$ instead of $\tilde{\mathbf{L}}_G$.

Lemma A.1. [19] Consider a polynomial filter $\mathbf{H}(\mathbf{L}_G) = \sum_{h=0}^R \alpha_h \mathbf{L}_G^h$, and perturbed Laplacian as $\hat{\mathbf{L}}_G = \mathbf{L}_G + \Delta \mathbf{L}_G$ with $\|\Delta \mathbf{L}_G\|_2 \leq \epsilon$ then

$$\|\mathbf{H}(\mathbf{L}_G) - \mathbf{H}(\hat{\mathbf{L}}_G)\|_2 \leq \frac{1}{4} \|\alpha\|_1 (R^2 - 1) \left(\frac{R-1}{R+1} \right)^R \epsilon, \quad (11)$$

where $\|\alpha\|_1 = [\alpha_0, \dots, \alpha_R] \in \mathbb{R}^{R+1}$.

Lemma A.1 shows that the error between the outputs of two filters fed with true and perturbed Laplacian is bounded and scales linearly with the error norm. We leverage the above Lemma to bound the difference between the prediction obtained from G-NAMRFF under perturbations.

Assume that the prediction of node i under the graph perturbation as $\hat{y}_i$. To begin with we evaluate the difference between the filter outputs. Considering the filter outputs with and without perturbation of graph as $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{X}}_{\text{per}}$. We have

$$\begin{aligned} \tilde{\mathbf{X}} &= \mathbf{H}(\mathbf{L}_G) \mathbf{X}, \\ \tilde{\mathbf{X}}_{\text{per}} &= \mathbf{H}(\hat{\mathbf{L}}_G) \mathbf{X}. \end{aligned} \quad (12)$$

Then the difference between the filtered outputs are bounded as

$$\begin{aligned} \|\tilde{\mathbf{X}}_{\text{per}} - \tilde{\mathbf{X}}\|_2 &= \|\mathbf{H}(\hat{\mathbf{L}}_G) \mathbf{X} - \mathbf{H}(\mathbf{L}_G) \mathbf{X}\|_2 \\ &\stackrel{(a)}{\leq} \|\mathbf{H}(\hat{\mathbf{L}}_G) - \mathbf{H}(\mathbf{L}_G)\|_2 \|\mathbf{X}\|_2 \\ &\stackrel{(b)}{\leq} \frac{1}{4} \|\alpha\|_1 (R^2 - 1) \left(\frac{R-1}{R+1} \right)^R \epsilon \|\mathbf{X}\|_2, \end{aligned} \quad (13)$$

where (13)(a) follows from a norm inequality and (13)(b) follows from (11). From (13)(b) it is clear that the difference of filter outputs is bounded linearly with the energy in the error term. Leveraging this we now evaluate the difference in the prediction output. We index the i, k element of $\tilde{\mathbf{X}}_{\text{per}}$ with $\tilde{x}_{i,k,\text{per}}$. Then,

$$\begin{aligned} |\hat{y}_i - y_i| &= \left| \sum_{k=1}^D \Phi_a^T(\tilde{x}_{i,k,\text{per}}) \mathbf{w}_k - \sum_{k=1}^D \Phi_a^T(\tilde{x}_{i,k}) \mathbf{w}_k \right| \\ &\leq \sum_{k=1}^D \|\Phi_a^T(\tilde{x}_{i,k,\text{per}}) - \Phi_a^T(\tilde{x}_{i,k})\|_2 \|\mathbf{w}_k\|_2 \\ &\stackrel{(a)}{\leq} C_{\text{RFF}} \sum_{k=1}^D |\tilde{x}_{i,k,\text{per}} - \tilde{x}_{i,k}| \|\mathbf{w}_k\|_2 \\ &\stackrel{(b)}{\leq} \sum_{k=1}^D C_{\text{RFF}} \max_k \{\|\mathbf{w}_k\|_2\} \underbrace{\frac{1}{4} \|\alpha\|_1 (R^2 - 1) \left(\frac{R-1}{R+1} \right)^R \epsilon}_K \|\mathbf{X}\|_2 \\ &\stackrel{(c)}{\leq} CK\epsilon D \|\mathbf{X}\|_2, \end{aligned} \quad (14)$$

