Cross-GCN: Enhancing Graph Convolutional Network with $k$-Order Feature Interactions

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Abstract—Graph Convolutional Network (GCN) is an emerging technique that performs learning and reasoning on graph data. It operates feature learning on the graph structure, through aggregating the features of the neighbor nodes to obtain the embedding of each target node. Owing to the strong representation power, recent research shows that GCN achieves state-of-the-art performance on several tasks such as recommendation and linked document classification. Despite its effectiveness, we argue that existing designs of GCN forgo modeling cross features, making GCN less effective for tasks or data where cross features are important. Although neural network can approximate any continuous function, including the multiplication operator for modeling feature crosses, it can be rather inefficient to do so (i.e., wasting many parameters at the risk of overfitting) if there is no explicit design. To this end, we design a new operator named Cross-feature Graph Convolution, which explicitly models the arbitrary-order cross features with complexity linear to feature dimension and order size. We term our proposed architecture as Cross-GCN, and conduct experiments on three graphs to validate its effectiveness. Extensive analysis validates the utility of explicitly modeling cross features in GCN, especially for feature learning at lower layers.

Index Terms—Cross-Feature, Graph-based Learning, Graph Neural Networks

1 INTRODUCTION

As a data structure, graph has been intensively used in information retrieval applications, ranging from search engines [1], digital libraries [2], to recommender systems [3], [4] and question-answering systems [4]. For example, in Web search, the structure of Web-page graph has been mined to estimate the page importance [6]. in recommender systems, the interaction graph between users and items provides rich signal about collaborative filtering [4]. Along with the trend of deep learning, research on graph mining has been shifted from structure understanding to representation learning (aka. feature learning) [7], which offers a universal way to perform predictive analytics (e.g., node classification, and link prediction) on discrete and high-dimensional graph data.

Owing to the extraordinary representation ability, Graph Convolutional Networks (GCNs) have become a promising solution for representation learning over graphs [8], [9], [10]. Generally, GCNs learn node representations in a low-dimensional latent space from raw input features and node connections with multiple graph convolutional layers. As shown in Figure 1(a), a traditional GCN layer typically contains two components: node aggregation module and feature transformation module. The node aggregation module augments the representation of a targeted node via fusing information from its connected nodes based on the assumption that the properties of connected nodes would also reflect the property of the target node. The feature transformation module transforms the input features into higher-level hidden features that better describe the node. Current research on GCNs mainly focuses on developing node aggregation modules emphasizing different connection properties such as local similarity [8], multi-hop connectivity [11], and structural similarity [12], nevertheless, while simply performs feature transformation with matrix mapping.

We argue that existing GCN layers are hardly able to capture cross features [13], which are essential for the success of many graph applications [14], [15], [16], [17]. For example, by capturing a cross feature: gender= female & age=[20,25] & in-

1. In the following, we interchangeably use feature interaction and cross feature.
Fig. 2. Training (left) and testing (right) accuracy on a citation graph (described in Section 4.1.1) of GCN (two layers) with original features and cross features as inputs.

come= $10,000/month, a recommender system could obtain better user representation and make more accurate product recommendations (e.g., whether to purchase the latest version of iPhone) [18]. To date, the simple matrix mapping used in most existing GCN layers, while equipped with non-linear activation, can hardly capture such cross features. As such, despite the extraordinary ability of GCNs to incorporate connection properties, we argue that their representation ability could be substantially improved by sharpening the feature transformation module to also encode cross features.

Figure 2 provides an empirical evidence on the weak ability of GCN in capturing cross features. We train a two-layer GCN on a citation graph with raw features and cross features as inputs, respectively. As can be seen, for node classification, training GCN with cross features achieves much higher accuracy on both training and testing sets than training with original features. It validates that explicitly considering cross features can enhance the representation ability of GCNs. Nevertheless, heuristic methods that either manually construct and select cross features or brutally enumerate all interactions are unaffordable for many real-world graphs with a large number of features, which motivates us to develop new graph convolution operations with feature interactions considered in GCN.

The main challenge of modeling cross feature is efficiency since the number of cross features grows dramatically with feature dimension. To tackle this challenge, we first devise a new operator named Cross-feature Graph Convolution. The new operator contributes a new feature transformation module encoding cross features at arbitrary orders with a complexity linear to the feature dimension and order size. Thereafter, we develop a new solution for graph-based representation learning, named Cross-GCN (illustrated in Figure 1(b)), by stacking multiple Cross-feature Graph Convolutional layers. Experiments on three graphs of node classification demonstrate the remarkable effectiveness of Cross-GCN. Moreover, Cross-GCN achieves more significant improvements on data with sparse low-level features, indicating its proper application scenarios.

