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TOPOLOGY ADAPTIVE GRAPH CONVOLUTIONAL NETWORKS

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ABSTRACT

Spectral graph convolutional neural networks (CNNs) require approximation to the convolution to alleviate the computational complexity, resulting in performance loss. This paper proposes the topology adaptive graph convolutional network (TAGCN), a novel graph convolutional network defined in the vertex domain. We provide a systematic way to design a set of fixed-size learnable filters to perform convolutions on graphs. The topologies of these filters are adaptive to the topology of the graph when they scan the graph to perform convolution. The TAGCN not only inherits the properties of convolutions in CNN for grid-structured data, but it is also consistent with convolution as defined in graph signal processing. Since no approximation to the convolution is needed, TAGCN exhibits better performance than existing spectral CNNs on a number of data sets and is also computationally simpler than other recent methods.

1 INTRODUCTION

Convolutional neural network (CNN) architectures exhibit state-of-the-art performance on a variety of learning tasks dealing with 1D, 2D, and 3D grid-structured data such as acoustic signals, images, and videos, in which convolution serves as a feature extractor LeCun et al. (2015). However, the (usual) convolution operation is not applicable when applying CNN to data that is supported on an arbitrary graph rather than on a regular grid structure, since the number and topology of neighbors of each vertex on the graph varies, and it is difficult to design a fixed-size filter scanning over the graph-structured data for feature extraction.

Recently, there has been an increasing interest in graph CNNs Bruna et al. (2014); Defferrard et al. (2016); Kipf & Welling (2017); Monti et al. (2017); Levie et al. (2017), attempting to generalize deep learning methods to graph-structured data, specifically focusing on the design of graph convolution. In this paper, we propose the topology adaptive graph convolutional network (TAGCN), a unified convolutional neural network to learn nonlinear representations for the graph-structured data. It slides a set of fixed-size learnable filters on the graph simultaneously, and the output is the weighted sum of these filters' outputs, which extract both vertex features and strength of correlation between vertices. Each filter is adaptive to the topology of the local region on the graph where it is applied. TAGCN unifies filtering in both the spectrum and vertex domains; and applies to both directed and undirected graphs.

In general, the existing graph CNNs can be grouped into two types: spectral domain techniques and vertex domain techniques. In Bruna et al. (2014), CNNs have been generalized to graph-structured data, where convolution is achieved by a pointwise product in the spectrum domain according to the convolution theorem. Later, Defferrard et al. (2016) and Levie et al. (2017) proposed spectrum filtering based methods that utilize Chebyshev polynomials and Cayley polynomials, respectively. Kipf & Welling (2017) simplified this spectrum method and obtained a filter in the vertex domain, which achieves state-of-the-art performance. Other researchers (Atwood & Towsley, 2016; Monti et al., 2017) worked on designing feature propagation models in the vertex domain for graph CNNs. Yang et al. (2016); Dai et al. (2016); Grover & Leskovec (2016); Du et al. (2017) study transforming graph-structured data to embedding vectors for learning problems. More recently, (**?**) proposed graph attention networks leveraging masked self-attentional layers to address the approximation of

exiting graph convolutions networks. Nevertheless, it still remains open how to extend CNNs from grid-structured data to arbitrary graph-structured data with local feature extraction capability.

We define rigorously the graph convolution operation on the vertex domain as multiplication by polynomials of the graph adjacency matrix, which is consistent with the notion of convolution in graph signal processing. In graph signal processing Sandryhaila & Moura (2013), polynomials of the adjacency matrix are graph filters, extending to graph based data from the usual concept of filters in traditional time or image based signal processing. Thus, comparing ours with existing work on graph CNNs, our paper provides a solid theoretical foundation for our proposed convolution step instead of an ad-hoc approach to convolution in CNNs for graph structured data.

Further, our method avoids computing the spectrum of the graph Laplacian as in Bruna et al. (2014), or approximating the spectrum using high degree Chebyshev polynomials of the graph Laplacian matrix (in Defferrard et al. (2016), it is suggested that one needs a 25th degree Chebyshev polynomial to provide a good approximation to the graph Laplacian spectrum) or using high degree Cayley polynomials of the graph Laplacian matrix (in Levie et al. (2017), 12th degree Cayley polynomials are needed). We also clarify that the GCN method in Kipf & Welling (2017) is a first order approximation of the Chebyshev polynomials approximation in Defferrard et al. (2016), which is very different from our method. Our method has a much lower computational complexity than the spectrum based methods, since our method only uses polynomials of the adjacency matrix with maximum degree 2 as shown in our experiments. Finally, the method that we propose exhibits better performance than existing methods as no approximation is required. Our contributions are summarized as follows:

- The proposed TAGCN explores a general K-localized filter for graph convolution in the vertex domain to extract local features on a set of size-1 up to size-K receptive fields. The topologies of these filters are adaptive to the topology of the graph as they scan the graph to perform convolution. It replaces the fixed square filters in traditional CNNs for the grid-structured input data volumes in traditional CNNs. Thus, the convolution that we define in the convolution step for the vertex domain is consistent with convolution in traditional CNNs.
- We analyze the mechanisms of the graph convolutional layers and prove that if only a size-k filter is used, as the convolutional layers go deeper under certain condition, the output of the last convolutional layer is the projection of the output of the first convolutional layer along the eigenvector corresponding to the eigenvalue of the graph adjacency matrix with the largest amplitude. This linear approximation leads to information loss and classification accuracy degradation. In contrast, using a set of size-1 up to size-K filters (as in our TAGCN) can avoid the linear approximation and increases the representation capability. Therefore, it leads to improved classification accuracy.
- TAGCN is consistent with the convolution in graph signal processing. It applies to both directed and undirected graphs. Moreover, it has a much lower computational complexity compared with recent methods since it only needs polynomials of the adjacency matrix with maximum degree 2 compared with the 25th and 12th degree Laplacian matrix polynomials in Defferrard et al. (2016) and Levie et al. (2017).
- As no approximation to the convolution is needed in TAGCN, it achieves better performance compared with existing methods. We contrast TAGCN with recently proposed graph CNN including both spectrum filtering methods (Bruna et al., 2014; Defferrard et al., 2016) and vertex domain propagation methods (Kipf & Welling, 2017; Monti et al., 2017; Atwood & Towsley, 2016), evaluating their performances on three commonly used graph-structured data sets. Our experimental tests show that TAGCN consistently achieves superior performance on all these data sets.