where (14)(a) follows from Lipschitz continuity of Φ_a , (14)(b), follows from (13)(b). Whereas, (14)(c) follows by considering the $C = C_{\text{RFF}} \max_k \|\mathbf{w}_k\|_2$. From (14)(c), it is clear that difference in the node predictions scales linearly with the norm of the error term $\Delta \mathbf{L}_G$. $\square$

B Additional Discussion on Interpretability

B.1 Interpretability on Node Classification Task

In this section, we present additional examples of the learned univariate functions on the PubMed dataset for the node classification task. Specifically, in Fig. 5, we illustrate the univariate function

outputs for the features i.e., keywords as *insulin*, *fat*, *liver*, and *diet*. Recall that at any given feature value, the curve with the highest output indicates the class that the feature most strongly supports.

In Fig. 5a, we examine the influence of the presence of *diet* keyword in the document on the model's predictions. It can be observed that the model associates higher output with type 2 diabetes, suggesting that *diet* is a strong predictor for this class. This observation aligns well with existing medical literature, which indicates that type 2 diabetes is heavily influenced by dietary factors, whereas type 1 diabetes, being an autoimmune condition is less affected by diet [21]. Consistent with this, the model assigns less importance to type 1 diabetes for this feature. In Fig. 5b, we plot the influence of *fat* keyword in the document where it is clear that it contributes less significantly to the prediction of type 1 diabetes, further supporting the model's ability to capture medically relevant patterns. Similarly, in Fig. 5c and Fig. 5d we plot the impact of these features on model prediction where it is clear that presence of this word aligns prediction towards type 2 and gestational diabetes. Although for illustration purposes we have presented few examples one can follow a similar procedure to obtain the contribution of different features on different datasets.

