Non-parametric Diffusion for Scalable Node Classification on Graphs

Anonymous authors
Paper under double-blind review

Abstract

Deep Learning on Graphs was recently made possible with the introduction of Graph Neural Networks (GNNs). GNNs use learnable diffusion processes to propagate information through the graph and improve performance on downstream tasks. However, learning this diffusion process can be expensive in terms of memory and computation. To address this, some methods have proposed simplified diffusion processes to make GNNs more scalable. Methods like Simplified Graph Convolutional Network (SGCN) or the Scalable Inception Graph Network (SIGN) perform diffusion as a pre-processing step, while others like Correct and Smooth (C&S) do it as a post-processing step. In this paper we highlight that these kinds of diffusion are non-parametric, meaning that diffusion does not rely on learnable parameters. We identify this idea as the core of scalable GNNs and propose Graph Non-Parametric Diffusion (GNPD) as a method which combines ideas from SIGN, SGCN and C&S, to outperform all three of them on several benchmarking datasets. GNPD alternates non-parametric diffusion with simple linear models which can ignore the graph structure. This gives GNPD a high parameter efficiency, allowing it to compete with models with two orders of magnitude more parameters. Additionally GNPD can also forego spectral embeddings which are the computational bottleneck of the C&S method.

1 Introduction

Pairwise relationships between entities arise in many settings in the real world. From people following eachother on social networks, to citations between papers (Rossi & Ahmed, 2015)(Bhattacharya & Getoor, 2007), or links between atoms in a molecule (Hu et al., 2020). These relationships can be described by a network structure which is mathematically referred to as a graph with nodes connected by edges. Since graphs can be used to reflect the structure of real world data, they are increasingly used to make predictions and perform Machine Learning (ML) in settings where relationships between entities are important predictors (Hu et al., 2020). This has led to a rising interest in finding the best way to use this graph structure to make predictions.

Harnessing the structure of data to find local patterns has been key to the success of Deep Learning (DL) tasks on images (LeCun et al., 2015)(Szegedy et al., 2014) and text (Devlin et al., 2018). However, the input spaces for these tasks have a clear and rigid structure. Sentences are sequences of words, and images are grids of pixels. This is not the case for graphs, where each node can have a different number of neighbors which are not ordered in any particular way. Despite the challenges that come with a more complex structure, several methods have successfully implemented deep learning over graphs with Graph Neural Networks (GNNs). Common GNN methods include Graph Convolutional Networks (GCN) (Kipf & Welling, 2016), Graph Attention Networks (Veličković et al., 2018) and Message Passing GNNs (MPGNNs) (Gilmer et al., 2017). These GNNs outperformed preexisting methods on most benchmarking datasets for machine learning on graphs (Hu et al., 2020).

Despite the success of these methods, recent papers have pointed out that GNNs may have inherited some assumptions from Deep Learning, which do not hold on graphs. For example, Simplified GCN (SGCN) (Wu et al., 2019) and SIGN (Rossi et al., 2020) showed that network depth is not needed to achieve state of the art (SOTA) performance on graphs. By using shallow networks, these methods become substantially

faster while requiring less memory. Similarly, the Correct & Smooth (C&S) (Huang et al., 2020) method outperformed many GNNs by using a graph agnostic Multi Layer Perceptron (MLP) combined with residual and label propagation post-processing through the graph structure. This makes it orders of magnitude more scalable than most GNN methods since the graph structure is only used once during training.

While more scalable than traditional GNNs, these methods also have shortcomings. For optimal performance, C&S requires the calculation of spectral embeddings to encode the graph structure, which can be expensive for large graphs. On the other hand, SIGN trains several models for every task, resulting in millions of parameters for most datasets (Hu et al., 2020). Finally, SIGN and SGCN were the SOTA at the time of their publication but have since been left behind by newer methods.

To address these limitations we make the following contributions: 1) Re-framing scalable node classification methods as examples of non-parametric diffusion and highlighting their similarities; 2) Introducing the Graph Non-Parametric Diffusion (GNPD) method which outperforms preexisting scalable models using only 2 linear models and non-parametric diffusion; 3) Highlighting the sufficiency of performing diffusion in the prediction space to achieve a competitive performance in node classification tasks, particularly when additional text features are used.

2 Related Work

2.1 Graphs

A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a collection of nodes $v_i \in \mathcal{V}$ and edges $e_{i,j} \in \mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ between pairs of nodes. The degree of a node is its number of neighbors. In directed graphs nodes have an in-degree and an out-degree corresponding to the edges going in and out of the node respectively. A graph with $n = |\mathcal{V}|$ nodes can be described by an Adjacency Matrix $A \in \mathbb{R}^{n \times n}$ with $A_{i,j} \in \{0, 1\}$ where $A_{i,j} = 1$ if $e_{i,j} \in E$ and 0 else. It is important to note that there is no canonical ordering of the nodes in a graph but they are given an arbitrary order to create an adjacency matrix. The same ordering of nodes is used to create a feature matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ with a vector of dimension d representing the features of each node. In ML tasks, self-loops connecting each node to itself are often added $\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}_N$ and the Degree Matrix $\mathbf{D}$ with $\mathbf{D}_i = \Sigma_j \tilde{\mathbf{A}}_{i,j}$ is often used to create the normalized adjacency matrix $\mathbf{S} = \mathbf{D}^{-1/2} \tilde{\mathbf{A}} \mathbf{D}^{-1/2}$.

