Revisiting Graph Convolutional Network on Semi-Supervised Node Classification from an Optimization Perspective

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Abstract
Graph convolutional networks (GCNs) have achieved promising performance on various graph-based tasks. However, they suffer from over-smoothing when stacking more layers. In this paper, we present a quantitative study on this observation and develop novel insights towards the deeper understanding of GCN. First, we interpret the current graph convolutional operations from an optimization perspective and argue that over-smoothing is mainly caused by the naive first-order approximation of the solution to the optimization problem. Subsequently, we introduce two metrics to measure the over-smoothing on node-level tasks. Specifically, we calculate the fraction of the pairwise distance between connected and disconnected nodes to the overall distance respectively. Based on our theoretical and empirical analysis, we establish a universal theoretical framework of GCN from an optimization perspective and derive a novel convolutional kernel named GCN+ which has lower parameter amount while relieving the over-smoothing inherently. Extensive experiments on real-world datasets demonstrate the superior performance of GCN+ over state-of-the-art baseline methods on the node classification tasks.

1 Introduction
Graphs are ubiquitous in the real world, which can easily express various and complex relationships between objectives. In recent years, extensive studies have been conducted on deep learning methods for graph-structured data. There are several approaches on analyzing the graph, including network embedding (Perozzi, Al-Rfou, and Skiena 2014; Tang et al. 2015; Grover and Leskovec 2016), which only uses the graph structure, and graph neural networks (GNNs), which consider graph structure and node features simultaneously. GNNs have shown powerful ability on modeling the graph-structured data in a variety of graph learning tasks such as node classification (Gao, Wang, and Ji 2018; Hamilton, Ying, and Leskovec 2017, Ying and Leskovec 2017; Yang, Cohen, and Leskovec 2016; Kipf and Welling 2016a; Velickovic et al. 2018; Wu et al. 2019), link prediction (Zhang and Chen 2017; 2018; Cai and Ji 2020) and graph classification (Gilmer et al. 2017; Lee, Lee, and Kang 2019; Ma et al. 2019; Xu et al. 2018; Ying et al. 2018b; Zhang et al. 2018). GNNs have also been applied to a range of applications, including social analysis (Qiu et al. 2018; Li and Goldwasser 2019), recommender systems (Ying et al. 2018a; Monti, Bronstein, and Bresson 2017), traffic prediction (Guo et al. 2019; Li et al. 2019b), drug discovery (Zitnik and Leskovec 2017) and fraud detection (Li et al. 2020).

GNNs usually have different design paradigms, which include the spectral graph convolutional networks (Bruna et al. 2013; Defferrard, Bresson, and Vandergheynst 2016; Kipf and Welling 2016a), message passing framework (Gilmer et al. 2017), Hamiltonian, Ying, and Leskovec 2017), and neighbor aggregation via recurrent neural networks (Li et al. 2015; Dai et al. 2018). By using the idea of message passing framework, GNNs are to design various graph convolutional layers to update each node representation by aggregating the node representations from its neighbors.

However, most GNNs only consider the immediate neighbors for each node, which impedes their ability to extract the information of high-order neighbors. More layers usually lead to the performance degradation, which is caused by over-fitting and over-smoothing, of which the former is due to the increasing number of parameters when fitting a limited dataset whereas the latter is the inherent issue of the graph learning. How to make use of the high-order information of neighbors as well as achieving better performance remains a challenge. We need more insights to understand what GCN does and why over-smoothing occurs.

Several studies (Li, Han, and Wu 2018; Xu et al. 2018a; Klüner, Bojchevska, and Gunnemann 2019; Chen et al. 2020; Liu, Gao, and Ji 2020) have noticed over-smoothing, that is after multiple propagations, the final output of vanilla multi-layer GCN converges to a vector which only carries the information of the degree of graph and the node features are indistinguishable. Fig. 1 shows the node representations of vanilla multi-layer GCN on a small citation network Cora. We can observe that 2-layer GCN learns a meaningful embeddings which distinguish the different classes whereas more layers degrade the performance and lead to indistinguishable features.

Different from previous studies, we interpret the current graph convolutional operations from an optimization perspective, and argue that over-smoothing is mainly caused by the naive first-order approximation of the solution to the optimization problem. By solving it and applying the first-order approximation, we get the standard GCN kernel. This suggests that the original GCN kernel can be viewed as a simplified version of the solution. We argue that this sim-
We conduct extensive experiments on several public real-world datasets. Our results demonstrate the superior performance of GCN+ over state-of-the-art baseline methods.

