ON THE CHOICE OF GRAPH NEURAL NETWORK ARCHITECTURES

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ABSTRACT
Seminal works on graph neural networks have primarily targeted semi-supervised node classification problems with few observed labels and high-dimensional signals. With the development of graph networks, this setup has become a de facto benchmark for a significant body of research. Interestingly, several works have recently shown that in this particular setting, graph neural networks do not perform much better than predefined low-pass filters followed by a linear classifier. However, when learning from little data in a high-dimensional space, it is not surprising that simple and heavily regularized methods are near-optimal. In this paper, we show empirically that in settings with fewer features and more training data, more complex graph networks significantly outperform simple models, and propose a few insights towards the proper choice of graph network architectures. We finally outline the importance of using sufficiently diverse benchmarks (including lower dimensional signals as well) when designing and studying new types of graph neural networks.

Index Terms—Graph neural networks, Semi-supervised learning, High-dimensional classification, Node classification

1. INTRODUCTION
Machine learning on graphs has found many applications in domains such as quantum chemistry [1], reinforcement learning [2] or point cloud processing [3]. Recently, this research field has undergone a new technological revolution with the introduction of graph convolutional networks, which permitted to extend the success of deep learning to irregular domains [4]. However, there is no single definition of a graph convolution, and different methods have been proposed for different applications.

Convolutional networks for graphs were first introduced in the spectral domain using the graph Fourier transform [5]. This required to perform an eigendecomposition of the graph Laplacian, which is computationally too costly for large graphs. In [6,7], reparameterizations of the filters by Laplacian polynomials were proposed, which allowed efficient computations and opened the way to a large variety of applications. In order to benchmark their method, [6] tackled graph classification, a task that requires graph convolutions but also graph coarsening. This significantly complicates the method, thus making it more difficult to compare different types of convolutions.

This methodological problem was simplified by the authors of [8], who designed a simpler version of Laplacian polynomials called graph convolutional networks (GCN), and proposed to evaluate on node classification instead. Because it does not require coarsening, node classification allows for simpler architectures, and hence this became the reference task to compare graph networks. Since then, neural networks of increasing complexity have been designed and studied in a similar context.

However, the choice of the benchmark datasets has strong implications on the development of new methods. Indeed, in the standard setting, simple graph networks have been shown to perform on par with sophisticated ones when hyperparameters are tuned fairly [9]. Hence, some works [10,11] have advocated for simplifying GCNs even further, claiming that linear classification methods are powerful enough to solve this task.

In this work, we hypothesize that the success of simplified graph neural network architectures can be explained by the statistics of the benchmark datasets. Indeed, semi-supervised learning on a graph with \( N_{\text{obs}} \) observed nodes and \( D \) dimensional graph signals can be seen in a first approximation as a classification problem with \( N_{\text{obs}} \) training examples in \( \mathbb{R}^D \). When \( N_{\text{obs}} \ll D \), it is known that heavily regularized linear models are optimal, and \( D \) is typically of the order of \( 10 N_{\text{obs}} \) in standard benchmark datasets. By varying the number of training points or features in the dataset, we show experimentally [2] that more complex models becomes more effective when the ratio \( N_{\text{obs}}/D \) grows. This confirms that more diverse benchmarks are necessarily to evaluate fairly the performance of the different graph network architectures.

Finally, we provide some insights towards the proper design of graph neural networks. Whereas increasing the complexity of the neural network is beneficial when more data is available, we find that intertwining propagation and learning is not necessary to obtain good performance. This allows to use simpler architectures: since propagation can be treated as a preprocessing step, the graph structure is not used during training, which results in a computational gain.

\footnote{For this purpose, they used the Planetoid citation datasets, which consist of citation networks between scientific papers, where each node has a signal corresponding to a bag-of-word representation of the paper.}

\footnote{Our source code is available at \url{github.com/LTS4/gnn_statistics}}
2. PROBLEM STATEMENT

We consider a graph $\mathcal{G}$ with $N$ nodes and write its weighted adjacency matrix $A \in \mathbb{R}^{N \times N}$. We denote by $D = \text{diag}(A1)$ the matrix containing the degree of each node in its main diagonal, $1$ being the ones vector. We assume that each node carries a signal or feature vector $x_i \in \mathbb{R}^D$ and possibly a label $y_i \in \{1, \ldots, C\}$. These feature vectors are aggregated in $X \in \mathbb{R}^{N \times D}$.

The goal of node classification is the following: given $A$, $X$ and a small subset of labels, one tries to predict the value of the remaining labels of the graph. Node classification can be viewed as an example of semi-supervised learning [13], where unlabeled data observed during training can be leveraged to achieve better performance. The recently developed Graph Neural Networks are the most popular framework to address node classification. However, there is now a plethora of different graph networks [14], and it is important to develop insights about the proper design choice for a given dataset.