2.2 Graph Neural Networks

Intuitively, GNNs aggregate information from local neighborhoods to produce more accurate node property predictions. This is done by multiplying the messages $\mathbf{M} \in \mathbb{R}^{n \times m}$ of size m, to be sent from each node by a diffusion operator. If this operator is the normalized adjacency matrix $\mathbf{S}$, each node will receive a weighted average of the messages from neighboring nodes. This process can be viewed as an aggregation with each node receiving messages from it's neighbours, or a diffusion process with each node diffusing its message to the rest of the network. By multiplying the message vectors by the kth power of the normalized adjacency matrix $\mathbf{M}' = S^k \mathbf{M}$, the message from each node will reach any other node within k connections or less, this is called the k-hop neighborhood of a node. GNNs split this diffusion process into k GNN layers separated by non-linearities. A k layer GNN is then able to aggregate information from it's k-hop neighborhood. In practice, GNNs face diminishing returns from additional layers once the number of layers goes past 3 or 4 (Kipf & Welling, 2016). Beyond the reduced benefit of adding more layers, stacking them is also expensive in terms of computation and memory which is why network depth has not been as successful for GNNs as it has in traditional deep learning methods.

The main distinction between different GNN architectures is the kind of message each node sends to its neighbors. The most general approach is to design a Message Passing GNN that can learn the most relevant messages to send between two nodes given their features. In practice, however, learning message vectors can be expensive in terms of memory (Bronstein et al., 2021), so the message sent by each node can be restricted to a weighted copy of the features of the node. The weight of these restricted messages can be learned by gradient descent as in GAT, or fixed by some heuristic as in GCN.

GCNs use the node degrees d_u and d_v to determine the importance of node v for node u, with $c_{uv} = \frac{1}{\sqrt{d_u d_v}}$. While each layer of a GCN is non parametric, the update function between layers is learned. This means that for GCNs of more than one layer, the diffusion process has to be repeated for every training step. The update function of a GCN layer can be written in vectorized form as in Equation 1, for $\mathbf{H}^0 = \mathbf{X}$ and $\mathbf{W}^l$ a learnable, layer specific weight matrix.

$$\mathbf{H}^{(l+1)} = \sigma(\mathbf{S}\mathbf{H}^{(l)}\mathbf{W}^l) \tag{1}$$

For a GCN with k layers, the predicted labels are the softmax of the output from the last layer as denoted in Equation 2.

$$\hat{\mathbf{Y}}_{GCN} = softmax(\mathbf{S}\mathbf{H}^{(k)}\mathbf{W}^k) \tag{2}$$

2.2.1 Inductive Bias In GNNs

An inductive bias allows us to encode assumptions into our models which can be useful to generalize to unseen data (Battaglia et al., 2018). Using the graph structure to change the representations of the nodes in order to get better predictions can be viewed as the inductive bias underpinning GNNs. The GNNs explored in this section add an increasingly strong inductive bias to the Message Passing framework. Attentional GNNs assume that each node should send a weighted copy of it's current features as a message and convolutional GNNs use a heuristic to decide these attention weights. Choosing $c_{uv} = \frac{1}{\sqrt{d_u d_v}}$ as in Kipf & Welling (2016) presents an inductive bias which gives more importance to messages coming from nodes with fewer neighbors, while other choices for the value of c_{uv} result in other kinds of inductive bias. Different choices of diffusion operators like triangle based adjacency matrix (Rossi et al., 2020) can also bias the predictions in different directions.

Inductive bias reduces the size of the hypothesis space, making training more efficient. However, choosing the wrong inductive bias for a dataset can lead to a drop in performance (Battaglia et al., 2018). Recent methods (Rossi et al., 2020) (Sun & Wu, 2021) explicitly explore the idea of using prior knowledge about the data to design diffusion operators with the right inductive bias for the task.

2.3 Non-parametric Diffusion

For all the methods described in subsection 2.2, some parts of the aggregation process must be learned through gradient descent with back-propagation. This means the aggregation process is repeated for every training step, leading to slower training and the need for graph sampling when the graph does not fit into memory. To avoid this, Wu et al. (2019) proposed Simplified GCN (SGCN), where the non-linearities in the aggregation function are removed. This allows us to collapse the learnable matrices $\mathbf{W}^{(0)}, \mathbf{W}^{(1)}, ..., \mathbf{W}^{(k)}$ into a single matrix $\mathbf{W}$. So the prediction of a SGCN which aggregates information from its k-hop neighborhood becomes:

$$\hat{\mathbf{Y}}_{SGCN} = softmax(\mathbf{S}\mathbf{S}...\mathbf{S}\mathbf{X}\mathbf{W}^{(0)}\mathbf{W}^{(1)}...\mathbf{W}^{(k)}) \tag{3}$$

$$\Leftrightarrow \hat{\mathbf{Y}}_{SGCN} = softmax(\mathbf{S}^k\mathbf{X}\mathbf{W}) \tag{4}$$

Here, the matrix $\mathbf{S}^k\mathbf{X}$ can be pre-computed, so the classifier becomes a simple logistic regression model which can ignore the graph structure. This means we can use minibatches to parallelize the training process without any sampling issues. Figure 1 depicts the contrast between this approach and that of traditional GNNs.

Diffusion through the graph can be identified as the bottleneck of most GNN methods. Therefore, making the diffusion process non parametric to avoid having to repeat it during training has been at the core of recent attempts to make graph methods scalable (Wu et al., 2019)(Rossi et al., 2020)(Huang et al., 2020).