The main contributions of this paper are summarized as:

- We devise a new graph-oriented operator, Cross-feature Graph Convolution, which explicitly captures arbitrary-order feature interactions with linearly increased parameters and computation complexity.
- By equipping the Cross-feature Graph Convolution operator, we develop a new graph-based learning solution, named Cross-GCN, which has the same model, computation, and memory complexity as vanilla GCN.
- With node classification as the testing task, we conduct experiments on three graphs and demonstrate the effectiveness of the proposed Cross-GCN (implementation will be released upon acceptance).

In the remainder of this paper, Section 2 introduces preliminary knowledge about GCN and cross feature. In Section 3 we elaborate the methodology followed by discussion of experiments and related work in Section 4 and Section 5, respectively. Lastly, we conclude the paper, and envision some future work in Section 6.

## 2 PRELIMINARY

We first introduce some notions used in the following sections. We use bold capital letters (e.g., $\mathbf{X}$) and bold lowercase letters (e.g., $\mathbf{x}$) to denote matrices and vectors, respectively. In addition, bold capital script letters (e.g., $\mathcal{X}$) are used to represent tensors. Note that all vectors are in a column form if not otherwise specified, and $X_{ij}$ denotes the entry of matrix $\mathbf{X}$ at the row $i$ and column $j$. Lastly, element-wise product and tensor outer product are denoted as $\odot$ and $\otimes$, respectively. In Table 1 we summarize some of the terms and notations.

### 2.1 Graph Convolutional Networks

A graph with $N$ nodes is typically represented as an adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$ associated with a feature matrix $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N]^T \in \mathbb{R}^{N \times D}$. $\mathbf{A}$ is a binary matrix, where $A_{ij} = 1$ if there is an edge between node $i$ and $j$, otherwise $A_{ij} = 0$. $D$ is the dimension of the input features which varies in a wide range from hundreds to millions in different applications. Taking the graph data as inputs, each GCN layer learns node representations in a low-dimensional embedding space (the last layer makes predictions) [8], [9], [10]. Note that a node feature in a latent layer is one dimension of previous layer’s output. In the first layer, a node feature is one of the raw node features (i.e., one dimension of $\mathbf{x}$). To simplify the notations and presentation, in the following, we always take the first layer as example to elaborate the detail of a GCN layer.

As shown in Figure 1(a), a GCN layer mainly performs two operations: node aggregation and feature transformation, to learn

| Symbol | Definition |
|--------|------------|
| $\mathbf{X} \in \mathbb{R}^{N \times D}$ | features of $N$ nodes. |
| $\mathbf{Y} \in \mathbb{R}^{M \times L}$ | labels of $M$ nodes. |
| $\mathbf{A} \in \mathbb{R}^{N \times N}$ | adjacency matrix of a graph. |
| $\mathbf{D} \in \mathbb{R}^{N \times N}$ | degree matrix of a graph. |
| $\text{neighbor}(\mathbf{x})$ | neighbors of a node. |
| $\mathcal{F}$ | feature transformation operation. |
| $\mathcal{N}$ | node aggregation operation. |
| $f^k(\cdot)$ | $k$-order cross-feature transformation function. |
| $\mathbf{x}^k_{1i12\cdots i_k}$ | a $k$-order cross feature. |
| $h^k \in \mathbb{R}^E$ | a $k$-order tensor of cross features. |
| $\mathbf{W}, \mathbf{b}$ | hidden vector encodes $k$-order cross features. |
| $\Theta$ | parameters for 1-order feature transformation. |
| $\odot$ | all model parameters. |
| $\otimes$ | element-wise product. |
| $\circ$ | tensor outer product. |
| $\sigma$ | a non-linear activation function. |
node representations. For a target node, a GCN layer can be abstracted as:

\[ x = \mathcal{N}(\{x_n|n \in \text{neighbor}(x)\}), \quad h = \mathcal{F}(x), \]

where \( \mathcal{F} \) and \( \mathcal{N} \) denote the feature transformation and node aggregation operations, respectively. \( x \in \mathbb{R}^D \) is the feature representation of the target node after aggregating neighbor node features. \( h \in \mathbb{R}^E \) is the latent representation of the target node.

Node aggregation enriches the representation of a target node by aggregating information from its neighbor nodes. The rationale is that the properties of neighbor nodes could reflect the properties of a target node. For instance, in a social network, having connections with many nodes with male gender and interests in playing video games indicates that the target node might be a teenager boy. Note that \( \text{neighbor}(x) \) could also include the target node since self-connections \( \mathcal{N} \) are typically intentionally added. Research on GCN has been focusing on developing different formats of \( \mathcal{N} \) to distill distinct information from \( \text{neighbor}(x) \) \[8\], \[9\], \[10\]. For instance, an average pooling filter out common properties from combinations with many nodes with male gender and interests in playing video games indicates that the target node might be a teenager boy.