In supervised learning, the choice of the model is typically guided by complexity measures such as the VC dimension. In particular, two crucial parameters are the number of training points $N$ and the dimension of the space $D$: more complex classes of functions can be used when $N$ is large and $D$ small. In semi-supervised learning however, we currently do not have such complexity measures. As a first approximation, we can consider only the labeled nodes and view the problem as the classification of points in dimension $D$ given $N_{\text{obs}}$ training examples. The ratio $N_{\text{obs}}/D$ is however extremely small for common benchmark datasets (cf. Table 1). If we now use insights from supervised learning, we would expect heavily regularized linear methods to be optimal, or close to it, for this classification problem. This has been recently verified in [10]. However, the very specific properties of these benchmark datasets do not permit to confidently extend these insights to other settings. In particular, we believe that the good performance of simple graph neural networks is a consequence of the current evaluation strategies focusing on the small $N_{\text{obs}}/D$ regime. Therefore, we make the following hypothesis:

Depending on the data structure, and especially on the ratio $N_{\text{obs}}/D$, graph neural networks of different complexities are appropriate, with no model being universally superior to all other ones.

We will verify experimentally this hypothesis and show in particular that, in settings where $N_{\text{obs}}/D$ is high, non-linear models perform significantly better.

3. GRAPH NEURAL NETWORKS

Graph neural networks provide a general method to address node classification. They define a parameterized and differentiable function $h : \mathbb{R}^{N \times D} \rightarrow \mathbb{R}^{N \times C}$ that can efficiently be trained to minimize a relevant loss, e.g., empirical cross-entropy or mean squared error on the training data. In order to introduce some form of domain prior, virtually all graph neural networks are formed using a composition of i) propagation steps $\varphi : \mathbb{R}^N \rightarrow \mathbb{R}^N$, which are applied column-wise to $X$ using the structure of $A$, and ii) feature extractors $f : \mathbb{R}^D \rightarrow \mathbb{R}^{D'}$, which act row-wise on $X$.

In this sense, most graph neural networks only differ on the way they define $\varphi$ and $f$, and the way these two are composed. We briefly review the most relevant graph neural networks for this work.

Graph convolutional networks (GCN) Without any doubt, the de facto standard graph neural network is the GCN [8]. It consists in the consecutive application of one-hop aggregation steps $\varphi(X) = \tilde{A}X$, based on the normalized adjacency matrix with self-loops $\tilde{A} = (D + I)^{-1/2}(A + I)(D + I)^{-1/2}$, and simple non-linear feature extractors $f(X) = \sigma(XW)$, where $W \in \mathbb{R}^{D \times D'}$ represents a set of coefficients to be learned and $\sigma$ is a point-wise non-linearity, e.g., Rectified Linear Unit (ReLU). These two steps are applied iteratively, leading to:

$$h(X) = \text{softmax}\left(\tilde{A}\sigma\left(\ldots\sigma\left(\tilde{A}XW_1\ldots\right)W_K\right)\right)$$

(1)

Although GCN was one of the earliest model introduced, more complex extensions of this model [16–18] did not lead to significant improvements in the classification accuracy on standard datasets. For this reason, a recent trend has been to try to simplify it instead.

Simplified graph convolutions (SGC) Following this line of thought, [10] proposed to simplify the structure in (1) by removing the intermediate non-linearities. By doing this, the learnable parameters $W_1, \ldots, W_k$ collapse into a single matrix $W$, and the model becomes:

$$h(X) = \text{softmax}\left(\tilde{A}^KXW\right)$$

(2)

\(^3\)Compared to other approaches, graph neural networks have the advantage of using both the the graph structure (encoded in the adjacency matrix) and the information contained in the node features.
Hence, they reduced the propagation to $\varphi(X) = \tilde{A}^K X$, which can be interpreted as a low-pass spectral filter in the graph Fourier domain\cite{10} and they effectively simplify the learning task to a logistic regression on these filtered features. Despite its simplicity, SGC performs on par with GCN on standard benchmarks (cf. Table\textsuperscript{1}).

Approximate personalized propagation of neural predictions (APPNP). In theory, the number of layers $K$ of a GCN\cite{1} or a SGC\cite{2} can be arbitrary. However, high values of $K$ are rarely used in practice. The reason is that multiple applications of the adjacency operator on the features tend to produce an important smoothing effect on the signal used for learning, which harms classification accuracy\cite{20}. Inspired by the success of the personalized page rank algorithm, the authors of\cite{12} proposed to circumvent this issue by modifying the propagation strategy to $\varphi(X) = \alpha \left( I - (1 - \alpha)\tilde{A} \right)^{-1} X$.

This operation is approximated using fixed point iterations, while a simple neural network is chosen for the feature extractor $f$. State-of-the-art results on standard datasets were obtained using a linear feature extractor, in which case the model writes:

$$h(X) = \alpha \left( I - (1 - \alpha)\tilde{A} \right)^{-1} X W$$ (3)

Nevertheless, most performance reviews for graph networks have only been conducted on datasets with very similar properties. Hence, it is important that benchmarking results are considered beyond this specific context. By doing this, we will show that simple models do not perform well in all settings, and that the network complexity should be tuned depending on the training set size and number of features. Besides, we do not find any evidence confirming that propagation and learning should be intertwined.
4. EXPERIMENTAL RESULTS

All our experiments are based on the experimental platform introduced in [9] in which multiple graph neural networks can be tested against the standard benchmark datasets. We repeat experiments with different train-test splits (selected uniformly at random) for each configuration of parameters to avoid overfitting to a particular training scenario.