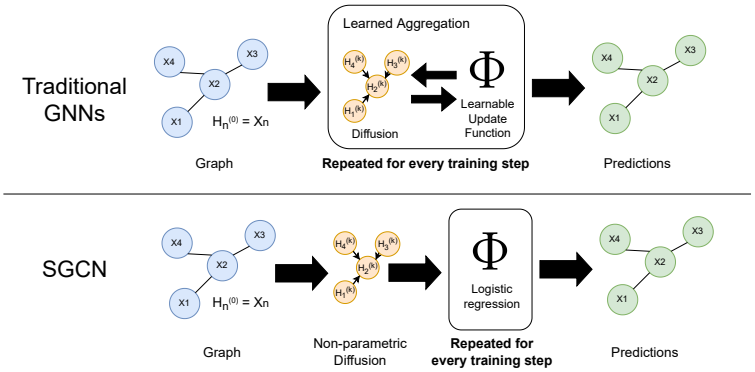


Figure 1: Schematic overview of traditional GNN methods and SGCN. In both cases the part of the method that is repeated for each training step is highlighted by a box. SGCN omits propagation from this highlighted section, resulting in classical, graph-agnostic ML classification.

While SGCN managed to achieve a comparable performance to GCN, both methods have fallen behind the state of the art on most benchmarks. However, newer non parametric methods like C&S, SIGN, and their variants (SAGN (Sun & Wu, 2021)) have outperformed the top learnable diffusion methods like GAT, and currently hold top spots on node classification leaderboards (Hu et al., 2020).

SIGN uses the same idea as SGCN and eliminates the non-linearities from the diffusion process, making it non parametric. Moreover, SIGN adds expressivity to its method by performing diffusion with different diffusion operators and making predictions based on a sequence of powers of these operators. The predictions are then aggregated in a final dense layer that makes the final prediction.

Correct & Smooth takes a different approach to non-parametric diffusion, instead of using it as a pre-processing step to create features for a traditional classifier, it takes the predictions from a traditional classifier and performs diffusion through the graph as a post processing step. A schematic overview of both SIGN and C&S is shown in Figure 2. These methods will be explored in more detail in subsections 2.4 and 2.5.

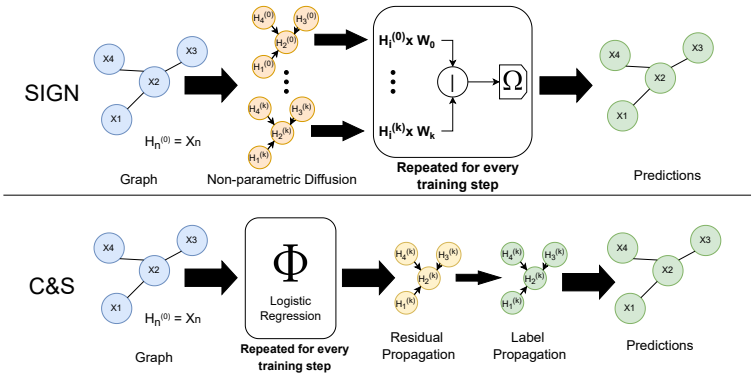


Figure 2: Schematic overview of SIGN and C&S. In both cases the part of the method that is repeated for each training step is highlighted by a box. In the case of SIGN, a non-parametric diffusion is performed before learning the matrices $\mathbf{W}_0$ to $\mathbf{W}_k$ and the classifier $\mathbf{\Omega}$. C&S trains a graph agnostic classifier and only then sends information across the graph, but the graph is still not used during training.

2.4 Correct & Smooth

Correct & Smooth (C&S) (Huang et al., 2020) uses a graph agnostic classifier, like an MLP or a linear model to make initial prediction based on the features of each node. Assuming that the classifier makes

similar mistakes on connected nodes, it uses residual propagation to address this. It further assumes that connected nodes are more likely to have the same labels and uses label propagation to enforce this. This method outperforms many GNNs with a fraction of the parameters. While C&S is accurate and fast, spectral embeddings of the graph are required as feature augmentation to achieve optimal performance.

Spectral embeddings are designed to be similar for connected nodes, therefore partially encoding the structure of the graph. They can be obtained by performing an eigendecomposition of the Laplacian of the graph, which can be computationally prohibitive for large graphs. Even with the approximation methods described in Kipf & Welling (2016), calculating the spectral embeddings is still the computational bottleneck of the C&S method.

For a dataset containing c classes, the C&S framework can be formally defined in the following way. An initial graph agnostic classifier $\mathbf{\Phi} : \mathbb{R}^{n \times d} \rightarrow \mathbb{R}^{n \times c}$, generates predictions $\mathbf{P}$ for every node, with $\mathbf{P} = \mathbf{\Phi}(\mathbf{X})$. Every row of $\mathbf{P}$ is a probability distribution for the different classes, generated by the softmax function.

These predictions are used along with a one-hot encoding of the labels $\mathbf{Y} \in \mathbb{R}^{n \times c}$ to obtain the errors $\mathbf{E}$ in the training data with $\mathbf{E}_t = \mathbf{Y}_t - \mathbf{P}_t$ for the training data and $\mathbf{E}_v = \mathbf{0}$ for the validation and test data. These residuals are the diffused through the graph by a sequence of diffusion steps until convergence:

$$\mathbf{E}^{(l+1)} = (1 - \alpha)\mathbf{E} + \alpha\mathbf{S}\mathbf{E}^{(l)} \tag{5}$$

Once the residuals are diffused through the graph, they are used to update the initial prediction $\mathbf{P}_r = \mathbf{P} - s\mathbf{E}$, with s a scaling coefficient.

The entries in $\mathbf{P}_r$ which correspond to training nodes, are replaced by the true labels to create the matrix $\mathbf{G}$, which is used to smooth the labels and predictions over the graph. The following equation is used, with $\mathbf{G}_0 = \mathbf{G}$:

$$\mathbf{G}^{(l+1)} = (1 - \alpha)\mathbf{G} + \alpha\mathbf{S}\mathbf{G}^{(l)} \tag{6}$$

This smoothing step differs from other label propagation methods in the combined use of predictions for the validation data, and true labels for the training data. The output of this smoothing step is taken as the prediction generated by the C&S method.