2 Convolution on Graph

We use boldface uppercase and lowercase letters to represent matrices and vectors, respectively. The information and their relationship on a graph $\mathcal{G}$ can be represented by $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \bar{\mathbf{A}})$, where $\mathcal{V}$ is the set of vertices, $\mathcal{E}$ is the set of edges, and $\bar{\mathbf{A}}$ is the weighted adjacency matrix of the graph; the graph can be weighted or unweighted, directed or undirected. We assume there is no isolated vertex in $\mathcal{G}$.

If $\mathcal{G}$ is a *directed weighted* graph, the weight $\bar{\mathbf{A}}_{n,m}$ is on the directed edge from vertex m to n. The entry $\bar{\mathbf{A}}_{n,m}$ reveals the dependency between node n and m and can take arbitrary real or complex values. The graph convolution is general and can be adapted to graph CNNs for particular tasks. In this paper, we focus on the vertex semisupervised learning problem, where we have access to very limited labeled vertices, and the task is to classify the remaining unlabeled vertices by feeding the output of the last convolutional layer to a fully connected layer.

2.1 Graph Convolutional Layer for TAGCN

Without loss of generality, we demonstrate graph convolution on the ℓ-th hidden layer. The results apply to any other hidden layers. Suppose on the ℓ-th hidden layer, the input feature map for each vertex of the graph has C_ℓ features. We collect the ℓ-th hidden layer input data on all vertices for the c-th feature by the vector $\mathbf{x}_c^{(\ell)} \in \mathbb{R}^{N_\ell}$, where $c = 1, 2, \ldots C_\ell$ and N_ℓ is the number of vertices[1]. The components of $\mathbf{x}_c^{(\ell)}$ are indexed by vertices of the data graph representation $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \bar{\mathbf{A}})$[2]. Let $\mathbf{G}_{c,f}^{(\ell)} \in \mathbb{R}^{N_\ell \times N_\ell}$ denote the f-th graph filter. The graph convolution is the matrix-vector product, i.e., $\mathbf{G}_{c,f}^{(\ell)}\mathbf{x}_c^{(\ell)}$. Then the f-th output feature map followed by a ReLU function is given by

$$\mathbf{y}_f^{(\ell)} = \sum_{c=1}^{C_\ell} \mathbf{G}_{c,f}^{(\ell)}\mathbf{x}_c^{(\ell)} + b_f \mathbf{1}_{N_\ell}, \tag{1}$$

where $b_f^{(\ell)}$ is a learnable bias, and $\mathbf{1}_{N_\ell}$ is the N_ℓ dimension vector of all ones. We design $\mathbf{G}_{c,f}^{(\ell)}$ such that $\mathbf{G}_{c,f}^{(\ell)}\mathbf{x}_c^{(\ell)}$ is a meaningful convolution on a graph with arbitrary topology.

In the recent theory on graph signal processing (Sandryhaila & Moura, 2013), the *graph shift* is defined as a local operation that replaces a graph signal at a graph vertex by a linear weighted combination of the values of the graph signal at the neighboring vertices:

$$\tilde{\mathbf{x}}_c^{(\ell)} = \bar{\mathbf{A}}\mathbf{x}_c^{(\ell)}.$$

The graph shift $\bar{\mathbf{A}}$ extends the time shift in traditional signal processing to graph-structured data. Following Sandryhaila & Moura (2013), a graph filter $\mathbf{G}_{c,f}^{(\ell)}$ is shift-invariant, i.e., the shift $\bar{\mathbf{A}}$ and the filter $\mathbf{G}_{c,f}^{(\ell)}$ commute, $\bar{\mathbf{A}}(\mathbf{G}_{c,f}^{(\ell)}\mathbf{x}_c^{(\ell)}) = \mathbf{G}_{c,f}^{(\ell)}(\bar{\mathbf{A}}\mathbf{x}_c^{(\ell)})$, if under appropriate assumption $\mathbf{G}_{c,f}^{(\ell)}$ is a polynomial in $\mathbf{A}$,

$$\mathbf{G}_{c,f}^{(\ell)} = \sum_{k=0}^{K} g_{c,f,k}^{(\ell)} \mathbf{A}^k. \tag{2}$$

In (2), the $g_{c,f,k}^{(\ell)}$ are the graph filter polynomial coefficients; the quantity $\mathbf{A} = \mathbf{D}^{-\frac{1}{2}}\bar{\mathbf{A}}\mathbf{D}^{-\frac{1}{2}}$ is the normalized adjacency matrix of the graph, and $\mathbf{D} = \text{diag}[\mathbf{d}]$ with the ith component being $\mathbf{d}(i) = \sum_j \mathbf{A}_{i,j}$.[3] We adopt the normalized adjacency matrix to guarantee that all the eigenvalues of $\mathbf{A}$ are inside the unit circle, and therefore $\mathbf{G}_{c,f}^{(\ell)}$ is computationally stable. The next subsection shows we will adopt $1 \times C_\ell, 2 \times C_\ell, \ldots,$ and $K \times C_\ell$ filters sliding on the graph-structured data. This fact coincides with GoogLeNet (Szegedy et al., 2015), in which a set of filters with different sizes are used in each convolutional layer. Further, It is shown in the appendix that the convolution operator defined in (2) is consistent with that in classical signal processing when the graph is in the 1D cyclic form, as shown in Fig. 3.

Following the CNN architecture, an additional nonlinear operation, e.g, rectified linear unit (ReLU) is used after every graph convolution operation:

$$\mathbf{x}_f^{(\ell+1)} = \sigma\left(\mathbf{y}_f^{(\ell)}\right),$$

where $\sigma(\cdot)$ denotes the ReLU activation function applied to the vertex values.

[1] Graph coarsening could be used and the number of vertices may vary for different layers.

[2] We use superscript (ℓ) to denote data on the ℓth layer and superscript ℓ to denote the ℓ-th power of a matrix.

[3] There is freedom to normalize $\mathbf{A}$ in different ways; here it is assumed that $\bar{\mathbf{A}}_{m,n}$ is nonnegative and the above normalization is well defined.