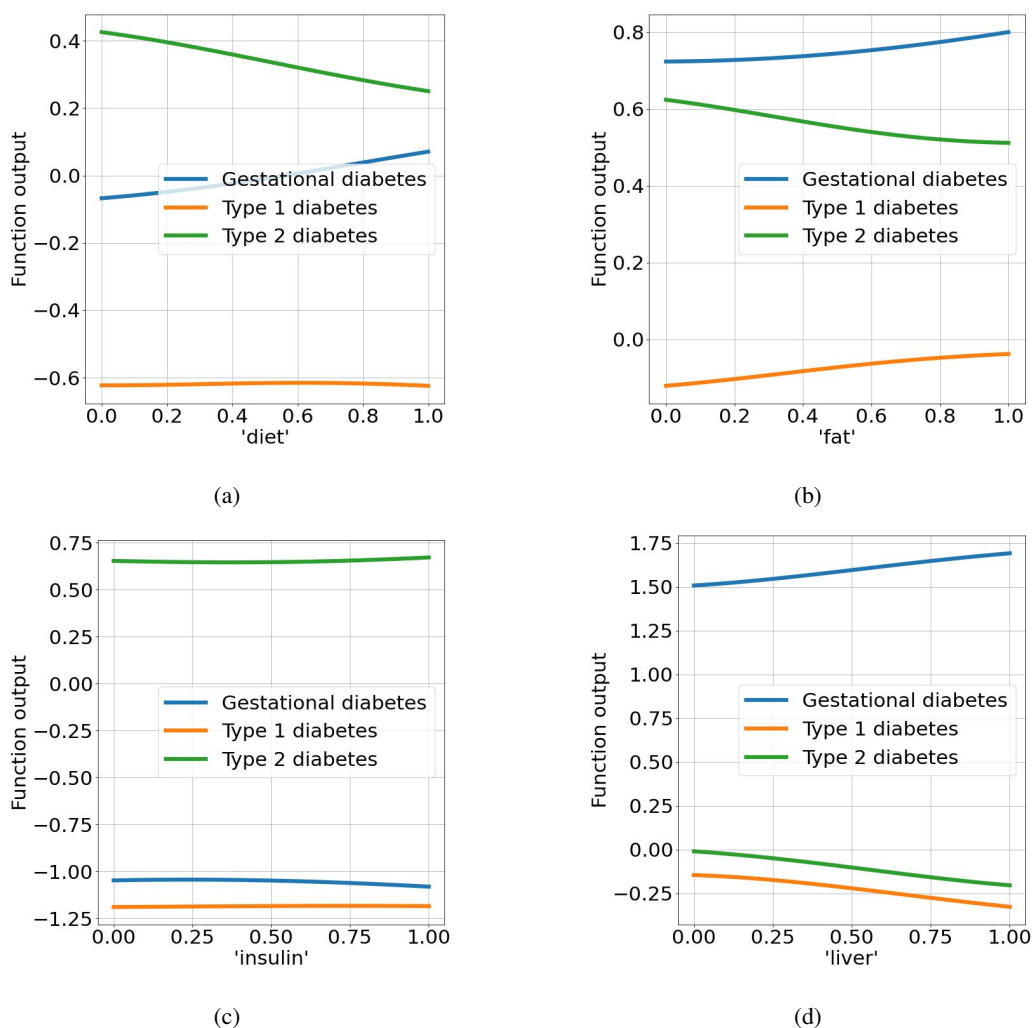


Figure 5: PubMed dataset: Univariate function outputs on features.

B.2 Interpretability on Graph Classification Task

In this section, we include more discussion on interpretability on the mutagenicity dataset. Here the main target is to give local level (structural) explanations and also compare them with the GNN-Explainer [37] which is a *post-hoc* explainer.

With the focus on mutagenic class, we give structure level explanations for the model prediction. In Figs. 6a, 6c and 6e we present three example molecules that are predicted as mutagenic and highlight predicted substructures responsible for the mutagenic prediction. It is clear that the NH_2 , NO_2 and aromatic rings act as key contributors to mutagenic class. These explanations align with the existing studies which advocate the presence of these substructures highly influences the mutagenicity [9]. For a fair comparison we present the substructures revealed from GNN-Explainer in Fig. 6b, 6d and 6f. It can be observed that compared to GNN-Explainer, our proposed model identifies NH_2 , NO_2 and aromatic rings more precisely.