2.2 Cross Feature

A \( k \)-order cross feature (aka. feature interaction) is a combination of \( k \) input features \[13\], which could be formulated as:

\[ x_{i_1i_2\ldots i_k}^k = \prod_{i \in \{i_1i_2\ldots i_k\}} x_i, \]

where \( x_i \) is the \( i \)-th dimension of the input features. For instance, a 3-order feature interaction could happen on three input features: \( \text{gender} \), \( \text{age} \), and \( \text{income} \). Such feature interaction could categorize users into more subgroups and might benefit the modeling of user profiles such as interests \[13\]. Given a feature vector \( x \in \mathbb{R}^D \) with \( D \) features, we consider all \( k \)-order crosses among the \( D \) features, which can be organized into a \( k \)-order tensor:

\[ \mathcal{X}^k = x \otimes \cdots \otimes x \in \mathbb{R}^{D \times \cdots \times D}. \]

Similar as Equation 2, a \( k \)-order cross-feature transformation calculates \( E \) hidden features from all the cross features in \( \mathcal{X}^k \). For the \( e \)-th hidden feature, the formulation is:

\[ h^k_e = \sigma \left( \text{sum}(\mathcal{X}^k \odot W^k_e) + b_e \right), \]

where \( W^k_e \) is a \( k \)-order tensor of parameters with the same size as \( \mathcal{X}^k \) to perform the transformation. Note that \( W^k_e \) would become the \( w^k_e \) in Equation 2 when \( k = 1 \). \( b_e \) is the bias for the \( e \)-th hidden feature. \text{sum} is a summation over all entries of a tensor. The computational complexity of the transformation is \( O(D^k) \), which makes it is unaffordable when \( D \) is large. Therefore, the key research challenge of cross-feature transformation is to devise an elegant mechanism that reduces the complexity while maintaining the representation capability. In the following, we omit the activation function \( \sigma \) and the bias \( b \) to simplify the presentation.

3 Cross-GCN

In this section, we elaborate the detail of the proposed Cross-feature Graph Convolution operator in Section 3.1 followed by its complexity analysis in Section 3.2. Lastly, we discuss the advantages of the proposed operator over existing solutions for modeling cross features in GCN.

3.1 Cross-feature Graph Convolution

The proposed operator Cross-feature Graph Convolution follows the general formulation of a GCN layer (Equation 1). That is to say, the operator also performs two operations: node aggregation and feature transformation, to learn hidden node representations.

- To efficiently and appropriately encode cross features, we devise a new cross-feature transformation module, which could calculate cross-feature transformation at arbitrary orders with complexity linear to feature dimension and order size.
- As our main target is to model cross features, we employ the node aggregation modules in existing GCNs. For instance, we could use the average pooling \[9\], LSTM \[9\], and Attention Networks \[19\].

3.1.1 Cross-feature Transformation Module

Incorporating cross features has been found to achieve significant success in many applications such as search engines \[14\], QA systems \[16\] and recommender systems \[13\]. This is because the cross features could enrich the representation of a wide range of entities including Web articles and user-item pairs. Inspired by its success, Cross-feature Graph Convolution performs cross-feature transformation with order size up to \( K \) to incorporate cross features. That is to say, the cross-feature transformation module simultaneously performs cross-feature transformations at orders from 1 to \( K \), and fuses the outputs of the \( K \) transformations into an overall output.

The key novelty of the proposed module is enabling cross-feature transformation in a linear complexity. Instead of directly evaluating Equation 3 which has a polynomial complexity of \( O(D^k) \), we propose a new operator by performing cross feature transformation in a recursive way:

\[ h^k = f^k(x) = (W^k x) \odot f^{k-1}(x), \quad \text{and } f^0(x) = 1. \]

\( x \in \mathbb{R}^D \) and \( h^k \in \mathbb{R}^E \) denotes the inputs and outputs of the \( k \)-order cross-feature transformation module, respectively. \( W^k \in \mathbb{R}^{E \times D} \). It is worthwhile to mention that we could also model feature interaction in node aggregation. That is to say, we consider interactions among different nodes. For simplicity, in this work, we only model feature interaction in feature transformation and will explore feature interaction in node aggregation in future work.
$R^{E \times D}$ is a matrix of transformation parameters. $f^k(\cdot)$ denotes a k-order cross-feature transformation function which encodes k-order cross features into a hidden vector $h^k \in R^E$. For instance, $f^2(x) = (W^2x) \odot (W^1x)$ performs the 2-order cross-feature transformation.