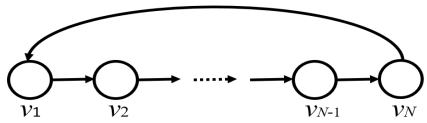

Figure 1: Graph topology of a 1-D cyclic graph.

2.2 Analysis of Graph Convolutional Layers

In the following, we analyze the mechanisms of the graph convolutional layers. We start from the graph filter with the form of a monomial $g_\ell \mathbf{A}^{k_\ell}$ for the ℓ-th layer and $C_\ell = F_\ell = 1$ with $\ell = 1, \ldots L$. In the following, we show that when the graph convolutional layers go deeper, the output of the last graph convolutional layer is proportional to the projection of the output data of the first convolutional layer along the eigenvector corresponding to the eigenvalue of the graph adjacency matrix with the largest amplitude.

Theorem 1 *For any filters $\boldsymbol{A}^{k_\ell}$, with $k_\ell \in \{1, 2, 3, \ldots\}$,*

$$\lim_{L \to +\infty} \underbrace{\sigma\left(\sigma \cdots \sigma\left(g_2 \boldsymbol{A}^{k_2} \sigma\left(g_1 \boldsymbol{A}^{k_1} \boldsymbol{x}\right)\right)\right)}_{L \text{ times } \sigma(\cdot)} = m \, \langle \boldsymbol{y}_1^{(1)}, \boldsymbol{v}_1 \rangle \boldsymbol{v}_1.$$

with $m = \prod_{\ell=1}^{\ell=L} g_\ell$ and $\boldsymbol{y}_1^{(1)} = \sigma\left(g_1 \boldsymbol{A}^{k_1} \boldsymbol{x}\right)$.

Proof For any input data $\mathbf{x} \in \mathbb{R}^N$ on the graph with N vertices, the output of the first graph convolutional layer is $\mathbf{y}_1^{(1)} = \sigma\left(g_1 \mathbf{A}^{k_1} \mathbf{x}\right)$. According to the definition of ReLU function, we know that each component in $\mathbf{y}_1^{(1)}$ is nonnegative. The data feeded to the fully connected layer for classification, which is the output of the L-th graph convolutional layer, is $\sigma\left(\sigma \cdots \left(\sigma\left(g_2 \mathbf{A}^{k_2} \mathbf{y}_1^{(1)}\right)\right)\right)$. It can be observed that all the learned g_i with $i \geq 2$ should be positive, otherwise, the output would be $\mathbf{0}$ resulting in an all-zero vector feeded to the fully connected layer for classification. Further, since all the components of $\mathbf{A}^{k_\ell}$ are nonnegative and $\mathbf{y}_1^{(1)}$ is nonnegative, by conduction, the input of ReLU function in each layer is nonnegative. Therefore, the output of the L-th graph convolutional layer can be written equivalently as

$$\begin{aligned}
&\underbrace{\sigma\left(\sigma \cdots \sigma\left(g_2 \mathbf{A}^{k_2} \sigma\left(g_1 \mathbf{A}^{k_1} \mathbf{x}\right)\right)\right)}_{L \text{ times } \sigma(\cdot)} \\
&= m \mathbf{A}^{\sum_{\ell=2}^{L} k_\ell} \mathbf{y}_1^{(1)} \\
&\overset{(a)}{=} m \mathbf{V} \mathbf{J}^{\sum_{\ell=2}^{L} k_\ell} \mathbf{V}^{-1} \mathbf{y}_1^{(1)} \\
&\overset{(b)}{=} m \mathbf{V} \mathbf{J}^{\sum_{\ell=2}^{L} k_\ell} \mathbf{V}^{-1} \left(c_1 \mathbf{v}_1 + c_2 \mathbf{v}_2 \ldots c_N \mathbf{v}_N\right) \\
&\overset{(c)}{=} m \mathbf{V} \mathbf{J}^{\sum_{\ell=2}^{L} k_\ell} \left(c_1 \mathbf{e}_1 + c_2 \mathbf{e}_2 \ldots + c_N \mathbf{e}_N\right).
\end{aligned} \tag{3}$$

In (a), we use eigendecomposition of $\mathbf{A}$, where $\mathbf{V} = [\mathbf{v}_1, \ldots, \mathbf{v}_N]$ with $\mathbf{v}_i$ the eigenvector of $\mathbf{A}$, and $\mathbf{J}$ is a diagonal matrix with diaonal elements being the eigenvalues of $\mathbf{A}$.[4] Equation (b) is due to the fact that the set of eigenvectors $\{\mathbf{v}_i\}_{i=1}^N$ form an orthogonal basis, and one can express $\mathbf{y}_1^{(1)} \in \mathbb{R}^N$ by a linear combination of those vectors, with $c_i = \langle \mathbf{y}_1^{(1)}, \mathbf{v}_i \rangle$. In (c), $\{\mathbf{e}_i\}_{i=1}^N$ is the standard basis.

Without loss of generality, the graph is assumed to be strongly connected, and we have the unique largest eigenvalue. Then, following the definition of $\mathbf{A}$, we have $\mathbf{J} = \text{diag}\left([1, \lambda_2, \ldots, \lambda_N]\right)$ with

[4] When $\mathbf{A}$ is asymmetric and rank deficient, Jordan decomposition is adopted to replace eigendecomposition, and then $\mathbf{J}$ is a block diagonal matrix. The remaining analysis also applies for the Jordan decomposition.

$|\lambda_k| < 1$ for all $k > 2$. Then we obtain

$$\begin{aligned} &\lim_{L\to+\infty} \mathbf{V}\mathbf{J}^{\sum_{\ell=2}^{L} k_\ell} \left(c_1\mathbf{e}_1 + c_2\mathbf{e}_2 \ldots + c_N\mathbf{e}_N\right) \\ &= c_1\mathbf{v}_1 = \langle \mathbf{y}_1^{(1)}, \mathbf{v}_1\rangle \mathbf{v}_1. \end{aligned} \tag{4}$$

■

Note that when $k_\ell = 1$ for all $\ell \in \{1, 2, \ldots L\}$, the graph convolutional filter reduces to $g_\ell \mathbf{A}$ which is used in Kipf & Welling (2017). Due to the linear approximation (projection along the eigenvector corresponding to the largest eigenvalue amplitude), the information loss would degrade the classification accuracy. However, if we choose the graph filter as a set of filters from size-1 to size-K, it is not a projection anymore, and the representation capability of graph convolutional layers is improved.