The choice of scaling coefficient s can have a significant impact on performance for some datasets. Huang et al. (2020) propose two scaling coefficients with the choice between the two as a hyperparameter: autoscale and fixed diffusion scaling. Autoscale scales the diffused errors to the magnitude of the average residuals in the training set. Fixed diffusion scaling fixes the residuals of the training nodes so they are not updated during diffusion. Fixed scale diffusion leads to label leakage which is a problem if one wants to perform learnable downstream tasks after label propagation, this will be elaborated on in Section 3.

While Huang et al. (2020) frame this method as label spreading of the kind described in Zhou et al. (2003), we can also see it as a sequence of two SGCN layers for which the features are predictions and residuals. The implications of this will be explored in Section 3.

2.5 SIGN

SIGN can also be seen as a set of SGCNs with different operators and receptive fields, and an additional dense layer to aggregate the outputs of all the SGCNs. The diffusion operators can be the normalized adjacency matrix $\mathbf{S}$, as in other methods, but Rossi et al. (2020) propose additional operators based on personalized page rank or a triangle based adjacency matrix. The set of linear diffusion operators is given by $\mathbf{A}^{(l)}$ for $l \in \{1, .., k\}$. The set of predictions from each SGCN is described in Equation 7.

$$\mathbf{P}^{(l)} = \mathbf{A}^{(l)}\mathbf{X}\mathbf{W}^{(l)} \tag{7}$$

With $W^{(l)}$ the learnable weight matrix, specific to each operator. A final dense layer $\mathbf{\Omega}$ is then learned to aggregate the outputs of the different SGCN layers after applying a non-linearity σ and the concatenation operator "|".

$$\hat{\mathbf{Y}}_{SIGN} = softmax(\sigma(\mathbf{P}^{(1)}|...|\mathbf{P}^{(k)})\mathbf{\Omega}) \tag{8}$$

3 Methodology

Building upon the aforementioned frameworks, we propose GNPD, a novel non-parametric diffusion model for learning on graphs. GNPD employs residuals and predictions akin to C&S with an aggregation model that combines inputs from the provided diffusion operators, similar to SIGN.

3.1 Our Approach

In designing our approach we aim to address the following limitations of existing non-parametric diffusion methods:

1. SGCN is scalable but has fallen behind other models in terms of accuracy (Hu et al., 2020).
2. C&S relies heavily on feature augmentation with spectral embeddings which are computationally expensive for large graphs.
3. SIGN trains a model for every power of each diffusion operator, resulting in millions of learnable parameters for most graphs (Hu et al., 2020).

To address these issues, we perform non-parametric diffusion in the prediction space, as in C&S, but use an aggregation model to combine different diffusion processes as in SIGN. By working in the prediction space we are able to encode prior knowledge in our diffusion process through Diffusion Bias. The result is a non-parametric diffusion method which outperforms SIGN, C&S and SGCN without the need for spectral embeddings and with orders of magnitude fewer parameters than SIGN.

3.2 Architecture

GNPD consists of 4 steps described in this section and depicted in Figure 3. An initial prediction is made, then used to perform residual and prediction diffusion. The outputs of the previous steps are then aggregated by a final model and smoothed with the true labels from the training data. In this section we explain each of these steps in detail.

3.2.1 Graph Agnostic Classifier

An initial prediction is made by a simple graph agnostic classifier using only the features of each node. In this paper we us a logistic regression model to make these predictions. Contrary to C&S, this model does not use additional spectral embeddings. The predictions are therefore given by $\mathbf{P} = softmax(\mathbf{XW})$ using the previously established notation.

3.2.2 Soft Non-parametric Diffusion

The predictions from this linear model are then corrected and smoothed using our proposed Soft Correct & Smooth (SoftC&S). This version of C&S propagates predictions in the smoothing step, instead of propagating the real labels. This allows us to train a downstream classifier, as the training loss no longer goes to zero in the smoothing process. Additionally, we bring C&S closer to other GNN methods by reducing its receptive field. The original C&S method uses 100 diffusion steps in total, resulting in each node potentially aggregating information from 100 hops away. We found that this is only viable if the spectral embeddings are included. Excluding these, a receptive field of 3 to 6 hops seems to be more adequate. This is in line with the findings of Kipf & Welling (2016) and Wu et al. (2019) which reported similar optimal receptive fields.

While the label smoothing can be replaced by prediction smoothing to avoid using the labels, the residuals cannot be computed without accessing the true labels. This is not problematic when using autoscale, since

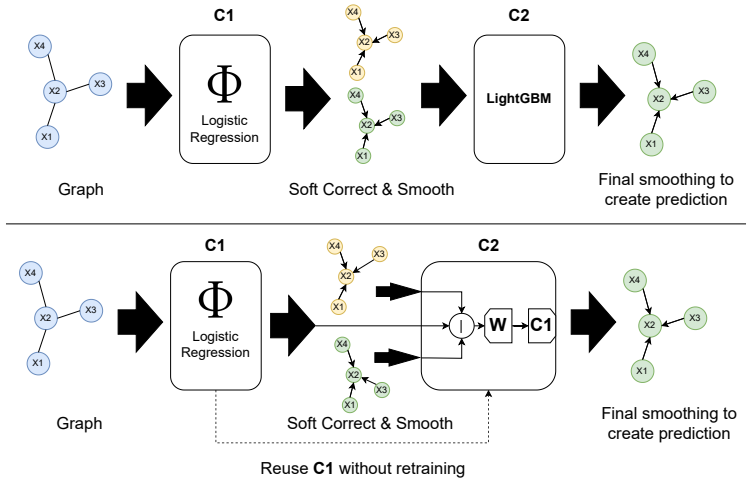


Figure 3: Schematic overview of the two versions of our method. Both present two classifiers which are trained independently, with a non-parametric diffusion of residuals and predictions in between the two. The parts of the each method that are repeated during training are shown in boxes. The symbol "|" represents the concatenation operator and $\mathbf{W}$ is a learnable weight matrix.

the residuals of the training nodes are also updated at every step without preserving their values from the previous step. This means the diffused residuals in the training set are representative of the residuals on the unlabeled nodes as they both arise from the same diffusion process. However, as fixed diffusion scaling treats training nodes differently from the rest, patterns found in the training data will no longer generalize to the validation and test sets. This makes fixed scaling incompatible with our method in its current form.