2 Notations

Given an undirected graph \( G = (V, E, X) \), \( V \) is node set with \( |V| = n \), \( E \) is edge set. Let \( A \in \mathbb{R}^{n \times n} \) denote the adjacency matrix, where \( A_{ij} = 1 \) if there is an edge between node \( i \) and node \( j \), otherwise 0. Let \( D \in \mathbb{R}^{n \times n} \) denote the diagonal degree matrix where \( D_{ii} = \sum_j A_{ij} \). Each node is associated with \( d \) features, and \( X \in \mathbb{R}^{n \times d} \) is the feature matrix of nodes, each row of \( X \) is a signal defined over nodes. The graph Laplacian matrix is defined as \( L = D - A \). Let \( \tilde{A} = A + I \) and \( \tilde{D} = D + I \) denote the adjacency and degree matrices of the self-loop graph respectively. We denote \( \tilde{A}_{sym} = \tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2} \) and \( \tilde{A}_{inv} = \tilde{D}^{-1} \tilde{A} \). Assume that each node \( v_i \) is associated with a class label \( y_i \in \mathbb{Y} \) where \( \mathbb{Y} \) is a set of \( c \) classes. Let \( N(v) \) denote the neighbors of \( v \) in graph, that is \( N(v) = \{ u \in V \mid \{ u, v \} \in E \} \) and \( \tilde{N}(v) = N(v) \cup \{ v \} \). \( L' \) is the Laplacian matrix of the graph \( G' = (V', E', X) \), which is the complement of \( G \), that means \( G' \) has the same nodes as \( G \) whereas if \( \{ u, v \} \in E \), then \( \{ u, v \} \notin E' \). Let \( A' \) and \( D' \) denote the corresponding adjacency and degree matrix respectively. We have \( A' = J_n - I_n \) and \( D' + D = (n - 1)I \) where \( J_n \) is a matrix whose element are all 1. Let \( \text{num}(E) \) denote the numbers of edges in \( G \) and \( G' \) respectively, we have \( \text{num}(E) + \text{num}(E') = \frac{n(n-1)}{2} \).

3 Perspectives of GCN

Here we provide three views to derive or understand the vanilla GCNs.

3.1 Spectral Graph Convolution

Bruna et al. (2013) define the spectral convolutions on graph by applying a filter \( g_0 \) in the Fourier domain to a graph signal. ChebNet (Bresson, Courbariaux, and Vandergheynst 2016) suggests that the graph convolutional operation can be further approximated by the \( k \)-th order Chebyshev polynomial of Laplacian. Kipf and Welling (2016a) simplify the ChebNet and obtains a reduced version of ChebNet by the renormalization trick:

\[
H^{l+1} = \sigma(\tilde{A}_{sym} H^{l}(W)) = \sigma(\tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2} H^{l}(W)),
\]

where \( \sigma \) denote the activation function such as ReLU. \( W^{l}(l) \) is a layer-specific trainable weight matrix. \( H^{l}(l) \) is the feature matrix of \( l \)-th layer and \( H^{0}(l) = X \).

3.2 Message Passing

Message passing (Gilmer et al. 2017) means that a node on the graph aggregates the message from neighbors and update its embedding:

\[
h^{l}(v) = U_{i} \left( h^{l-1}(v), \sum_{u \in N(v)} M_l(h^{l-1}(u), h^{l-1}(v), e_{uv}) \right),
\]

where \( M_l(\cdot) \) and \( U_l(\cdot) \) are message aggregation function and vertex update function, respectively. \( h^{l}(v) \) denotes the hidden state of node \( v \) at \( l \)-th layer, and \( e_{uv} \) is the edge features.

In this way, GCN layer can be decomposed into two steps, including the neighbors’ message aggregation and update:

\[
h^{l}(v) = \sigma \left( W^{l}(v) \sum_{u \in N(v)} \frac{h^{l-1}(u)}{\sqrt{|N(v)||N(u)|}} \right).
\]
Here a GCN layer can be viewed as a weighted average of all neighbors’ message where the weighting is proportional to the inverse of the number of neighbors.