2.3 Filter Design for TAGCN Convolutional Layers

In this section, we would like to understand the proposed convolution as a feature extraction operator in traditional CNN rather than as embedding propagation. Taking this point of view helps us to profit from the design knowledge/experience from traditional CNN and apply it to grid structured data. Our definition of weight of a path and the following filter size for graph convolution in this section make it possible to design a graph CNN architecture similar to GoogLeNet (Szegedy et al., 2015), in which a set of filters with different sizes are used in each convolutional layer. In fact, we found that a combination of size 1 and size 2 filters gives the best performance in all three data sets studied, which is a polynomial with maximum order 2.

In traditional CNN, a $K \times K \times C_\ell$ filter scans over the input grid-structured data for feature extraction. For image classification problems, the value K varies for different CNN architectures and tasks to achieve better performance. For example, in VGG-Verydeep-16 CNN model (Simonyan & Zisserman, 2015), only $3 \times 3 \times C_\ell$ filters are used; in ImageNet CNN model (Krizhevsky et al., 2012), $11 \times 11 \times C_\ell$ filters are adopted; and in GoogLeNet (Szegedy et al., 2015), rather than using the same size filter in each convolutional layer, different size filters, for example, $1 \times 1 \times C_\ell$, $3 \times 3 \times C_\ell$ and $5 \times 5 \times C_\ell$ filters, are concatenated in each convolution layer. Similarly, we propose a general K-localized filter for graph CNN.

For a graph-structured data, we cannot use a square filter window since the graph topology is no longer a grid. In the following, we demonstrate that the convolution operation $\mathbf{G}_{c,f}^{(\ell)}\mathbf{x}_c^{(\ell)}$ with $\mathbf{G}_{c,f}^{(\ell)}$ a polynomial filter $\mathbf{G}_{c,f}^{(\ell)} = \sum_{k=0}^{K} g_{c,f,k}^{(\ell)}\mathbf{A}^k$ is equivalent to using a set of filters with filter size from 1 up to K. Each k-size filter, which is used for local feature extraction on the graph, is k-localized in the vertex domain.

Define a *path* of length m on a graph $\mathcal{G}$ as a sequence $v = (v_0, v_1, ..., v_m)$ of vertices $v_k \in \mathcal{V}$ such that each step of the path (v_k, v_{k+1}) corresponds to an (directed) edge of the graph, i.e., $(v_k, v_{k+1}) \in \mathcal{E}$. Here one path may visit the same vertex or cross the same edge multiple times. The following adjacency matrix $\mathbf{A}$ is one such example:

$$\mathbf{A} = \begin{bmatrix} 0&1&0&2&3&0&0&\cdots \\ 1&0&4&5&0&0&0&\cdots \\ 0&1&0&0&0&0&1&\cdots \\ 1&1&0&0&6&0&0&\cdots \\ 1&0&0&1&0&1&0&\cdots \\ 0&0&0&0&1&0&0&\cdots \\ 0&0&0&1&0&0&0&\cdots \\ \vdots&\vdots&\vdots&\vdots&\vdots&\vdots&\vdots&\ddots \end{bmatrix}.$$

Since $\mathbf{A}$ is asymmetric, it represents a directed graph, given in Fig. 2. In this example, there are 6 different length 3-paths on the graph from vertex 2 to vertex 1, namely, $(2, 1, 4, 1)$, $(2, 1, 2, 1)$, $(2, 1, 5, 1)$, $(2, 3, 2, 1)$, $(2, 4, 2, 1)$, and $(2, 4, 5, 1)$.

We further define the *weight of a path* to be the product of the edge weights along the path, i.e., $\phi(p_{0,m}) = \prod_{k=1}^{m} \mathbf{A}_{v_{k-1},v_k}$, where $p_{0,m} = (v_0, v_1, \ldots v_m)$. For example, the weight of the path $(2, 1, 4, 1)$ is $1 \times 1 \times 2 = 2$. Then, the (i, j)th entry of $\mathbf{A}^k$ in (2), denoted by $\omega(p_{j,i}^k)$, can be interpreted as the sum of the weights of all the length-k paths from j to i, which is

$$\omega(p_{j,i}^k) = \sum_{j \in \left\{\tilde{j} \mid \tilde{j} \text{ is } k \text{ paths to } i\right\}} \phi(p_{j,i}).$$

In the above example, it can be easily verified that $\mathbf{A}^3_{1,2} = 18$ by summing up the weights of all the above six paths from vertex 2 to vertex 1 with length 3. Then, the ith component of $\mathbf{A}^k \mathbf{x}_c^{(\ell)}$ is the weighted sum of the input features of each vertex $\mathbf{x}_c^{(\ell)}$ that are length-k paths away to vertex i. Here, k is defined as the *filter size*. The output feature map is a vector with each component given by the size-k filter sliding on the graph following a fixed order of the vertex indices.

The output at the i-th component can be written explicitly as $\sum_{c=1}^{C_\ell} \sum_j g_{c,f,k}^{(\ell)} \omega(p_{j,i}^k) \mathbf{x}_c^{(\ell)}(j)$. This weighted sum is similar to the dot product for convolution for a grid-structured data in traditional CNNs. Finnaly, the output feature map is a weighted sum of convolution results from filters with different sizes, which is

$$\mathbf{y}_f^{(\ell)}(i) = \sum_{k=1}^{K_\ell} \sum_{c=1}^{C_\ell} \sum_{j \in \{\tilde{j} | \tilde{j} \text{ is } k \text{ paths to } i\}} g_{c,f,k}^{(\ell)} \omega(p_{j,i}^k) \mathbf{x}_c^{(\ell)}(j) + b_f \mathbf{1}_{N_\ell}. \tag{5}$$

The above equation shows that each neuron in the graph convolutional layer is connected only to a local region (local vertices and edges) in the vertex domain of the input data volume, which is adaptive to the graph topology. The strength of correlation is explicitly utilized in $\omega(p_{j,i}^k)$. We refer to this method as topology adaptive graph convolutional network (TAGCN).