SoftC&S can be written as a correction step shown in Equation 10 followed by a smoothing step shown in Equation 11.

$$\mathbf{E} = \mathbf{Y} - softmax(\mathbf{X}\mathbf{W}_p) \tag{9}$$

$$\hat{\mathbf{Y}}_{Correct} = softmax(\mathbf{X}\mathbf{W}_p) + s\mathbf{S}^k\mathbf{E} \tag{10}$$

$$\hat{\mathbf{Y}}_{Smooth} = \mathbf{S}^k\hat{\mathbf{Y}}_{Correct} \tag{11}$$

3.2.3 Aggregation

We hypothesized that, while C&S fixes errors at a local level in the graph, this process must also be introducing errors, which could be addressed by looking at the dataset as a whole. We propose using an additional classifier after SoftC&S which will be able to address the global patterns in the errors introduced by C&S. This final aggregation can be performed by any traditional classifier, in this work we propose two approaches which are depicted in Figure 3. The first is to add a gradient boosted model (LightGBM (Ke et al., 2017)) to make the final predictions, this allows us to capture complex patterns while enabling parallelization during training to make it more scalable. We also propose a lightweight version of our method which reuses the initial text based linear model without retraining it. We change it's input with another linear model which takes the output of the diffusion steps as input. These two approaches are shown in Figure 3.

We design the aggregation classifier $\mathbf{\Omega} : \mathbb{R}^{(3c+2)\times n} \rightarrow \mathbb{R}^{c\times n}$ to take in a concatenation of the original prediction $\mathbf{P}$, the prediction after the correct step and the prediction after smoothing, along with node features like the in-degree d_{in} and out-degree d_{out} of the nodes. This results in the feature matrix $\mathbf{H}$ shown in Equation 12 and an aggregator prediction depicted in Equation 13.

$$\mathbf{H} = (\mathbf{P}|\hat{\mathbf{Y}}_{Correct}|\hat{\mathbf{Y}}_{Smooth}|d_{in}|d_{out}) \tag{12}$$

$$\hat{\mathbf{Y}}_{Aggregator} = \mathbf{\Omega}(\mathbf{H}) \tag{13}$$

For the second version of our method shown in Figure 3, we reuse the initial classifier $\mathbf{\Phi}$ along with the initial node features $\mathbf{X}$. The predictions from this version of our method are described in Equation 14.

$$\hat{\mathbf{Y}}_{Aggregator} = \mathbf{\Phi}(\mathbf{\Omega}(\mathbf{H}) + \mathbf{X}) \tag{14}$$

3.2.4 Final Smoothing

Finally we perform 2 additional smoothing steps of the kind described in Equation 6, this time including the real labels for the training set, as no further classifiers need to be trained on this data. For the data from the validation and test sets, the true labels are not available so the predictions $\mathbf{P}$ are used.

3.3 Diffusion Bias

An advantage of performing diffusion in the prediction space is that predictions can be easily interpreted as the probabilities assigned by the model of each node belonging to each class. Each node is represented by a probability distribution and aggregates information from the classes assigned to it's neighbors. The interpretability of these representations allows us to introduce our background knowledge into the diffusion process in what we call Diffusion Bias. We do this in two main ways which are relevant for most real world applications, but this can be extended by using dataset specific insights.

3.3.1 Class Specific Homophily

We observe that, for most graphs, homophily is not homogeneous across classes. For example, in graph citation networks, some paper topics can lend themselves to citations from a diverse set of research areas, while other research areas predominantly cite papers with the same topic. To reflect this, we add a class specific homophily coefficient based on the External-Internal (EI) homophily index (Coleman, 1964). This index looks at Internal edges which connect nodes of the same class, and External edges which connect nodes of different classes, the formula for the index is shown in Equation 15.

$$EI = \frac{External - Internal}{External + Internal} \tag{15}$$

We use the training set to calculate the EI_c index of each class c, an index of -1 corresponds to complete homophily while an index of 1 corresponds to the opposite (heterophily). We then set the importance of messages to be proportional to $1 - \lambda EI_c$, with $\lambda \in [0, 1]$ as a hyperparameter.

3.3.2 Confidence

We also want predictions which are made confidently by the initial model to be less affected by the diffusion process than predictions for which the confidence is low. Therefore, we update the prediction with the diffused residuals proportionally to $1 - \frac{C}{max(C)}$ with $C \in \mathbb{R}^n$ the maximum probability assigned to a class for a given node.

3.4 Relationship to SGCN

We argue that the smoothing used in our method and in C&S (Equation 17) has common features with SGCN (Equation 16). The main difference between the two is whether the weight matrix $\mathbf{W}$ is learned before or after the diffusion process. SGCN aggregates node features and then makes a prediction with a logistic regression model whereas our model, like Linear + C&S aggregates the predictions of a logistic regression model.

$$\hat{\mathbf{Y}}_{SGCN} = softmax(\mathbf{S}^k\mathbf{X}\mathbf{W}) \tag{16}$$

$$\hat{\mathbf{Y}}_{Smooth} = \mathbf{S}^k softmax(\mathbf{X}\mathbf{W}_p) \tag{17}$$

When learning $\mathbf{W}$ before aggregating the node features, the model loses some information about the features of the neighboring nodes. However, the number of classes in a classification task is often lower than the dimension of the node feature vectors. Therefore, propagating predictions through the graph often requires less memory than propagation of the node features. Additionally it seems from the findings of Huang et al. (2020) and our findings in this paper, that performing a simplified convolution over the predictions is more effective than a simplified convolution over the features.