In the next, we prove that the proposed Equation 6 provides a low-rank approximation to the k-order cross-feature transformation of Equation 5.

**Theorem.** Let $C : R^D \to R^E$ be a k-order cross-feature transformation $h^k = C(x)$, which calculates each output dimension $h^k$ as: $h^k = \sum (\mathcal{X}^k \odot W^k)$ (Equation 3). We have: $C(x) \approx (W^x) \odot \cdots \odot (W^1x)$ where $W^k \in R^{E \times D}$.

**Proof.** To facilitate understanding, we first take the cross-feature transformation at second-order as an example to present the derivation. Originally, 2-order cross-feature transformation (Equation 3) calculates a hidden feature as:

$$h^2 = \sum (\mathcal{X}^2 \odot W^2) = \sum ((x^x) \odot W) \tag{7}$$

where $W \in R^{D \times D}$ is the mapping matrix. Note that $h^2$ is just one dimension of $h^2 \in R^E$. In total, the number of needed parameters to calculate $h^2$ would be $E \cdot D^2$. The key of accelerating the transformation is to reduce the number of parameters. According to the theory of matrix factorization [20], we can decompose parameter matrix ($W$) into latent factors $w$ and $\bar{w} \in R^D$ such as $W \approx w \bar{w}^T$. Subsequently, we can approximate Equation 7 as:

$$h^2 \approx \sum ((x^x) \odot (w \bar{w}^T)) = \sum ((w \odot x)(\bar{w} \odot x)^T). \tag{8}$$

Furthermore, we can transform it into:

$$h^2 \approx \sum_{i=1}^{D} \sum_{j=1}^{D} w_i x_i \odot \bar{w}_j x_j = \sum_{i=1}^{D} w_i x_i \odot \sum_{j=1}^{D} \bar{w}_j x_j = \sum_{i=1}^{D} w_i x_i \odot (\bar{w}^T x) = (\bar{w}^T x)(\bar{w}^T x) \tag{9}$$

Following the same procedure, we can transform the calculation of all $E$ hidden features into the format based on latent factors (i.e., $(\bar{w}^T x)(\bar{w}^T x)$). In total, we need $E$ pairs of latent factors. By organizing the latent factors into two parameter matrices $W$ and $\bar{W} \in R^{E \times D}$ (one row for each hidden feature), the 2-order cross-feature transformation can be transformed into:

$$h^2 = (W^x) \odot (\bar{W}^x), \tag{10}$$

which has the same form as the proposed transformation module $h^2 = f^2(x) = (W^2x) \odot (W^1x)$.

**k-order ($k \geq 2$).** For a k-order cross-feature transformation, directly calculating a hidden feature needs the number of $D^k$ parameters ($\mathcal{W}^k$ in Equation 3). By extending the matrix factorization to canonical tensor factorization [21], we can factorize $\mathcal{W}^k$ into $k$ vectors of latent factors with dimension of $D$: $\{w^1, \cdots, w^K\}$ subject to $\mathcal{W}^k \approx w^1 \otimes \cdots \otimes w^K$. Following Equations 8 and 9, we can calculate $h^k$ by:

$$h^k = \sum (\mathcal{X}^k \odot \mathcal{W}^k) = \sum ((w^k \odot x) \otimes (w^l \odot x)) = (w^k \bar{w}^T x) \odot \cdots \odot (w^1 \bar{w}^T x), \tag{11}$$

where the number of parameters is $kD$. Similarly, we use $E$ sets of latent factors to calculate $E$ hidden features. We organize the latent factors into $k$ different matrices, and obtain: $h^k = (W^kx) \odot \cdots \odot (W^1x)$ which is the proposed $f^k(x)$.

It is worthwhile to emphasize that the proposed module does not explicitly conduct the decomposition — instead of learning a costly k-order tensor $\mathcal{W}^k \in R^{D \times \cdots \times D}$, we learn $k$ latent vectors $\{w^1, \cdots, w^K\}$, which can be seen as approximating $\mathcal{W}^k$ with canonical tensor factorization [21].

### 3.1.2 Order Aggregation

Research on cross features has shown that cross features in different orders might have different impacts on the prediction [13]. In other words, in the cross-feature transformation, hidden features transformed from cross features at different orders might contribute differently to the output. As such the cross-feature transformation module further performs order aggregation which is denoted as a function $a(\cdot)$. The order aggregation function $a(\cdot)$ first aggregates hidden features transformed from interactions at different orders ($\{h^k|k = 1, \cdots, K\}$) into a single vector. We can perform the aggregation using many operations such as a pooling function (e.g., mean pooling) or a neural modeling component (e.g., LSTM [22]). After aggregation, $a$ then adds bias and performs non-linear activation on the hidden vector to obtain the output ($h$).