In Fig. 2, we show TAGCN with an example of 2-size filter sliding from vertex 1 (figure on the left-hand-side) to vertex 2 (figure on the right-hand-side). The filter is first placed at vertex 1. Since paths $(1, 2, 1)$ $(5, 4, 1)$ and so on (paths with red glow) are all 2-length paths to vertex 1, they are covered by this 2-size filter. Since paths $(2, 3)$ and $(7, 3)$ are not on any 2-length path to vertex 1, they are not covered by this filter. Further, when this 2-size filter moves to vertex 2, paths $(1, 5)$, $(4, 5)$ and $(6, 5)$ are no longer covered, but paths $(2, 3)$ and $(7, 3)$ are first time covered and contribute to the convolution with output at vertex 2.

Further, $\mathbf{y}_f^{(\ell)}(i)$ is the weighted sum of the input features of vertices in $\mathbf{x}_c^{(\ell)}$ that are within k-paths away to vertex i, for $k = 0, 1, \ldots K$, with weights given by the products of components of $\mathbf{A}^k$ and $g_{c,f,k}^{(\ell)}$. Thus the output is the weighted sum of the feature map given by the filtered results from 1-size up to K-size filters. It is evident that the vertex convolution on the graph using Kth order polynomials is K-paths localized. Moreover, different vertices on the graph share $g_{c,f,k}^{(\ell)}$. The above local convolution and weight sharing properties of the convolution (5) on a graph are very similar to those in traditional CNN.

Though the convolution operator defined in (2) is defined on the vertex domain, it can also be understood as a filter in the spectrum domain, and it is consistent with the definition of convolution in graph signal processing. We provide detailed discussion in the appendix.

3 Relation with Other Existing Formulations

In general, there are two types of graph convolution operators for the CNN architecture. One defines the convolution in the spectrum domain, whose output feature map is the multiplication of the inverse Fourier transform matrix with the filtered results in the spectrum domain (Bruna et al., 2014; Defferrard et al., 2016; Levie et al., 2017). By doing further approximations based on this spectrum domain operator, a simplified convolution was obtained in Kipf & Welling (2017). The other defines convolution by a feature propagation model in the vertex domain such as MoNet in Monti et al. (2017) and the diffusion CNN (DCNN) in Atwood & Towsley (2016). We investigate in detail each alternative.

In Bruna et al. (2014); Defferrard et al. (2016); Levie et al. (2017), the convolution operation was defined using the convolution theorem and filtering operation in the spectrum domain by computing the eigendecomposition of the normalized Laplacian matrix of the graph. The Laplacian matrix $\mathbf{L}$ is defined as $\mathbf{L} = \mathbf{D} - \mathbf{A}$ with the further assumption that $\mathbf{A}$ is symmetric to guarantee that $\mathbf{L}$ is positive semi-definite. The convolution defined by the multiplication in the spectrum domain is approximated by Defferrard et al. (2016) by

$$\mathbf{U} g_\theta \mathbf{U}^T \mathbf{x} \approx \sum_{k=0}^{K} \theta_k T_k \left[\frac{2}{\lambda_{\max}} \mathbf{L} - \mathbf{I} \right] \mathbf{x}_c^{(\ell)}, \tag{6}$$

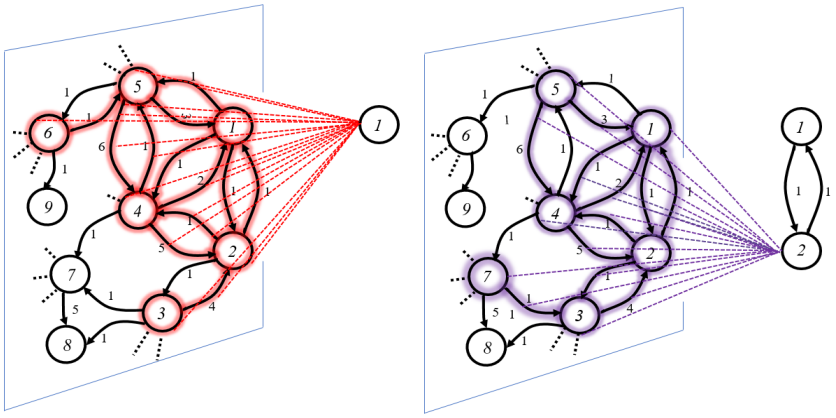

Figure 2: An example of a directed graph with weights along directed edges corresponding to $\mathbf{A}$. The parts with glow on left(right)-hand-side represent filters at different locations. The figure on the left-hand-side denotes the filtering/convolution starting from vertex 1, then the filter slides to vertex 2 as shown on the right-hand-side with filter topology adaptive to the new local region.

where $T_k[\cdot]$ is the kth order matrix Chebyshev polynomial (Shuman et al., 2013) where

$$T_k(\mathbf{L}) = 2\mathbf{L}T_{k-1}[\mathbf{L}] - T_{k-2}[\mathbf{L}], \tag{7}$$

with the initial values defined as $T_0[\mathbf{L}] = \mathbf{I}$ and $T_1[\mathbf{L}] = \mathbf{L}$. We refer later to this method as ChebNet for performance comparison. Note that the Laplacian matrix can be seen as a differentiator operator. The assumption of symmetric $\mathbf{A}$ restricts the application to undirected graphs. Note that in Defferrard et al. (2016), Laplacian matrix polynomials with maximum order $K = 25$ is needed to approximate the convolution operation on the left-hand side in (6), which imposes the computational burden. While TAGCN only needs an adjacency matrix polynomials with maximum order 2 to achieve better performance as shown in the experiment part.