3.5 Relationship to SIGN

A SIGN model with k distinct operators also requires k models like the one described in Equation 2 with k distinct learnable $\mathbf{W}$ matrices. By using the kind of smoothing described in Equation 17, the $\mathbf{W}_p$ matrix is learned before diffusion in GNPD, meaning the same matrix can be used for every diffusion operator. This allows our model to combine different kinds of diffusion operators without increasing the number of parameters. In our current method, we perform two kinds of diffusion, prediction and residual diffusion. However, our approach could be extended to include other diffusion operators, like the ones used in SIGN (Rossi et al., 2020), while keeping the same amount of learnable parameters.

3.6 Relationship to C&S

Our method uses the same kind of residual and prediction diffusion as C&S, with the differences described in Subsection 3.2.2. While C&S is framed as performing smoothing until convergence, as in Zhou et al. (2003), we view it as the same kind of diffusion as the one performed in a SGCN. This puts the focus away from convergence of the diffusion process and puts emphasis on the choice of receptive field determined by the number of diffusion steps. Our method is also different in the lack of spectral embeddings, the use of an aggregation classifier after the diffusion process, as well as the added diffusion bias.

4 Experimental Setup

4.1 Datasets

Dataset	Nodes	Edges	Classes	Train/Val/Test
arxiv	169,343	1,166,243	40	54%/18%/28%
Products	2,449,029	61,859,140	47	10%/2%/88%
Pubmed	19,717	44,338	3	92%/3%/5%
Citeseer	3,327	4,732	6	55%/15%/30%

Table 1: Summary statistics for the datasets used in this paper.

The statistics of the datasets used in this paper are described in Table 1.

4.2 Additional Text Features

As described in Subsection 4.1, most graph benchmarking datasets come with text embeddings to represent the node features instead of using the raw text corresponding to each node. This equalizes the information that each method can extract from the text and puts the focus on learning from the graph structure. However, recent methods (Chien et al., 2021) have started making use of additional text features to learn better node representations, outperforming any models that do not use these additional features (Hu et al., 2020). In

this work we evaluate our models on all datasets in the originally intended setting, without additional text features. However, we also use the text of the papers to generate better text encodings for ogbn-arxiv using a sentence transformer (Reimers & Gurevych, 2019). This allows us to evaluate how much our method can benefit from additional text features and how it compares to state of the art ensemble models based on GIANT (Chien et al., 2021) which are designed to make use of these additional features.

5 Results

Performance metrics and model parameter counts for experiments on ogbn-arxiv without additional text features are denoted in Table 2. Our method is compared to the SOTA and the architectures it draws inspiration from, SIGN and C&S. Notably, our method outperforms SIGN, all iterations of C&S and achieves close to SOTA performance with only 1% of the parameters. This parameter efficiency is highlighted in Figure 4a.

Method	Validation Accuracy	Test Accuracy	Parameters
MLP + C&S	72.42% ±0.06	71.04% ±0.09	85,323
SIGN	73.23 ± 0.06	71.95% ±0.11	3,566,128
Linear + C&S + embeddings	73.68% ±0.04	72.22% ±0.02	15,400
MLP + C&S + embeddings	73.91% ±0.15	73.12 ±0.12	175,656
GNPD (Linear)	74.49% ±0.06	73.51% ±0.04	**15,400**
GNPD (LightGBM)	<u>74.68 ±0.08</u>	<u>73.72% ±0.04%</u>	_
AGDN+BoT+self-KD+C&S	**75.19** ±0.09	**74.31** ±0.14	1,513,294

Table 2: Validation and test metrics on ogbn-arxiv. Reported accuracy scores are averages over 10 runs along with the corresponding standard deviations. Best performing results are depicted in **bold**, while the best results out of our baselines are <u>underlined.</u>

Method	Validation Accuracy	Test Accuracy	Parameters
GIANT-XRT+DRGAT+KD	**77.25%** ±0.08	**76.33** ±0.06	2,685,527
GNDP (Linear)	76.20% ±0.04	74.76% ±0.03	**15,400**
GIANT-XRT+GraphSAGE	75.95% ±0.11	74.35% ±0.14	546,344

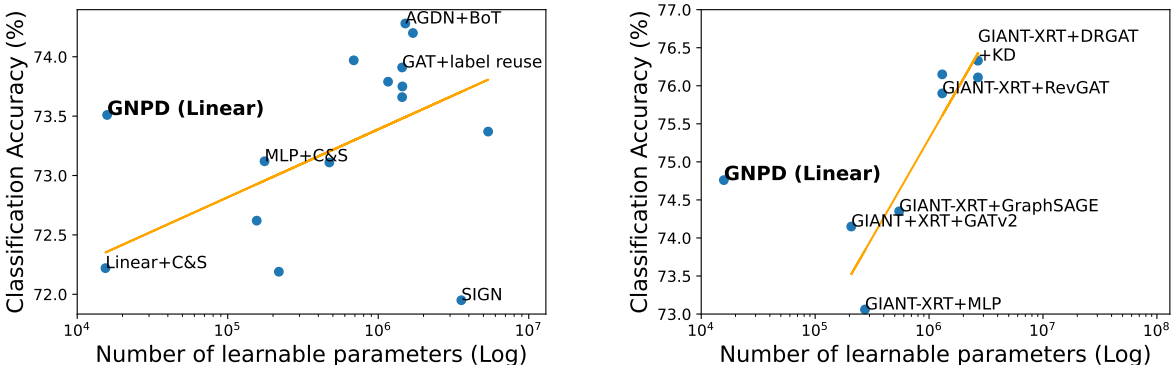
Table 3: Accuracies over 10 runs and number of parameters on ogbn-arxiv using additional text features.