3.3 Graph Regularized Optimization

Let $\bar{X} \in \mathbb{R}^{n \times d}$ denote the final node embeddings matrix, and $\bar{x}_i$ is the $i$-th row of $\bar{X}$. We consider the following optimization problem:

$$f = \min \left( \sum_{i \in V} \| \bar{x}_i - x_i \|^2_D + \alpha \sum_{(i,j) \in E} \| \bar{x}_i - \bar{x}_j \|^2_D \right), \tag{4}$$

where $(x, y)_D = \sum_{i \in V} d(i) x(i) y(i)$, if $x = y$, we have $\| x \|_D = \sqrt{(x, x)_D}$.

The first term in the above optimization problem is the fitting constraint, which means the output features (also called embeddings) should not be too far off of the input features, while the second term is the smoothness constraint, which means the connected nodes should have similar embeddings. $\alpha > 0$ is a hyperparameter to balance the importance of two objectives. It is worth noting that there is no limit to the specific transformation from $X$ to $\bar{X}$.

Before solving the optimization problem, we have the following lemma.

**Lemma 1** $\tilde{A}_{rw}$ and $\tilde{A}_{sym}$ always have the same eigenvalues $|\lambda| \leq 1$.

**Corollary 1** $(I_n - \tilde{A}_{rw})$ and $(I_n - \tilde{A}_{sym})$ are invertible if $\alpha \in [0, 1)$.

**Lemma 2** Given a graph with adjacency matrix $A$, the powers of $A$ give the number of walks between any two vertices.

**Corollary 2** $A^k$ includes the information of high-order neighbors.

Next, we derive the closed-form solution of Eq. 4. Specifically, we rewrite Eq. 4 as

$$f = \min \left( \text{Tr}((\bar{X} - X)(\bar{X} - X)^T \tilde{D}) + \alpha \text{Tr}((\bar{X}^T L \bar{X}) \right).$$

Differentiating $f$ with respect to $\bar{X}$, we have

$$\frac{df}{d\bar{X}} = \tilde{D}(\bar{X} - X) + \alpha L \bar{X} = 0.$$

Notice Corollary 1 we have

$$\bar{X} = (1 - \mu)(I - \mu \tilde{A}_{rw})^{-1} X,$$

where $\mu = \frac{\alpha}{1 - \alpha}$.

Actually, the solution is also the personalized PageRank (Page et al. 1999)'s limiting distribution. If we set $\mu = 0.5$, we get $X = (2I - \tilde{A}_{rw})^{-1} X$, and $\tilde{A}_{rw} X$ is the first-order Taylor approximation. By replacing $\tilde{A}_{rw}$ with $\tilde{A}_{sym}$, we get standard graph convolution kernel. In other words, we lose the information from high-order neighbors, which is contained in the error series of the Taylor expansion. (See Corollary 2).

In a nutshell, we obtain the well-known kernel or resemble form of the graph convolution from different ways.

Figure 2: $M_{\text{over}}$, $M_{\text{smooth}}$ and $M_{\text{non-smooth}}$ of the output node embeddings of vanilla GCN with increasing layers on Cora.

4 Over-smoothing in Vanilla Deep GCN

Neural network usually performs better when stack more layers while graph neural network does not benefit from the depth. On the contrary, more layers often result in significant degradation in performance.

Previous work illustrates the over-smoothing by computing the limiting distribution of $A_k$ when $k \rightarrow \infty$. Actually, this is not identical with vanilla deep GCN, which contains non-linear transformation among different layers. Littler work considers the non-linearity in multi-layer GCN. [Ono and Suzuki] (2019) extend the linear analysis to the non-linearity firstly, which considers the ReLU activation function. They suggest that the node features of a $k$-layer GCNs will converge to a subspace and incur information loss, which makes the node feature indistinguishable.

At first, one main reason we introduce the deep architecture in GCN is that we want to use the long-range neighbor’s information. We argue that vanilla deep GCN is not the correct way to capture this information. However, it does not mean that deep architecture is useless. [Chen et al. 2020] and [Liu, Gao, and Ji 2020] have shown that more layers can boost the performance of GCN on several datasets and tasks.