In this work, to avoid introducing additional model parameters, we simply implement the order aggregation function $a(\cdot)$ as:

$$h = a(\{h^k|k = 1, \cdots, K\}) = \sigma \left( \sum_{k=1}^{K} \alpha_k h^k \right) + b. \tag{12}$$

$\alpha_k$ regulates the information from k-order cross features flowing into the final node representation. When assigned with a larger value, the k-order cross features contribute more to the final output $h$. We leave the exploration of advanced implementations of $a(\cdot)$ to future work since this work is focused on the cross-feature transformation.

### 3.2 Complexity Analysis

For practical applications, in addition to effectiveness, the usability of a neural network operator also depends on three complexity criteria: 1) model complexity, 2) computation complexity, and memory complexity. As such, we carefully analyze the complexity of the proposed cross-feature transformation module. Note that we omit the cost of order aggregation function $a(\cdot)$ since it is only affected by the output dimension ($E$) which is typically small. We focus on the complexity of the transformation functions ($f^k(\cdot)$) which is sensitive to input dimension ($D$) where $E \ll D$.

- **Model complexity.** As shown in Equation 3 a cross-feature transformation module considering K-order cross features contains $K$ parameter matrices $\{W^k|k = 1, \cdots, K\}$ where $W^k \in R^{E \times D}$. Therefore, the overall number of model parameters is $O(KE D)$ which increases linearly with feature dimension and order size. In addition, it means that the model parameters is $K$ times as many as that of the conventional feature transformation module (Equation 2) in existing GCNs.

- **Computation complexity.** The computation cost mainly comes from the $K$ times matrix multiplication between $W^k$ and $x$. The computation complexity is $O(KE D)$ which increases linearly with $D$. It should be noted that the computation can be
easily accelerated by simply computing the $K$ matrix multiplications in parallel.

- **Memory complexity.** The main memory cost comes from storing model parameters which have the complexity of $O(KED)$. Note that most neural networks rely back-propagation algorithm (BP) to learn the model parameters. As such, in the training phase, storing gradients would bring additional memory cost of which the complexity depends on the implementation of BP. Roughly, the additional cost should also be in order of $O(KED)$.

We conclude that the proposed cross-feature transformation module has complexities linear to feature dimension and order size. In addition, the overhead of the proposed module as compared to the conventional feature transformation module (Equation 2) is linearly dependent on $K$. Considering that order size ($K$) is a hyper-parameter typically smaller than 5, the overhead should be acceptable.

**Discussion.** To the best of our knowledge, Graph Isomorphism Network (GIN) 10 adopting a Multi-layer Perceptron (MLP) as the feature transformation module in each layer is the only existing GCN having the potential to capture cross features. The reason is that a MLP can approximate any arbitrary transformation according to the universal approximation theorem. However, existing research has shown that it might take a large number of hidden units to appropriately approximate feature interactions, which could be much larger than the dimension of input features (i.e., $D$). Therefore, the computational overhead is unaffordable. In addition, implicitly modeling feature interactions with MLP may lead to downsides that a GIN layer cannot control the maximum order of feature interactions and the strength of different orders.

**4 EXPERIMENTS**

We evaluate the proposed method in the node classification task, which covers a wide range of applications such as user profiling, fraud detection, and text classification. Note that it could be easily adapted to solve the other tasks such as link prediction and community detection. In the problem setting of node classification, a graph $G = \{A, X\}$ with $N$ nodes, associated with labels ($Y$) of a portion of nodes. For simplification, we index the labeled nodes and unlabeled nodes in the range of $[1, M]$ and $(M, N]$. We train our model on the labeled nodes by optimizing:

$$
\Gamma = \sum_{i=1}^{M} l(\tilde{y}_i, y_i) + \lambda \|\Theta\|^2_F,
$$

where $l$ is a classification loss function such as cross-entropy. $\Theta$ denotes all the model parameters.

**4.1 Experimental Settings**

**4.1.1 Datasets**

In accordance with [8], we test our model on citation graph.

- **Citation graphs.** Citation graphs represent documents and their citation relations with nodes and edges where features (extracted from document contents) and labels (topic of the document) are associated with each node. Following [8], we adopt three citation graphs, Cora, Citeseer, and Pubmed, with sparse bag-of-word document features. We follow the extreme data split in [8], that is, 20 labeled nodes per class are used for training; 500 and 1,000 nodes are used for validation and testing, respectively.