Table 3 compares GNDP performance on ogbn-arxiv using additional text features to that of the overall SOTA ensemble using this feature augmentation. This inclusion boosts our test accuracy to $74.76 \pm 0.03\%$. Figure 4b depicts the contrast in parameter efficiency between GNDP and the overall best performing architectures on ogbn-arxiv.

In Table 4 we evaluate our method on three additional datasets. We see improvement over our baselines in Pubmed and Citeseer, but not on ogbn-products. While our method outperforms the autoscale version of C&S along with the other baselines, it does not outperform C&S with Fixed Diffusion (FixedDiff) Scaling on ogbn-products. FixedDiff makes a minor difference on every dataset reported in Huang et al. (2020) except for ogbn-products where it leads to an increase in accuracy of 5.58%. Since our method is incompatible with FixedDiff Scaling, it cannot benefit from this boost in performance and therefore only outperforms the autoscale version of C&S on ogbn-products.

For ogbn-products, the SOTA model listed in Table 4 corresponds to GAMLP+RLU+SCR+C&S, an ensemble model with 3,335,831 parameters. For Citeseer and Pubmed, the SOTA models are currently versions of Snowball (Luan et al., 2021).

With respect to model runtimes, avoiding the use of spectral embeddings results in a substantial increase in efficiency, with our model scaling better to larger datasets than methods using spectral embeddings, like



(a) Parameter efficiency of top methods without additional text features.

(b) Parameter efficiency of top methods using additional text features.

Figure 4: Parameter efficiency of the top methods on the ogbn-arxiv leaderboard with and without using additional text features. A regression line is added to show the exponential relationship (linear in log scale) between parameters, and accuracy.

Method	Pubmed	Citeseer	ogbn-products
SGCN	84.04	72.04	—
GCN	88.13	73.68	75.64
MLP+C&S+embeddings autoscale	89.33%	76.31%	78.60%
MLP+C&S+embeddings FixedDiff	89.23%	76.42%	<u>84.18%</u>
GNPD (Linear) autoscale	<u>90.02% ±0.04</u>	<u>79.32% ±0.21</u>	82.80% ±0.08
SOTA	**91.44%** ±0.59	**82.07%** ±1.04	**85.20%** ±0.08

Table 4: Test accuracies averaged over 10 runs with the corresponding standard deviation when available. SOTA results are shown in **bold**, while the best results out of our baselines are <u>underlined</u>.

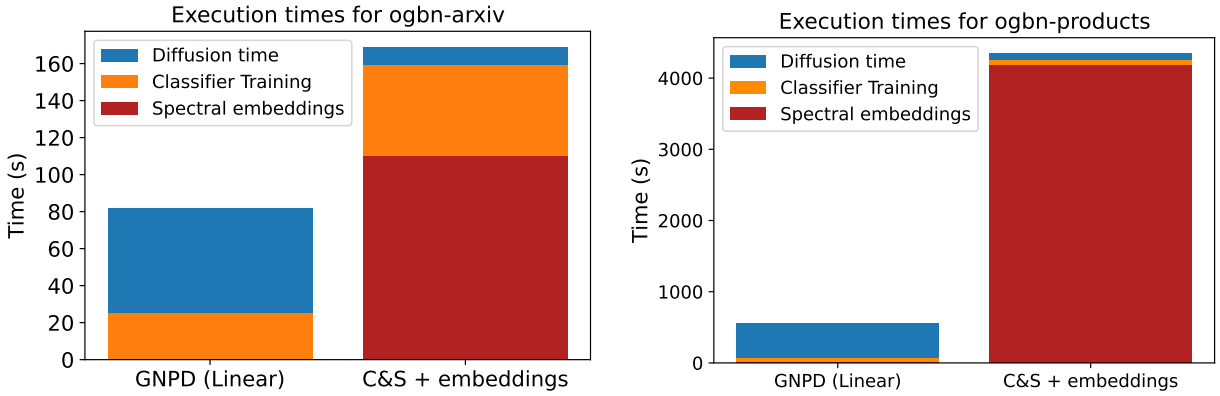
C&S. The benefits of spectral embedding removal due to increasing computational cost for larger datasets is highlighted in Figure 5a.

6 Conclusion

We introduced GNPD, a novel method for non-parametric diffusion, designed to enable scalable node classification while improving accuracy over existing non-parametric diffusion models. In doing this, we grounded the C&S method in the same theoretical framework as other GNNs, allowing us to draw from insights in the GNN literature to design our method and forego the computational bottleneck of spectral embeddings. Our work shows that graph agnostic scalable models can be alternated with non-parametric diffusion to achieve competitive results with an unmatched parameter efficiency. Further work could explore the possibility of adding different diffusion operators to our method as in SIGN (Rossi et al., 2020), since our method makes it possible to do this without multiplying the number of learnable parameters.

References

Peter W. Battaglia, Jessica B. Hamrick, Victor Bapst, Alvaro Sanchez-Gonzalez, Vinícius Flores Zambaldi, Mateusz Malinowski, Andrea Tacchetti, David Raposo, Adam Santoro, Ryan Faulkner, Çaglar Gülçehre, H. Francis Song, Andrew J. Ballard, Justin Gilmer, George E. Dahl, Ashish Vaswani, Kelsey R. Allen, Charles Nash, Victoria Langston, Chris Dyer, Nicolas Heess, Daan Wierstra, Pushmeet Kohli, Matthew M.