To quantify the over-smoothing in vanilla deep GCN, we compute the overall pairwise distance of node embeddings as follows:

$$M_{\text{over}} = \sum_{i,j \in V} ||\bar{x}_i - \bar{x}_j||_2^2 = \sum_{(i,j) \in E} ||\bar{x}_i - \bar{x}_j||_2^2 + \sum_{\{i,j\} \notin E} ||\bar{x}_i - \bar{x}_j||_2^2$$

$$= \text{Tr}(\bar{X}^T L \bar{X}) + \text{Tr}(\bar{X}^T L' \bar{X}).$$

Fig. 2(a) depicts the pairwise distance distribution of vanilla GCN with increasing layers on Cora. We can see that $M_{\text{over}}$ decreases as the model goes deeper. Revisit the two parts of $M_{\text{over}}$, we propose two fine quantitative metrics to measure the over-smoothing of graph representation.

$$M_{\text{smooth}} = D_{\text{smooth}} / D_{\text{over}},$$

$$M_{\text{non-smooth}} = D_{\text{non-smooth}} / D_{\text{over}}, \tag{5}$$

where

$$D_{\text{smooth}} = \text{Tr}(\bar{X}^T L \bar{X}) / \text{num}(E),$$

$$D_{\text{non-smooth}} = \text{Tr}(\bar{X}^T L' \bar{X}) / \text{num}(E'),$$

$$D_{\text{over}} = D_{\text{smooth}} + D_{\text{non-smooth}}. \tag{6}$$
Here, num\((E)\) and num\((E')\) in the denominator are used to eliminate the impact of unbalanced edge numbers in \(G\) and \(G'\). \(M_{\text{smooth}}\) measures the smoothness of the graph representation of connected pair nodes while \(M_{\text{non-smooth}}\) measures the smoothness of the graph representation of disconnected pair nodes.

Fig. 2(b) compares \(M_{\text{smooth}}\) and \(M_{\text{non-smooth}}\). We see that \(M_{\text{smooth}}\) contributes to quite a few parts of the overall distance, which seems counter-intuitive. We will discuss this two metrics of GCN+ in Section 6.3 again.

5 A General Framework of GCN

Recall the graph regularized optimization problem, we add a negative term to constrain the sum of distances between disconnected pairs as follows:

\[
f = \min_{X} \left( \sum_{i \in V} \| \bar{x}_i - x_i \|^2_2 + \alpha \sum_{(i,j) \in E} \| \bar{x}_i - \bar{x}_j \|^2_2 + \beta \sum_{(i,j) \notin E} \| \bar{x}_i - \bar{x}_j \|^2_2 \right),
\]

where \(\alpha\) and \(\beta\) are hyperparameters to balance the importance of the corresponding terms.

We consider two cases: \(\beta = 0\) and \(\beta \neq 0\).

5.1 Case 1: \(\beta = 0\)

In this situation, \(\bar{X} = (1 - \mu)(I_n - \mu \bar{A})^{-1}X\) where \(\mu = \frac{\alpha + \beta}{1 + \alpha + \beta} \in (0, 1)\). Directly calculating such an intractable expression is not only computationally inefficient but also results in a dense \(\mathbb{R}^{n \times n}\) matrix. It would lead to a high computational complexity and memory requirement when we apply such operator on large graphs. We can achieve linear computational complexity via power iteration.

We use \(\bar{A}\) to denote \(\bar{A}_{\text{sym}}\) and \(\bar{A}_{\text{rw}}\). Here we consider a more general expression \((1 - \mu)(I_n - \mu \bar{A})^{-1}H\) where \(H = f_\theta(X)\).

**Theorem 1** \((I_n - \mu \bar{A})\) is invertible. Consider the following iterative scheme

\[
Z^{(0)} = H,
\]

\[
Z^{(k)} = \mu \bar{A} Z^{(k-1)} + (1 - \mu)H,
\]

where \(\mu \in (0, 1)\). When \(k \to \infty\),

\[
Z^{(\infty)} = (1 - \mu)(I_n - \mu \bar{A})^{-1}H.
\]

**Proof** Using corollary 1 we can see that \((I_n - \mu \bar{A})\) is invertible. Combining the two equation of 7 we have

\[
Z^{(k)} = \left( \mu^k \bar{A}^k + (1 - \mu) \sum_{i=0}^{k-1} \mu^i \bar{A}^i \right) H.
\]

Notice that

\[
\lim_{k \to \infty} \mu^k \bar{A}^k = 0,
\]

\[
\lim_{k \to \infty} \sum_{i=0}^{k-1} \mu^i \bar{A}^i = (I - \mu \bar{A})^{-1}.
\]

Hence, the proof is finished.