In Kipf & Welling (2017), a graph convolutional network (GCN) was obtained by a first order approximation of (6). In particular, let $K = 1$ and make the further assumptions that $\lambda_{\max} = 2$ and $\theta_0 = \theta_1 = \theta$. Then a simpler convolution operator that does not depend on the spectrum knowledge is obtained as

$$\mathbf{U}g_\theta\mathbf{U}^T\mathbf{x} \approx \sum_{k=0}^{1}\theta_k T_k\left[\frac{2\mathbf{L}}{\lambda_{\max}} - \mathbf{I}\right]\mathbf{x}_c^{(\ell)} \approx \theta(\mathbf{I} + \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}})\mathbf{x}_c^{(\ell)}.$$

Note that $\mathbf{I} + \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}$ is a matrix with eigenvalues in $[0, 2]$. A renormalization trick is adopted here by letting $\widetilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}$ and $\widetilde{\mathbf{D}}_{i,i} = \sum_j \widetilde{\mathbf{A}}_{i,j}$. Finally, the convolutional operator is approximated by

$$\mathbf{U}g_\theta\mathbf{U}^T\mathbf{x} \approx \theta\widetilde{\mathbf{D}}^{-\frac{1}{2}}\widetilde{\mathbf{A}}\widetilde{\mathbf{D}}^{-\frac{1}{2}}\mathbf{x}_c^{(\ell)} = \theta\widehat{\mathbf{A}}, \tag{8}$$

where $\widehat{\mathbf{A}} = \widetilde{\mathbf{D}}^{-\frac{1}{2}}\widetilde{\mathbf{A}}\widetilde{\mathbf{D}}^{-\frac{1}{2}}$. It is interesting to observe that this method though obtained by simplifying the spectrum method has a better performance than the spectrum method (Defferrard et al., 2016). The reason may be because the simplified form is equivalent to propagating vertex features on the graph, which can be seen as a special case of our TAGCN method, though there are other important differences.

As we analyzed in Section 2.2, GCN as in (8) or even extending it to higher order, i.e., $\theta\widehat{\mathbf{A}}^k$ only project the input data to the graph eigenvector of the largest eigenvalue when the convolutional layers go deeper.

Our TAGCN is able to leverage information at a farther distance, but it is not a simple extension of GCN Kipf & Welling (2017). First, the graph convolution in GCN is defined as a first order Chebyshev polynomial of the graph Laplacian matrix, which is an approximation to the graph convolution defined in the spectrum domain in Defferrard et al. (2016). In contrast, our graph convolution is

rigorously defined as multiplication by polynomials of the graph adjacency matrix; this is not an approximation, rather, it simply is filtering with graph filters as defined and as being consistent with graph signal processing.

Next, we show the difference between our work and the GCN method in Kipf & Welling (2017) when using 2nd order (K=2, 2 steps away from the central node) Chebyshev polynomials of Laplacian matrix. In the GCN paper Kipf & Welling (2017), it has been shown that $\sum_{k=0}^{1} \theta_k T_k(\mathbf{L}) \approx \widehat{\mathbf{A}}$ as repeated in (8), and $T_2[\mathbf{L}] = 2\mathbf{L}^2$ by the definition of Chebyshev polynomial. Then, extending GCN to the second order Chebyshev polynomials (two steps away from a central node) can be obtained from the original definition in T. Kipfs GCN (Kipf & Welling, 2017, eqn (5)) as $\sum_{k=0}^{2} \theta T_k(L) = \widehat{\mathbf{A}} + 2\mathbf{L}^2 - \mathbf{I}$, which is different from our definition as in (2). Thus, it is evident that our method is not a simple extension of GCN. We apply graph convolution as proposed from basic principles in the graph signal processing, with no approximations involved, while both GCN in Kipf & Welling (2017) and Defferrard et al. (2016) Levie et al. (2017) are based on approximating the convolution defined in the spectrum domain. In our approach, the degree of freedom is the design of the graph filter-its degree and its coefficients. Ours is a principled approach and provides a generic methodology. The performance gains we obtain are the result of capturing the underlying graph structure with no approximation in the convolution operation.

Simonovsky & Komodakis (2017) proposed the edge convolution network (ECC) to extend the convolution operator from regular grids to arbitrary graphs. The convolution operator is defined similarly to (8) as

$$\mathbf{y}_f^{(\ell)}(i) = \sum_{j \in \mathcal{N}(i)} \frac{1}{|\mathcal{N}(i)|} \mathbf{\Theta}_{j,i}^{(\ell)} \mathbf{x}_c^{(\ell)}(j) + b_f^{(\ell)},$$

with $\mathbf{\Theta}_{j,i}^{(\ell)}$ is the weight matrix that needs to be learned.

A mixture model network (MoNet) was proposed in Monti et al. (2017), with convolution defined as

$$\mathbf{y}_f^{(\ell)}(i) = \sum_{f=1}^{F} \sum_{j \in \mathcal{N}(i)} g_f \kappa_f \mathbf{x}_c^{(\ell)}(j),$$

where κ_f is a Gaussian kernel with $\kappa_f = \exp\left\{-\frac{1}{2}(\mathbf{u} - \boldsymbol{\mu}_f)^T \mathbf{\Sigma}_f^{-1} (\mathbf{u} - \boldsymbol{\mu}_f)\right\}$ and g_f is the weight coefficient for each Gaussian kernel κ_f. It is further assumed that $\mathbf{\Sigma}_f$ is a 2×2 diagonal matrix.

GCN, ECC, and MoNet all design a propagation model on the graph; their differences are on the weightings used by each model.

Atwood & Towsley (2016) proposed a diffusion CNN (DCNN) method that considers a diffusion process over the graph. The transition probability of a random walk on a graph is given by $\mathbf{P} = \mathbf{D}^{-1}\mathbf{A}$, which is equivalent to the normalized adjacency matrix.

$$\mathbf{y}_{c,f}^{(\ell)} = \mathbf{g}_{c,f}^{(\ell)} \mathbf{P}^f \mathbf{x}_c^{(\ell)}.$$

By comparing the above methods with TAGCN in (5), it can be concluded that GCN, ECC and MoNet can be seen as a special case of TAGCN because in (5) the item with $k = 1$ can be seen as an information propagation term. However, as shown in Section 2.2, when the convolutional layers go deeper, the output of the last convolutional layer of GCN, ECC and MoNet are all linear approximations of the output of the corresponding first convolutional layer which degradates the representation capability. TAGCN overcomes this by designing a set of fixed size filters that is adaptive to the input graph topology when performing convolution on the graph. Further, compared with existing spectrum methods (Bruna et al., 2014; Defferrard et al., 2016; Levie et al., 2017), TAGCN satisfies the convolution theorem as shown in the previous subsection and implemented in the vertex domain, which avoids performing costly and practically numerical unstable eigendecompositions.