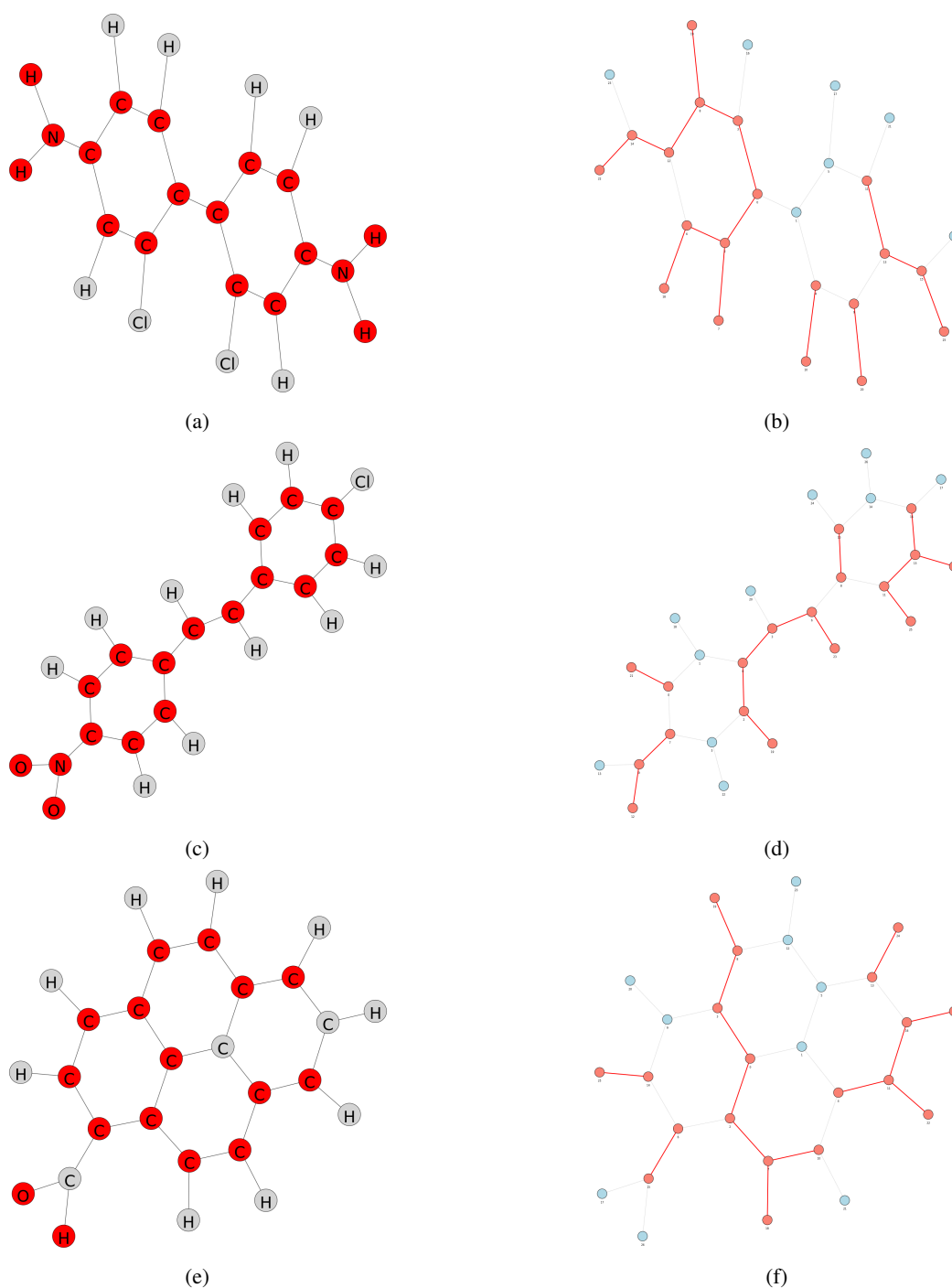


Figure 6: Mutagenicity dataset: Local level explanations.

C Hyperparameter Details and Ablation Studies

In this section, we first present the hyperparameter details used in our node and graph classification tasks. Then we analyze how each of these hyperparameters affects G-NAMRFF performance across datasets.

C.1 Hyperparameter Details

We have conducted all the experiments using an *NVIDIA* A30 GPU. In particular, we set the tuning range as follows: Number of RFFs (M)- $\{20, 40, 50, 100, 200\}$, filter order (R) - $[1, 7]$, kernel width (Θ)- $[1.0, 4.0]$, learning rate (Lr)- $[1e-4, 2e-1]$ and weight decay (Wd)- $[1e-5, 1e-2]$. The hyperparameter configurations that yielded the best validation performance are detailed in Table 3. For node classification tasks, we follow the standard dataset splits as specified in [16, 20, 23]. In the case of graph classification tasks, where no standard splits are available, we employ 10-fold cross-validation. All models are trained for 1000 epochs using the *AdamW* optimizer with randomly initialized parameters. The specific learning rates and weight decay values used across different experiments are also reported in Table 3. For node classification, we report the mean classification accuracy computed over five independent random seeds. For graph classification, we report the mean classification accuracy across 10 folds, with each fold averaged over three random seeds.