Actually, the prevalent GCN, SGC and APPNP can be viewed as the special variant of Case 1.

5.2 Case 2: \(\beta \neq 0\)

In this situation, \(\bar{X} = Q^{-1} (1 + \alpha + \beta)I - (\alpha + \beta) \bar{D}^{-1} \bar{A} - \beta n \bar{D}^{-1} \bar{A} \bar{D}^{-1} I_n\) is invertible when we choose a suitable \(\beta\). We will introduce the conditions later.

First we use the first-order Taylor approximation of above convolutional kernel (GCN*) directly without any tricks such as Batch Normalization (Ioffe and Szegedy 2015) or residual connection (He et al. 2016) on two small citation datasets Cora and Citeseer. We compare the performance of the vanilla deep GCN and GCN* as the model layer increases. Fig. 3 shows the result of GCN and GCN*. Dashed lines illustrate the performance of GCN, which shows that deep GCN suffers from performance drop. We can see that the performance decay with GCN* kernel is much slower.

[Oono and Suzuki (2019)] have proved that the node feature of vanilla \(k\)-layer GCN will converges to an invariant subspace which only carry the information of the connected component and node degree. The convergence speed is proportional to the \(\lambda^k\), where \(\lambda\) is the supreme of eigenvalue of \(\bar{A}\). In GCN*, \(\lambda > 1\) (see the proof of Theorem 2), which implies that \(\lambda^k\) is large, thus the information loss and over-smoothing are relieved.

Although the modified graph kernel relieves over-smoothing to some extent, more layers do not boost the performance, which is not our focus. However the above result demonstrates that it is an efficient way to tackle the over-smoothing issue. We can achieve linear computational complexity via power iteration similar to Case 1.

**Theorem 2** \((I_n - \mu \bar{A})\) is invertible when \(\beta < \frac{1}{n}\) where \(\mu = \frac{\alpha + \beta}{1 + \alpha + \beta}\) and \(\bar{A} = \bar{A} + \beta n \bar{D}^{-1} \bar{A} \bar{D}^{-1} I_n\). Consider the following iterative scheme

\[
Z^{(0)} = H,
\]

\[
Z^{(k)} = \mu \bar{A} Z^{(k-1)} + (1 - \mu)H,
\]

where \(\mu \in (0, 1)\). When \(k \to \infty\),

\[
Z^{(\infty)} = (1 - \mu)(I_n - \mu \bar{A})^{-1}H.
\]
Proof Let $M = \frac{\beta_n D - I}{\alpha + \beta} (n I - J_n)$. Note that $(n I - J_n)$ has the largest eigenvalue $n$. Suppose that $\lambda$ is the eigenvalue of $M$, we have $\lambda \leq \frac{\beta_n}{\alpha + \beta}$. Then eigenvalue of $A$ is less than $1 + \frac{\beta_n}{\alpha + \beta}$, $(I_n - \mu A)$ is invertible if $\frac{1}{\mu}$ is not an eigenvalue of $A$. Note that $\frac{1}{\mu} = 1 + \frac{\alpha + \beta}{\alpha + \beta}$, when $\beta < \frac{1}{\mu}$. We have $1 + \frac{\beta_n}{\alpha + \beta}$, hence $\frac{1}{\mu}$ cannot be an eigenvector of $A$ and $(I_n - \mu A)$ is invertible. The proof of the iterative scheme follows the similar procedure of case 1 with a slight difference, as it is trivial, we omit the proof.

5.3 Why GCN+ relieve the over-smoothing? We have no assumptions on the specific transformation from $X$ to $\tilde{X}$. In our implementation, the mathematical expression of GCN+ is defined as
\begin{equation}
Z^{(0)} = H = \sigma(XW_1),
\end{equation}
\begin{equation}
Z^{(k)} = \mu AZ^{(k-1)} + (1 - \mu)H,
\end{equation}
\begin{equation}
X_{out} = \text{softmax}(Z^{(k)}W_2),
\end{equation}
where $W_1 \in \mathbb{R}^{d \times m}$ and $W_2 \in \mathbb{R}^{m \times c}$ are learnable weight matrices, $k$ is the dimension of the hidden layers.