- **Citeseer-Cross.** Moreover, we construct a semi-real dataset based on the Citeseer citation graph to test whether cross feature are properly considered. We intentionally compile features for nodes so that labels are highly correlated with 2-order cross features. In particular, we use a feature vector $x$ with dimension of 12 to describe each node, which is initialized with random values sampled from a standard Gaussian distribution. We then intentionally change the sign of feature values according to the label of a node so that there would be a cross feature that clearly indicates the value of label. For a node in class $c \in [1, 6]$, i.e., $y_i = c$ for $i = 1, \ldots, 6$, the edited feature would satisfy:

$$
\begin{cases}
  x_{i+2} > 0, & i = c (y_i = 1), \\
  x_{i+2} \leq 0, & i \neq c \in [1, 6] (y_i = 0).
\end{cases}
$$

Note that the sign of a cross feature (e.g., $x_1 \times x_2$) is highly correlated with the label of a class (e.g., $c = 1$). As such, a method would benefit from modeling 2-order feature interactions. Note that Citeseer-Cross and Citeseer have the same graph structure and data splits.

**4.1.2 Methods**

- **SemiEmb [31]:** It is a representative graph-based learning method based on Laplacian regularization which encourages connected nodes to have close embeddings and predictions. Here, we use a MLP with graph Laplacian regularization on the predictions.

- **DeepWalk** [32]: DeepWalk is a widely used graph representation learning method based on the skip-gram technique, which learns node representation by predicting node contexts that are generated by performing random walk on graph. The learned embeddings are fed into a MLP for label prediction.

- **GCN** [8]: is a general GCN model performing feature transformation with matrix mapping without explicit feature interactions, and node aggregation with a pooling function.

- **GIN [10]:** GIN is a generalization of vanilla GCN, performing feature transformation with a MLP in each convolution layer.

- **Cross-GCN:** is the simplest implementation of the proposed method with $K = 2$ as order size.

Note that we omit potential graph convolution-based baselines revolving on the modeling of node aggregation such as [19], since we focus on the modeling of feature transformation. In addition, for each model, we only test the single layer and two layer versions leaving the exploration of deeper models in future work.
4.1.3 Parameter Settings

We implement Cross-GCN, GIN, and SemiEmb with Tensorflow 1.8.0 and adopt the public implementation of GCN. Following the implementation of GCN, we apply dropout and weight decay on each layer to prevent overfitting. To avoid over-tuning of hyper-parameters, we set Cross-GCN and GIN with the optimal hyper-parameters of GCN released in the original paper [8] except the size of hidden layers ($E$). In other words, we set dropout ratio ($p$) and weight decay ($\lambda$) for the $L_2$-norm with values of 0.5 and 5e-4, respectively. For the size of hidden layer ($E$), we perform grid-search within the range of [16, 32, 64, 128]. All the models are optimized via Adam [34] with initial learning rate of 0.01. Following prior work [35], we also test the methods on 20 random splits of the training set while keeping the validation and test sets unchanged. For each run, the epoch a model achieves best performance on the validation is selected to report performance.

4.2 Citeseer-Cross

4.2.1 Performance Comparison

Recall that the target of this work is to explicitly consider cross features in GCN. To investigate the effect of modeling feature crosses, we first test GCN, GIN, and Cross-SGCN on the semi-real dataset (Citeseer-Cross). Table 3 presents the performance of the models with single layer and two layers. Note that the main difference across the compared models is the feature transformation module. From the results, we have the following observations:

- In all cases, the proposed Cross-GCN outperforms GCN with significant improvements. This validates the effectiveness of the cross-feature transformation module. Moreover, this result demonstrates the benefit of explicitly modeling feature crosses in each layer as compared to relying totally on the multi-layer structure.

- Cross-GCN also beats GIN which indicates the advantages of the proposed cross-feature transformation module over a MLP in modeling feature crosses. Similar observation has been presented in previous research [25]. Such observations suggest that we should pay more attention on explicit cross-feature modeling.

- The performance of Cross-GCN with a single layer surpasses GCN GIN with two layers. This result further verifies the benefit of explicit cross-feature modeling. In addition, it indicates that modeling feature crosses would help to reduce network depth in some situations, which would facilitate model optimization.

4.2.2 Impact of Model Complexity

We then investigate the impact of model complexity by testing GCN, GIN, and Cross-GCN with different numbers of hidden units ($E$ for the first layer). Figure 3 shows the performance w.r.t. test accuracy with $E = [16, 32, 64, 128]$. From the results, we have the following observations:

- In all cases, Cross-GCN achieves significantly better performance than GCN and GIN. It further justifies the effectiveness of the proposed cross-feature transformation module.

- Moreover, Cross-GCN with $E = 16$ shows inspiring performance, which is consistently better than GCN and GIN with much larger hidden layers (e.g., $E = 64$ and $E = 128$). This result further justifies the strong representation ability of Cross-GCN and indicates that the advanced representation ability is due to considering cross features rather than additional model parameters. Note that Cross-GCN doubles the model parameter of GCN when they have the same hidden layer size.