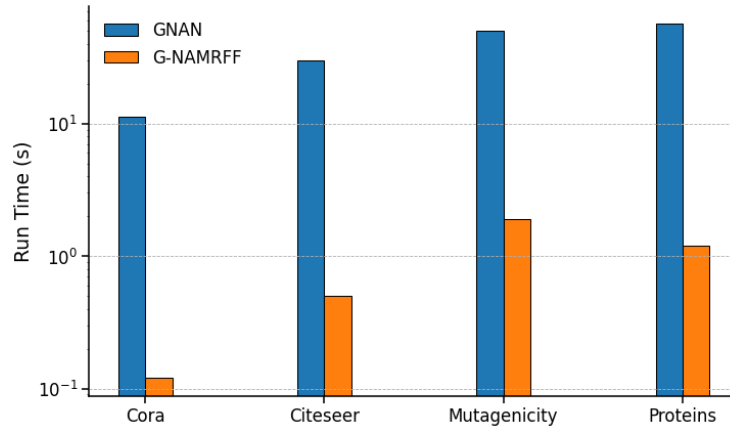


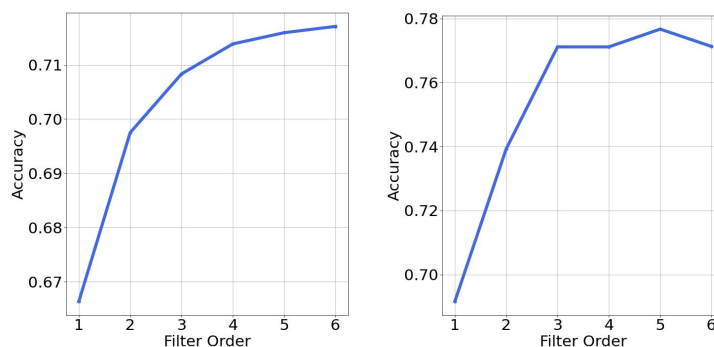
Figure 7: Run time comparison.

C.2 Run time analysis

In this section, we compare the runtime performance of G-NAMRFF, against GNAN, which is the only existing *glass-box* GNN architecture. In Fig. 7, we present the per-epoch runtime comparison on both node and graph classification tasks. Notably, it can be observed that even when GNAN is configured

Dataset	Number of RFFs (M)	Filter Order (R)	Kernel width (Θ)	Learning rate (Lr)	Weight Decay (Wd)
Cora	100	7	2.2	1.8e-1	2.4e-4
Citeseer	100	5	2.5	5.1e-1	3.1e-4
Pubmed	100	5	3.8	2.7e-2	4e-4
Cornell	100	6	2.9	7.3e-2	3.7e-4
ogbn-arxiv	100	4	3.4	5.2e-2	1.3e-4
ogbn-products	40	5	2.3	2.9e-2	5e-4
Proteins	50	5	1.9	3.2e-3	5e-3
Mutag	200	7	1.2	3.7e-2	5e-3
Mutagenicity	200	6	1.4	1.1e-2	5e-4
NCI1	50	7	3.7	1.6e-2	5e-4
PTC	50	5	1.7	2.9e-3	2.5e-5

Table 3: Hyperparameter details.



(a) Mutagenicity (b) Pubmed
Figure 8: Classification accuracy against filter order.

with a relatively small hidden dimension of 32, it still requires 10 to 100 times more runtime per epoch compared to G-NAMRFF.