In practice, we use Pytorch (Paszke et al. 2019) and Pytorch Geometric (Fey and Lenssen 2019) for an efficient implementation. The statistics of datasets are summarized in Table 1. It is worth nothing that OGB includes enormous challenging and large-scale datasets than Planetoid. We refer readers to Hu et al. (2020) for more details about OGB datasets.

Table 1. Dataset statistics.

| Dataset           | Nodes | Edges | Classes | Features | Metric      |
|-------------------|-------|-------|---------|----------|-------------|
| Cora              | 2708  | 5429  | 7       | 1433     | Accuracy    |
| Citeseer          | 3327  | 4732  | 7       | 2703     | Accuracy    |
| Pubmed            | 19717 | 44338 | 3       | 500      | Accuracy    |
| ogb-arxiv         | 169343| 1166243| 40     | 128      | Accuracy    |
| ogb-proteins      | 132534| 39561252| 112   | 8        | ROC-AUC     |

6 Experiments

In this section, we evaluate the performance of GCN+ on several benchmark datasets against various graph neural networks on semi-supervised node classification tasks.

6.1 Experimental Setup

Datasets: We conduct extensive experiments on the node-level tasks on two kinds commonly used networks: Planetoid: Cora, Citeseer, Pubmed (Sen et al. 2008) and recent Open Graph Benchmark (OGB) (Hu et al. 2020): ogb-arxiv, ogb-proteins. The statistics of datasets are summarized in Table 1. For SGC, we vary number of layers in {1, 2, ..., 10, 15, ..., 60}; and for GCN and GAT in {2, 4, ..., 10, 15, ..., 30}. For $\alpha$ in APPNP, we search it from {0.1, 0.2, 0.3, 0.4, 0.5}. For DAGNN and JKNet, we search layers from {2, 3, ..., 10}. For learning rate, we choose from {0.001, 0.005, 0.01}. For dropout rate, we choose from {0.1, 0.2, 0.3, 0.4, 0.5}. We perform a grid search to tune the hyperparameters for other models based on the accuracy on the validation set. We run each experiment 10 times and report the average.

In practice, we use Pytorch (Paszke et al. 2019) and Pytorch Geometric (Fey and Lenssen 2019) for an efficient GPU-based implementation of GCN+. All experiments in this study are conducted on NVIDIA TITAN RTX 24GB GPU.

6.2 Comparison with SOTA

The evaluate metric of various datasets are listed in Table 1. Actually it is commonly used to evaluate the model by the community.

Planetoid: We use standard fixed and random training/validation/testing splits. Specifically, we use 20 labeled nodes per class as the training set, 500 nodes as the validation set, and 1000 nodes as the test set for all models. For fixed split, we follow the experimental setup in (Yang, Cohen, and Salakhudinov 2016). We compare Multiplayer Perception (MLP), GCN (Kipf and Welling 2016a), GAT (Kipf and Welling 2016a), GAT
Table 2: Summary of classification accuracy(%) on Planetoid datasets of semi-supervised node classification.

| Dataset      | ogb-arxiv | ogb-proteins |
|--------------|-----------|--------------|
| GCN          | 71.74 ± 0.29 | 72.51 ± 0.35 |
| GraphSAGE    | 71.49 ± 0.25 | 77.68 ± 0.20 |
| GCN+(β = 0)  | 71.85 ± 0.23 | 78.63 ± 0.28 |
| GCN+(β ≠ 0)  | **71.95 ± 0.28** | **79.07 ± 0.34** |

Table 3: Summary of classification performance(%) on OGB datasets. For ogb-arxiv, it indicates accuracy and for ogb-proteins, it indicates ROC-AUC.

Figure 4: $M_{non-smooth}$ of GCN+ with increasing hops on Cora.

forms slightly better than it.

**OGB** We adopt the setting of [Hu et al. 2020], which is more challenging and realistic. We consider the following representative models GCN (Kipf and Welling 2016a), GraphSAGE (Hamilton, Ying, and Leskovec 2017) and GCNII (Chen et al. 2020) as our baselines. In particular, we use the reported metric of the leaderboards of OGB team, which provide an open benchmark on several tasks and datasets.

Table 3 compares the average test accuracy/ROC-AUC on OGB datasets. As shown, GCN+ outperforms the GCN and GraphSAGE. It is clear that our proposed GCN+ outperforms SOTA in two middle scale datasets.