- GIN does not perform as well as expected when $E > 16$. We find that, during training, it always sticks at some sub-optimal points even though we try different learning rates and techniques like batch-normalization. It indicates that there are more optimization issues as we increase the depth of GIN. We leave the exploration of solutions in future work.

4.2.3 Cross Feature at Different Layers

We then investigate the impact of considering cross features at different layers by performing ablation study. Table 4 shows the performance of different combinations of Cross-GCN with different layers by performing ablation study. Table 4 shows the performance of different combinations of Cross-GCN with different layers by performing ablation study.
There is a clear gap between the performance of considering feature crosses at the first layer only. The result is reasonable since the semi-real dataset is intentionally designed to benefit modeling of second-order interactions on raw features.

4.2.4 Impact of Cross Features
We investigate the impact of cross features by adjusting the values of $\alpha_1$ and $\alpha_2$ that control the contributions of 1-order feature transformation and 2-order cross-feature transformation to the output representation. Figure 4 shows the performance of Cross-GCN (single layer) as we set $\alpha_1 = 1$ and adjust the value of $\alpha_2$ from 0 to 32. As can be seen, the prediction accuracy increases substantially (roughly from 20% to 60%) when $\alpha_2/\alpha_1$ is in the range of [0, 1], while it is relatively stable when $\alpha_2/\alpha_1 > 1$. Findings on this results are twofold: 1) it demonstrates the necessity of regulating the contribution of feature interactions; and 2) we can simply set both $\alpha_1$ and $\alpha_2$ with fixed values of 1.0 to get an acceptable prediction performance.

4.3 Real-world Datasets
We further test the GCN models on three real-world datasets where the prediction performance is not only determined by the consideration of feature crosses.

4.3.1 Performance Comparison
Here, we compare three more methods: SemiEmb, DeepWalk, and Cross-GCN_Fix. Cross-GCN_Fix is a variant of Cross-GCN with fixed value (1.0) of $\alpha_1$ and $\alpha_2$. Table 5 shows the performance of the compared methods. From the results, we have the following observations:

- With single layer, in most cases, all models with consideration of feature crosses, i.e., GIN1, Cross-GCN1_Fix, and Cross-GCN1, outperform GCN1, which signifies the effectiveness and rationality of considering feature crosses in a graph convolution operator. Note that single layer means that the model only considers the 1-hop neighbors when calculating the representation of a target node, rather than the total number of network layers of the model. As such, the GCN1 model that employs an MLP to perform feature transformation can better capture non-linear feature transformation. On dataset where such non-linear feature important is important, GIN1 achieves better performance on both Cross-GCN1 and Cross-GCN1_Fix.
- In most cases, graph convolution-based models outperform conventional graph representation learning methods. In addition, these models with two layers achieves better performance than the corresponding single layer models. Similar observations have been presented in previous research [8], [9]. Moreover, as compared to the origin GCN paper [8], all the results have large variances. This should not be a concern since recent works [35] have shown consistent results, and can be easily avoided by removing the runs with outlier performance [35]. In addition, our reproduction of GCN (two layers) achieves inconsistent performance as compared to the origin GCN paper.
- Note that, while our GCN reproduction performs worse on Cora and Pubmed, it performs better on Citeseer. Moreover, previous work [35] has also reported inconsistent reproducing results, which thus should also not be a concern.

4.3.2 In-depth Analysis on GIN
As aforementioned, according to the universal approximation theorem [24], an MLP can approximate any arbitrary transformation including the cross-feature transformation even though it may take a large number of hidden units [25]. We study the impact of hidden layer size on the effectiveness of GIN. As shown in Figure 5, GIN achieves better performance as we increase the hidden size from 32 to 256. This result indicates that feature crosses (i.e., multiplication operation) indeed require more hidden units, which is consistent with previous work [25]. Moreover, the performance of GIN with hidden size of 256 is still not comparable as Cross-GCN_Fix which further validates the rationality of considering feature crosses in an explicit manner.
4.3.3 Impact of Hyper-parameters

We then study the impact of hyper-parameters on the effectiveness of the proposed cross-feature graph convolution. We select the drop ratio ($p$) of dropout during model training as an example. Figure 6 illustrates the performance of Cross-GCN and Cross-GCN_Fix as increasing the drop ratio from 0 to 0.8 on Citeseer (a), Cora (b), and Pubmed (c). From the results, we have the following observations, 1) in all the cases, both Cross-GCN and Cross-GCN_Fix achieve better performance when increasing the drop rate, which reflects the importance of preventing over-fitting during the training of such GCN models. 2) As compared to Cross-GCN, on each dataset, the performance of Cross-GCN_Fix varies in a smaller range. This result is reasonable since Cross-GCN_Fix performs order aggregation without introducing any additional parameters, making the model less sensitive to the risk of over-fitting.