The main hypothesis we want to test is if, depending on the ratio of observed nodes to feature dimensionality $N_{obs}/D$, the methods introduced earlier show different behaviours. We are especially interested in the scenario in which $N_{obs}/D$ is high, since this is different from the standard evaluation regime for graph neural networks. To tune $N_{obs}/D$ we control independently the proportion of observed nodes and the dimensionality of the features. To avoid any bias in the feature selection, we change the dimensionality of our feature matrix using a random sketching matrix. That is,

$$X' = \frac{1}{\sqrt{D'}} X W_r,$$

where $W_r \in \mathbb{R}^{D \times D'}$ is a random matrix with entries drawn from a normal distribution, and $D'$ is the target dimension. We use the same set of randomly scrambled features $X' \in \mathbb{R}^{N \times D'}$ as input to the different methods.

4.1. Changing the dataset statistics

We compare the performance of a GCN and a SGC on different ratios $N_{obs}/D$. Both networks are built using their standard hyperparameters [9] and $K = 2$. We recall that in the standard setting for citation data, $N_{obs}/D$ is of the order of 0.1 and both methods perform equally well (cf. Table 1).

We test separately the effect of reducing $D$ (cf. Figure 1a) and increasing $N_{obs}$ (cf. Figure 1b). Clearly, both methods only perform on par in the small data and high-dimensional regime. When we start to increase $N_{obs}/D$, the model based on a GCN tends to perform significantly better than the SGC, while the previously reported similarity [10] is only retained for the original configuration. The reason for these differences is rooted in the complexity of the two classifiers. Indeed, the GCN has the potential to fit non-linear functions and the bias in this estimation decreases when we increase $N_{obs}/D$.

4.2. Decoupling feature extraction and propagation

Furthermore, we evaluate the benefits of using non-linear classification methods and the need to intertwine propagation and feature extraction layers. To this end, we compare the performance of the GCN and the SGC from the previous experiments. We also study the APPNP architecture, and two models (APPNP-MLP and SGC-MLP) where the feature extractor $f$ is a two-layer neural network (MLP) instead of a logistic regression. Contrary to the original APPNP model, feature propagation is treated as a preprocessing step and performed before learning, so as to make gradient backpropagation faster during training. In our configuration, 50% of the nodes are observed and the nodes have 300 random features in order to explore different settings than those of standard benchmarks.

Table 2 summarizes the results. First, we find that GCN and SGC-MLP perform similarly, suggesting that there is no need to use multilayer architectures that intertwine propagation and feature extraction. Indeed, the only difference between the two methods is that $\varphi$ and $f$ are alternated in GCN on not in GCN-MLP. Furthermore, we find that non-linear classification methods (GCN, SGC-MLP) can significantly outperform linear ones (SGC) and that, in high $N_{obs}/D$ scenarios, non-linear feature extractors also boost the accuracy of methods with a complex propagation step such as APPNP.

Overall these results support our claim that depending on the setup, graph neural networks of different complexities perform best. Furthermore, it is clear that having the possibility to tune the complexity of $\varphi$ and $f$ independently gives rise to a rich set of classification behaviours that can be optimized to better fit the structure of the data. Our study further outlines that the choice of the benchmark dataset is really critical when comparing the performance of different graph neural networks.

| Ratio $N_{obs}/D$ | Pubmed | Citeseer | Cora |
|------------------|--------|---------|------|
| SGC              | 76.3 ± 3.2 | 68.4 ± 2.5 | 70.0 ± 3.2 |
| SGC-MLP          | 80.2 ± 1.9 | 70.8 ± 2.8 | 79.3 ± 2.9 |
| GCN              | 78.2 ± 3.0 | 71.3 ± 2.6 | 80.9 ± 3.8 |
| APPNP            | 80.4 ± 2.7 | 72.8 ± 2.4 | 82.3 ± 3.2 |
| APPNP-MLP        | **84.0 ± 1.2** | 70.9 ± 2.6 | 78.8 ± 2.6 |

Table 2: Accuracy and 95% confidence interval over 100 splits with 300 features and 50% of the nodes in the training set.

5. CONCLUSIONS

We have empirically demonstrated that the surprising good performance of simple graph neural networks reported in the recent literature is essentially driven by the characteristics of the benchmark datasets. In particular, both the high-dimensionality of the features and the scarcity of labels in the standard setup make simple methods based on feature smoothing and linear classification nearly optimal. For richer datasets (in terms of $N_{obs}/D$), complex GNN models do outperform simpler ones. However, we find no evidence that intertwining propagation and feature extraction is necessary to obtain good performance: it is sufficient to tune the complexity of the feature extractor depending on the data statistics. Overall, when designing new types of graph neural networks, it is very important to use benchmarks with lower dimensional features and more observed nodes as well, and to assess performance on data whose statistics are suited to the complexity of the proposed method.
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