(a) Compared run-times on ogbn-arxiv.

(b) Compared runtimes on ogbn-products

Figure 5: Compared runtimes of GNPD (Linear) and the closest version of C&S in terms of accuracy (MLP+C&S+embeddings), averaged over 10 runs on 2 datasets. We see the spectral embeddings are the most computationally expensive part of C&S and that by removing them, our model divides the training time by 2 in the case of ogbn-arxiv and by 10 in the case of ogbn-products.

Botvinick, Oriol Vinyals, Yujia Li, and Razvan Pascanu. Relational inductive biases, deep learning, and graph networks. *CoRR*, abs/1806.01261, 2018. URL `http://arxiv.org/abs/1806.01261`.

Indrajit Bhattacharya and Lise Getoor. Collective entity resolution in relational data. *ACM Trans. Knowl. Discov. Data*, 1(1):5–es, mar 2007. ISSN 1556-4681. doi: 10.1145/1217299.1217304. URL `https://doi.org/10.1145/1217299.1217304`.

Michael M. Bronstein, Joan Bruna, Taco Cohen, and Petar Velickovic. Geometric deep learning: Grids, groups, graphs, geodesics, and gauges. *CoRR*, abs/2104.13478, 2021. URL `https://arxiv.org/abs/2104.13478`.

Eli Chien, Wei-Cheng Chang, Cho-Jui Hsieh, Hsiang-Fu Yu, Jiong Zhang, Olgica Milenkovic, and Inderjit S Dhillon. Node feature extraction by self-supervised multi-scale neighborhood prediction. *arXiv preprint arXiv:2111.00064*, 2021.

James Samuel Coleman. *Introduction to mathematical sociology [by] James S. Coleman.* Free Press of Glencoe [New York], 1964.

Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. BERT: pre-training of deep bidirectional transformers for language understanding. *CoRR*, abs/1810.04805, 2018. URL `http://arxiv.org/abs/1810.04805`.

Justin Gilmer, Samuel S. Schoenholz, Patrick F. Riley, Oriol Vinyals, and George E. Dahl. Neural message passing for quantum chemistry. *CoRR*, abs/1704.01212, 2017. URL `http://arxiv.org/abs/1704.01212`.

Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. Open graph benchmark: Datasets for machine learning on graphs. *arXiv preprint arXiv:2005.00687*, 2020.

Qian Huang, Horace He, Abhay Singh, Ser-Nam Lim, and Austin R. Benson. Combining label propagation and simple models out-performs graph neural networks. *CoRR*, abs/2010.13993, 2020. URL `https://arxiv.org/abs/2010.13993`.

Guolin Ke, Qi Meng, Thomas Finley, Taifeng Wang, Wei Chen, Weidong Ma, Qiwei Ye, and Tie-Yan Liu. Lightgbm: A highly efficient gradient boosting decision tree. In I. Guyon, U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett (eds.), *Advances in Neural Information Processing*

Systems, volume 30. Curran Associates, Inc., 2017. URL https://proceedings.neurips.cc/paper/2017/file/6449f44a102fde848669bdd9eb6b76fa-Paper.pdf.

Thomas N. Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. *CoRR*, abs/1609.02907, 2016. URL http://arxiv.org/abs/1609.02907.

Yann LeCun, Yoshua Bengio, and Geoffrey Hinton. Deep learning. *nature*, 521(7553):436, 2015.

Sitao Luan, Chenqing Hua, Qincheng Lu, Jiaqi Zhu, Mingde Zhao, Shuyuan Zhang, Xiao-Wen Chang, and Doina Precup. Is heterophily A real nightmare for graph neural networks to do node classification? *CoRR*, abs/2109.05641, 2021. URL https://arxiv.org/abs/2109.05641.

Nils Reimers and Iryna Gurevych. Sentence-bert: Sentence embeddings using siamese bert-networks. In *Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing*. Association for Computational Linguistics, 11 2019. URL http://arxiv.org/abs/1908.10084.

Emanuele Rossi, Fabrizio Frasca, Ben Chamberlain, Davide Eynard, Michael M. Bronstein, and Federico Monti. SIGN: scalable inception graph neural networks. *CoRR*, abs/2004.11198, 2020. URL https://arxiv.org/abs/2004.11198.

Ryan A. Rossi and Nesreen K. Ahmed. The network data repository with interactive graph analytics and visualization. In *AAAI*, 2015. URL https://networkrepository.com.

Chuxiong Sun and Guoshi Wu. Scalable and adaptive graph neural networks with self-label-enhanced training. *CoRR*, abs/2104.09376, 2021. URL https://arxiv.org/abs/2104.09376.

Christian Szegedy, Wei Liu, Yangqing Jia, Pierre Sermanet, Scott E. Reed, Dragomir Anguelov, Dumitru Erhan, Vincent Vanhoucke, and Andrew Rabinovich. Going deeper with convolutions. *CoRR*, abs/1409.4842, 2014. URL http://arxiv.org/abs/1409.4842.

Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio. Graph attention networks, 2018.

Felix Wu, Tianyi Zhang, Amauri H. Souza Jr., Christopher Fifty, Tao Yu, and Kilian Q. Weinberger. Simplifying graph convolutional networks. *CoRR*, abs/1902.07153, 2019. URL http://arxiv.org/abs/1902.07153.

Dengyong Zhou, Olivier Bousquet, Thomas Lal, Jason Weston, and Bernhard Schölkopf. Learning with local and global consistency. In S. Thrun, L. Saul, and B. Schölkopf (eds.), *Advances in Neural Information Processing Systems*, volume 16. MIT Press, 2003. URL https://proceedings.neurips.cc/paper/2003/file/87682805257e619d49b8e0dfdc14affa-Paper.pdf.