4.3.4 Comparison of Efficiency

Finally, we study the computational complexity by comparing the training time of GCN, GIN, and Cross-GCN on Reddit400K. Table 6 shows the average training time over 50 continues epochs. Note that we omit the standard deviation since its value is tiny. Compared to GIN that implicitly encodes feature interactions, Cross-GCN achieves comparable running time. This result indicates that explicitly modeling cross feature is as efficient as the implicit manner. In addition, the average time of training Cross-GCN is roughly at most 1.5 times that of GCN which means the overhead is affordable. In addition, it is consistent with the analysis in Section 3.2 and further validates the strong usability of Cross-GCN.

5 RELATED WORK

5.1 Graph Neural Networks

The recent year has witnessed the success of representation learning over graphs with neural networks owing to their extraordinary ability of non-linear modeling. The recent methods can be roughly divided into three main categories regarding their technique to encode graph structure: 1) skip-gram, 2) autoencoder, and 3) graph convolution.

Skip-gram. Inspired by the skip-gram model [38], which is proposed to learn word embeddings from large-scale documents, many recent methods learn the node embeddings based on a large scale of node sequences generated by random walk [32], [39], [40], [8], [41]. Most of the existing methodologies in this line implement the idea by optimizing a classifier of which the target is to predict the co-occurred node (positive/target node) of a given node (context node), such as DeepWalk [32] and node2vec [39]. Finding that negative sampling plays crucial role in training skip-gram model, a line of work has been focusing on exploring new sampling techniques. In particular, recent work [40] uses node-anchored sampling as an alternative of the uniform sampler in vertex2vec, which incorporates the connectedness to the context node during the sampling. More recently, dynamic negative sampling scheme is adopted, which adaptively selects hard negative samples (i.e., similar to the context node) to boost the training process [8], [41]. The main restriction of skip-gram-based methods is learning embedding independently from the predictive analysis, i.e., in a two-phase fashion. As such, different applications on the same graph have to use the same node embedding while different applications might highlight different connection properties such as local similarity and structural similarity.

Autoencoder. Inspired by the success of Autoencoder (AE) in learning embedding from original features, various works use AE to learn node embedding. Sparse Autoencoder (SAE) [42] is the first work in this line of research, which takes each column of the adjacency matrix as node features. Structure Deep Network Embedding SDNE [43] enhances SAE by further incorporating Laplacian regularization. Furthermore, DNGR [44] employs the positive pointwise mutual information between nodes as the features. As a natural extension of AE, recently, Variational Autoencoder (VAE) has also been introduced to learn node embeddings [45], [46], so that to learn more robust embeddings owning to its inherent generation model. Although AE-based methods could be end-to-end trained, their performance largely relies on designing graph-oriented node features which is typically labor intensive.

Graph Convolution. Recently, research attention on graph representation learning has been shifted to convolution-based methods inspired by its extraordinary success in computer vision. Most of existing research focuses on developing node aggregation modules satisfying different requirements. For instance, GCN [8] and GraphSAGE [9] use pooling functions to aggregate directly connected neighbors. To enlarge the reception field, ChebNet [11] and MixHop [47] aggregate k-hop neighbors. Some other works focus on calculating weights for different nodes during the aggregating. For instance, DCNN [33] uses the transition probability of a length $k$ diffusion process. GAT [19] and CAO [48] adopt attention modules. Another line of research is to extend GCN from simple graphs to more complex graphs such as hypergraph [49] and heterogeneous graph [50], [51]. Despite effectiveness, the existing designs of GCN forgo modeling the cross of features, which is the key difference to the proposed method.

5.2 Cross-feature Modeling

In the literature, two existing neural networks for non-graph data: Cross Network [17] and Compressed Interaction Network...
Cross-feature Graph Convolution, which models feature crosses with complexity linear to feature dimension and order size. Furthermore, we developed a new solution, named Cross-GCN, for graph-based learning tasks such as node classification. Experiments on three graphs demonstrated the effectiveness of Cross-GCN. In addition, the results indicate that applying Cross-GCN in applications with sparse low-level node features is promising.

In the future, we would test Cross-GCN with higher-order feature interactions and deeper structures. In addition, we plan to test Cross-GCN in other graph-based learning tasks such as link prediction. Moreover, we will further consider cross features in the node aggregation operation of GCNs. Furthermore, we are interested in exploring the effectiveness of the cross-feature transformation module with different node aggregation methods such as Attention Networks. Lastly, we will explore methods to learn the weights (α) in the order aggregation function and implementations of the function advanced than the employed weighted sum.

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