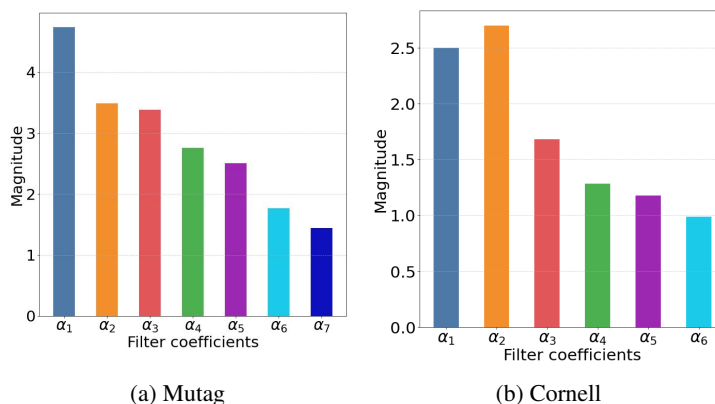
Furthermore, it is worth emphasizing that on small-scale datasets such as Citeseer and Pubmed, increasing the hidden dimension to 64 can already result in out-of-memory (OOM) errors when training GNAN. On large-scale datasets like ogbn-products, training GNAN becomes entirely infeasible due to excessive memory requirements.

C.3 Ablation studies

In this section, we analyze the impact of hyperparameters on the model performance. Recall the key hyperparameters in G-NAMRFF includes the filter order (R) and number of RFF (M).

Filter Order: In Fig. 8, we illustrate the effect of the filter order on classification accuracy for two tasks: node classification on the Pubmed dataset and graph classification on the Mutagenicity dataset. Recall that a filter of order R aggregates information from R -hop neighborhoods in the graph. It can be observed that as the filter order increases, the model is able to incorporate information from larger receptive fields, leading to an initial improvement in classification accuracy. However, beyond a certain point, further increasing the filter order causes the accuracy to saturate or decline, likely due to oversmoothing. Notably, we observe that using higher-order filters ($R > 1$) significantly improves performance compared to $R = 1$, highlighting the benefit of aggregating information from larger graph neighborhoods.

To further highlight the relative importance of different node neighborhoods, we present the magnitudes of the learned filter coefficients for a fixed filter order in Fig. 9, using the Mutagenicity and Cornell datasets. It can be observed that the model assigns higher weights to closer neighborhoods, emphasizing the greater importance of immediate node interactions in the classification task.



(a) Mutag (b) Cornell
Figure 9: Filter coefficients magnitude against filter order.

Random Fourier Features:

We analyze the effect of the number of RFFs on classification accuracy. Figures. 10a, 10b, and 10c show the performance variation on the Cornell, PubMed, and NCI1 datasets, respectively. As the number of random Fourier features (M) increases, the classification accuracy initially improves due to better kernel approximation. However, beyond a certain point, performance drops as the model may begin to overfit with larger M . Across all datasets, we observe that good performance can be achieved with relatively small values of M , which translates to a lower number of learnable parameters. Recall that the total number of parameters in G-NAMRFF is $D \times M + R + 1$. As observed M being small the model remains lightweight while being effective.

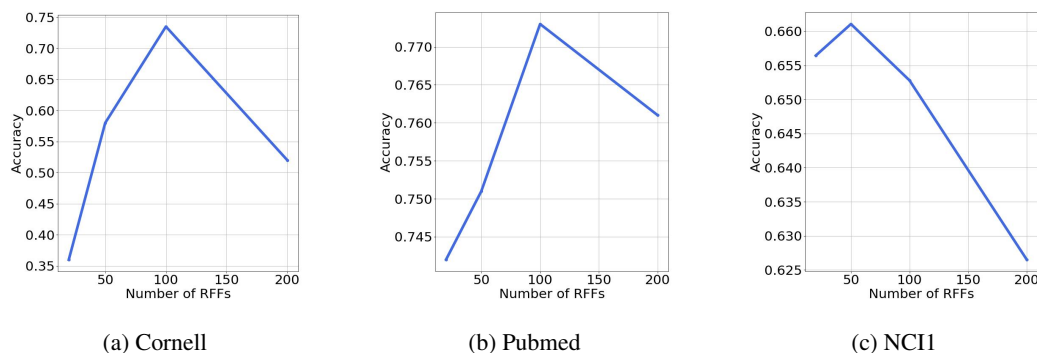


Figure 10: Classification accuracy vs number of RFFs.