We further compare the number of weights that need to be learned in each hidden layer for these different methods in Table 1. As we show later, $K = 2$ is selected in our experiments using cross validation. However, for ChebNet in (Defferrard et al., 2016), it is suggested that one needs a 25th degree Chebyshev polynomial to provide a good approximation to the graph Laplacian spectrum. Thus we have a moderate number of weights to be learned. In the following, we show that our method achieves the best performance for each of those commonly used graph-structured data sets.

Table 1: Number of weights need to be learned for the ℓ-th layer.

DCNN	ECC	ChebNet	GCN	MoNet	TAGCN
$F_\ell C_\ell$	$F_\ell C_\ell$	$25F_\ell C_\ell$	$F_\ell C_\ell$	$4F_\ell C_\ell$	$2F_\ell C_\ell$

Table 2: Dataset statistics, following Yang et al. (2016)

Dataset	Nodes	Edges	Classes	Features	Label Rate
Pubmed	19,717	44,338	3	500	0.003
Citeseer	3,327	4,732	6	3,703	0.036
Cora	2,708	5,429	7	1,433	0.052

4 EXPERIMENTS

The proposed TAGCN is general and can be fit to the general graph CNN architectures for different tasks. In the experiments, we focus on the vertex semisupervised learning problem, where we have access to only a few labeled vertices, and the task is to classify the remaining unlabeled vertices. To compare the performance of TAGCN with that of existing methods, we extensively evaluate TAGCN on three graph-structured datasets, including the Cora, Citesser and Pubmed datasets. The datasets split and experiments setting closely follow the standard criteria in Yang et al. (2016).

In each data set, the vertices are the documents and the edges are the citation links. Each document is represented by sparse bag-of-words feature vectors, and the citation links between documents are provided. Detailed statistics of these three data sets are summarized in Table 2. It shows the number of nodes and edges that corresponding to documents and citation links, and the number of document classes in each data set. Also, the number of features at each vertex is given. Label rate denotes the number of labeled documents that are used for training divided by the total number of documents in each data set.

4.1 EXPERIMENTAL SETTINGS

We construct a graph for each data set with nodes representing documents and undirected edges[5] linking two papers if there is a citation relationship. We obtain the adjacency matrix $\bar{\mathbf{A}}$ with 0 and 1 components and further obtain the normalized matrix $\mathbf{A}$.

In the following experiments, we design a TAGCN with two hidden layers (obtained from cross validation) for the semi-supervised node classification. In each hidden layer, the proposed TAGCN

[5]We use undirected graphs here as citation relationship gives positive correlation between two documents. However, in contrast with the other approaches surveyed here, the TAGCN method is not limited to undirected graphs if directed graphs are better suited to the applications.

Table 3: Summary of results in terms of percentage classification accuracy with standard variance

Dataset	Pubmed	Citeseer	Cora
DeepWalk	65.3	43.2	67.2
Planetoid	77.2	64.7	75.7
DCNN	73.0±0.5	-	76.8±0.6
ChebNet	74.4	69.8	79.5
GCN	79.0	70.3	81.5
MoNet	78.81±0.4	-	81.69±0.5
GAT	79.0±0.3	**72.5± 0.7**	83.0±0.7
TAGCN (ours)	**81.1±0.4**	71.4± 0.5	**83.3±0.7**

is applied for convolution, followed by a ReLU activation. 16 hidden units (filters) are designed for each hidden layer, and dropout is applied after each hidden layer. The softmax activation function is applied to the output of the second hidden layer for the final classification. For ablation study, we evaluate the performance of TAGCN with different filter sizes from 1 to 4. To investigate the performance for different number of parameters, we also design a TAGCN with 8 filters for each hidden layer and compare its classification accuracy with all the baselines and TAGCN with 16 filters. We train our model using Adam (Kinga & Ba, 2015) with a learning rate of 0.01 and early stopping with a window size of 45. Hyperparameters of the networks (filter size, dropout rate, and number of hidden layers) are selected by cross validation.

To make a fair comparison, we closely follow the same split of training, validation, and testing sets as in Kipf & Welling (2017); Yang et al. (2016), i.e., 500 labeled examples for hyperparameters (filter size, dropout rate, and number of hidden layers) optimization and cross-entropy error is used for classification accuracy evaluation. The performance results of the proposed TAGCN method are an average over 100 runs.

4.2 Quantitative Evaluations

We compare the classification accuracy with other recently proposed graph CNN methods as well as a graph embedding methods known as DeepWalk and Planetoid **?**Yang et al. (2016). The recent published graph attention networks (GAT) **?** leveraging masked self-attentional layers is also compared.

The quantitative results are summarized in Table 3. Reported numbers denote classification accuracy in percentage. Results for DeepWalk, Planetoid, GCN, and ChebNet are taken from Kipf & Welling (2017), and results for DCNN and MoNet are taken from Monti et al. (2017). All the experiments for different methods are based on the same data statistics shown in Table 2. The datasets split and experiments settings closely follow the standard criteria in Yang et al. (2016); Kipf & Welling (2017). Table 3 shows that our method outperforms all the recent state-of-the-art graph CNN methods (DCNN, ChebNet, GCN, MoNet) by obvious margins for all the three datasets.

These experiment results corroborate our analyses in Section 2.2 and Section 3 that as no approximation to the convolution is needed in TAGCN, it achieves better performance compared with spectrum approximation method such as ChebNet and GCN. Further, using a set of size-1 up to size-2 filters avoids the linear approximation by the simply size-1 filter ($\mathbf{A}$ in GCN Kipf & Welling (2017)), which further verify the efficacy of the proposed TAGCN. Compared with the most recent GAT method **?**, our method exhibit obvious advantage for the largest dataset Pubmed. It should be note that GAT suffers from storage limitation in their model and not scale well for large-scale graph as explained by the authors.