In summary, GCN+ achieves superior performance on several benchmarks, which shows that considering the information of high-order neighbors makes sense and we need more reasonable way to deepen GCNs or make use of the high-order neighbors. Note that GCN+(β ≠ 0) is slightly better than GCN+(β = 0) which is benefit from the third term of Eq. (7).
6.3 Over-smoothing Analysis
We employ the two proposed metrics to measure the node embeddings learned by GCN+. The results on Cora are shown in Fig. 4. We can observe that as the number of hops increases, the $M_{\text{smooth}}$ values nearly remains a small constant which is lower than vanilla deep GCN. This implies that GCN+ use the information of long-range neighbors and do not suffer from over-smoothing.

Fig. 1 also compares the final output embeddings of GCN+ with multiple hops, which shows different behaviors with GCN. GCN+ relieves the over-smoothing and learns the meaningful embeddings with the increasing hops.

6.4 Hyperparameter Analysis
In the previous sections, we use $A$ to refer the $\tilde{A}_{\text{sym}}$ and $\tilde{A}_{\text{rw}}$. Here we compare the different choices of propagation matrix $\tilde{A}$. Fig. 5 depicts the test accuracy achieved by varying the hops of different propagation matrices. The result illustrates that $\tilde{A}_{\text{sym}}$ is slightly better than $\tilde{A}_{\text{rw}}$.

We consider three hyperparameter of GCN+, that is $\alpha$, $\beta$ and number of power iteration steps $\bar{k}$. For Cora, when $\alpha = 9$ (that means the fraction of retained initial node features is 0.1.), GCN+ achieve the best performance. The value of $\alpha$ varies by different datasets. More results and details listed in the supplementary material.

7 Related Work
7.1 Graph Neural Networks
Graph neural networks (GNNs) have been extensively studied for the past years. There are different views on designing new architecture, including the spectral-based, spatial-based and others, such as understanding the GNN using dynamic system (Xhonneux, Qu, and Tang 2019). Numerous methods are proposed to model the graph-structure data and apply on a wide range of applications. Besides the GCNs, there are also other types of GNNs, such as attention-based GNN (Velickovic et al. 2018) which use multiple attention to aggregate information from neighbors, autoencoder-based GNN (Kipf and Welling 2016b), which use a GCN encoder and decoder to learn meaningful embeddings, and dynamic GNNs (Seo et al. 2018; Hajiramezanali et al. 2019; Yan et al. 2020) which learn the node embedding over time.

7.2 Deep GCN and Over-smoothing
Most GNNs are shallow models as deep architecture suffers from over-smoothing. Several studies explore deep GCNs. Xu et al. (2018b) introduce Jumping Knowledge Networks, which uses residual connection to combine the output of each layer. Klicpera, Bojchevski, and Günnemann (2019) use Personalized PageRank, which consider the information of root node to replace the graph convolution operator to solve the over-smoothing. DropEdge (Rong et al. 2019) suggests that randomly removing the edge of original graph impedes over-smoothing. PairNorm (Zhao and Akoglu 2019) is another scheme which uses a normalization layer to scale the node features after the convolution layer. Li et al. (2019a) build on ideas from ResNet to train very deep GCNs; Li et al. (2020) further propose MsgNorm, which boosts the performance on several datasets. Yang et al. (2020) present NodeNorm to scale the node features. Chen et al. (2020) propose a deep GNN models which use initial residual connection and identity mapping.

A few works analyzes the cause and behaviors of over-smoothing theoretically. Oono and Suzuki (2019) investigate the asymptotic behaviors of GCNs as the layer size tends to infinity and reveals the information loss in deep GCNs. Cai and Wang (2020) further extend analysis of Oono and Suzuki (2019) from linear GNNs to the nonlinear architecture.

8 Conclusion
We summarize the existing different views on the mechanism of GCNs, which help us understand and design the graph convolutional kernel. We further provide a general optimization framework named GCN+. Based on this framework, we derive two forms of GCN+ and propose two metrics to measure the smoothness of output node representations. Extensive empirical studies on several real-world datasets demonstrate that GCN+ compares favorably to state of the art with a small amount of parameters. For future work, we will consider different optimization objectives which encode the graph structure and node features adaptively. As we do not limit the transformation from $X$ to $\tilde{X}$, another reasonable formulas can be further explored.
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