For ablation study, we further compare the performance of different filter sizes from $K = 1$ to $K = 4$ in Table 4. It shows that the performances for filter size $K = 2$ are always better than that for other filter sizes. The value $K = 1$ gives the worst classification accuracy. As $K = 1$ the filter is a monomial, this further validates the analysis in Section 2.2 that monomial filter results in a very rough approximation. In Table 4, we also compare the performance of different number of filters, which reflects different number of network parameters. Note, we also choose filer size $K = 2$ and filter number $F_\ell = 8$ that results in the same number of network parameters as that in GCN, MoNet, ECC and DCNN according to Table 1. It shows that the classification accuracy using 8 filters is comparable with that using 16 filters in each hidden layer for TAGCN. Moreover, TAGCN with 8 filters can still achieve higher accuracy than GCN, MoNet, ECC and DCNN methods. This proves that, even with a similar number of parameters or architecture, our method still exhibits superior performance than GCN.

As we analyzed and explained in Section 2.2 and Section 3, TAGCN in our paper is not simply extending GCN Kipf & Welling (2017) to k-th order. Nevertheless, we implement $\mathbf{A}^2$ and compare its performance with ours. For the data sets Pubmed, Cora, and Citeseer, the classification accuracies are $79.1(80.8)$, $81.7(83.0)$ and $70.8(71.2)$, where the numbers in parentheses are the results obtained with our method. Our method still achieves a noticeable performance advantage over $\mathbf{A}^2$; in particular, we note the significant performance gain with the Pubmed database that has the largest number of nodes among these three data sets.

Table 4: TAGCN classification accuracy (ACC) with different parameters

Data Set	Filter Size	Filter Number	ACC
Citeseer	1	16	68.9
	2	16	**71.4**
	3	16	70.0
	4	16	69.8
	2	**8**	**71.2**
Cora	1	16	81.4
	2	16	**83.3**
	3	16	82.1
	4	16	81.8
	2	**8**	**83.0**
Pubmed	1	16	79.4
	2	16	**81.1**
	3	16	80.9
	4	16	79.5
	2	**8**	**80.8**

5 CONCLUSIONS

We have defined a novel graph convolutional network that rearchitects the CNN architecture for graph-structured data. The proposed method, known as TAGCN, is adaptive to the graph topology as the filter scans the graph. Further, TAGCN inherits properties of the convolutional layer in classical CNN, i.e., local feature extraction and weight sharing. On the other hand, by the convolution theorem, TAGCN that implements in the vertex domain offers implement in the spectrum domain unifying graph CNN in both the spectrum domain and the vertex domain. TAGCN is consistent with convolution in graph signal processing. These nice properties lead to a noticeable performance advantage in classification accuracy on semi-supervised graph vertex classification problems with low computational complexity.

6 APPENDIX: SPECTRUM RESPONSE OF TAGCN

In classical signal processing (Oppenheim & Schafer, 2009), the convolution in the time domain is equivalent to multiplication in the spectrum domain. This relationship is known as the convolution theorem. Sandryhaila & Moura (2013) showed that the graph filtering defined in the vertex domain satisfies the generalized convolution theorem naturally and can also interpret spectrum filtering for both directed and undirected graphs. Recent work (Bruna et al., 2014; Defferrard et al., 2016) used the convolution theorem for undirected graph-structured data and designed a spectrum graph filtering.

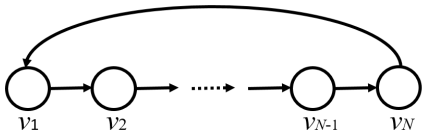

Figure 3: Graph topology of a 1-D cyclic graph.

Assume that the adjacency matrix $\mathbf{A}$ for a graph is diagonalizable, i.e., $\mathbf{A} = \mathbf{F}^{-1}\mathbf{J}\mathbf{F}$ with $\mathbf{J}$ a diagonal matrix. The components on the diagonal of $\mathbf{J}$ are eigenvalues of $\mathbf{A}$, and the column vectors of $\mathbf{F}^{-1}$ are the right eigenvectors of $\mathbf{A}$; the row vectors of $\mathbf{F}$ are the left eigenvectors of $\mathbf{A}$ [6]. By diagonalizing

[6] When $\mathbf{A}$ is not diagonalizable, the columns of $\mathbf{F}^{-1}$ and the rows of $\mathbf{F}$ are the generalized right and left eigenvectors of $\mathbf{A}$, respectively. In this case, $\mathbf{F}$ is no longer a unitary matrix. Also, $\mathbf{J}$ is a block diagonal matrix;

$\mathbf{A}$ in (2) for TAGCN, we obtain

$$\mathbf{G}_{c,f}^{(\ell)}\mathbf{x}_c^{(\ell)} = \mathbf{F}^{-1}\left(\sum_{k=0}^{K} g_{c,f,k}^{(\ell)}\mathbf{J}^k\right)\mathbf{F}\mathbf{x}_c^{(\ell)}. \tag{9}$$

The expression on the left-hand-side of the above equation represents the filtering/convolution on the vertex domain. Matrix $\mathbf{F}$ defines the graph Fourier transform (Sandryhaila & Moura, 2013; 2014), and $\mathbf{F}\mathbf{x}_c^{(\ell)}$ is the input feature spectrum map, which is a linear mapping from the input feature on the vertex domain to the spectrum domain. The polynomial $\sum_{k=0}^{K} g_{c,f,k}^{(\ell)}\mathbf{J}^k$ is the spectrum of the graph filter. Relation (9), which is equation (27) in Sandryhaila & Moura (2013) generalizes the classical convolution theorem to graph-structured data: convolution/filtering on the vertex domain becomes multiplication in the spectrum domain. When the graph is in the 1D cyclic form, as shown in Fig. 3, the corresponding adjacency matrix is of the form

$$\mathbf{A} = \begin{bmatrix} & & & 1 \\ 1 & & & \\ & \ddots & & \\ & & 1 & \end{bmatrix}.$$

The eigendecomposition of $\mathbf{A}$ is

$$\mathbf{A} = \frac{1}{N}\mathrm{DFT}^{-1}\begin{bmatrix} e^{-j\frac{2\pi 0}{N}} & & \\ & \ddots & \\ & & e^{-j\frac{2\pi(N-1)}{N}} \end{bmatrix}\mathrm{DFT},$$

where DFT is the discrete Fourier transform matrix. The convolution operator defined in (2) is consistent with that in classical signal processing.

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