Connecting Graph Convolutional Networks and Graph-Regularized PCA

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Abstract

Graph convolution operator of the GCN model is originally motivated from a localized first-order approximation of spectral graph convolutions. This work stands on a different view; establishing a connection between graph convolution and graph-regularized PCA. Based on this connection, GCN architecture, shaped by stacking graph convolution layers, shares a close relationship with stacking graph-regularized PCA (GPCA). We empirically demonstrate that the unsupervised embeddings by GPCA paired with a logistic regression classifier achieves similar performance to GCN on semi-supervised node classification tasks. Further, we capitalize on the discovered relationship to design an effective initialization strategy for GCN based on stacking GPCA.

1. Introduction

Graph neural networks (GNNs) are neural networks designed for the graph domain. Since the breakthrough of GCN (Kipf & Welling, 2017) notably improving performance on the semi-supervised node classification problem, many GNN variants have been proposed; including GAT (Veličković et al., 2018), GraphSAGE (Hamilton et al., 2017), DGI (Veličković et al., 2019), GIN (Xu et al., 2019), to name a few.

Despite the empirical successes of GNNs in both nodelevel and graph-level tasks, peculiar issues remain not well understood due to the lack of systematic and theoretical analysis of GNNs. For example, researchers have found that GNNs, unlike their non-graph counterparts, suffer from performance degradation with increasing depth, losing their expressive power exponentially in number of layers (Oono & Suzuki, 2020). Such behavior is only partially explained by the oversmoothing phenomenon (Li et al., 2018; Zhao & Akoglu, 2020). Another surprising observation shows that

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a Simplified Graph Convolution model, named SGC (Wu et al., 2019), can achieve similar performance to various more complex GNNs on a variety of node classification tasks. Moreover, a simple baseline that does not utilize the graph structure altogether performs similar to state-of-the-art GNNs on graph classification tasks (Errica et al., 2020). These observations call attention to studies for a better understanding of GNNs (NT & Maehara, 2019; Morris et al., 2019; Xu et al., 2019; Oono & Suzuki, 2020; Loukas, 2020; Srinivasan & Ribeiro, 2020). (See sec.2 for more on understanding GNNs.)

Toward a systematic analysis and better understanding of GNNs, we establish a connection between the graph convolution operation of GCN and Graph-regularized PCA (GPCA), and show the similarity between GCN and stacking GPCA. This connection provides a deeper understanding of GCN's power and limitation. Empirically, we also find that GPCA performance matches that of GCN on benchmark semi-supervised node classification tasks. What is more, the unsupervised stacking GPCA can be viewed as "unsupervised GCN" and provides a straightforward, yet systematic way to initialize GCN training. We summarize our contributions as follows:

- Mathematical connection btwn. GCN & GPCA: We establish the connection between the graph convolution operator of GCN and the closed-form solution of graph-regularized PCA formulation. We demonstrate that a simple graph-regularized PCA can achieve similar results to GCN over several benchmark datasets.
- New parameter-free stacking GPCA model: We propose GPCANET, a simple unsupervised embedding model shaped by stacking multiple GPCA layers and nonlinear transformations, which shares the same architecture as multi-layer GCN. We argue that this simple model should be used as a baseline along GCN, as it achieves on par performance.
- New GCN initialization strategy: Capitalizing on the GCN-GPCA connection, we design a new strategy to initialize GCN training based on stacking GPCA, outperforming the popular Xaiver initialization (Glorot & Bengio, 2010).

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2. Related Work

Understanding GNNs. We discuss related work that provide a more systematic understanding of GNNs in a number of fronts. GCN's graph convolution is originally motivated from the approximation of graph filters in graph signal processing (Kipf & Welling, 2017). NT et al. (2019) show that graph convolution only performs low-pass filtering on original feature vectors, and also states a connection between graph filter and Laplacian regularized least squares. Motivated by the oversmoothing phenomenon of graph convolution, Oono et al. (2020) theoretically prove that GCN can only preserve information of node degrees and connected components when the number of layers goes to infinity, under some conditions of GCN weights. At graph-level, Xu et al. (2019) show that GNNs cannot have better expressive power than the Weisfeiler-Lehman (WL) test of graph isomorphism, and develop the GIN model that is as powerful as the WL test. Morris et al. (2019) extend the work by (Xu et al., 2019) and establish a connection to the higher-order WL algorithm. When given distinguishable node features, Loukas (2020) has shown that the GNN models can be Turing universal with sufficient depth and width.

Graph-regularized PCA. PCA and its variants are standard linear dimensionality reduction approaches widely used for i.i.d. vectors. Several works extend PCA to graph-structured data, such as Graph-Laplacian PCA and Manifold-regularized Matrix Factorization (Zhang & Zhao, 2012). For other variants, see Shahid et al. (2016).

Stacking PCA and Deep Learning. The connection between CNN and stacking PCA has been explored in PCANet (Chan et al., 2015), which demonstrated that the (unsupervised) simple stacking PCA works as good as supervised CNN over a large variety of vision tasks. The original PCANet is shallow and does not have nonlinear transformations, PCANet+ (Low et al., 2017) overcomes these limitations and pushes the architecture much deeper.

PCA initialization. The heavily non-convex property of deep neural networks requires good initialization for better convergence and escaping bad local minima. Lots of data-independent initialization approaches exist and have been widely used in practice. As a data-dependent method, using PCA to initialize deep neural networks has been explored by (Krähenbühl et al., 2016). In similar lines, we explore initializing graph neural networks using GPCA.

3. Graph Convolution and GPCA

3.1. Graph Convolution

Similar to other neural networks stacked with repeated layers, GCN (Kipf & Welling, 2017) contains multiple graph convolution layers each of which is followed by a nonlinear

activation. Let $H^{(l)}$ be the l-th layer hidden representation, then GCN follows:

$$H^{(l+1)} = \sigma(\tilde{A}_{\text{sym}}H^{(l)}W^{(l)}) \tag{1}$$

where $\tilde{A}_{\mathrm{sym}} = \tilde{D}^{-1/2}(A+I)\tilde{D}^{-1/2}$ denotes the symmetrically normalized adjacency matrix with self-loops, $W^{(l)}$ is the l-th layer parameter (to be learned), and σ is the nonlinear activation function.

Graph convolution operation is defined as the formulation before activation in Eq. (1). Formally, let $X \in \mathbb{R}^{n \times d}$ be the feature matrix with n samples and d features. The graph convolution (parameterized with W) mapping X to a new representation Y is defined as

$$Y = \tilde{A}_{\text{sym}} X W . (2)$$

3.2. Graph-regularized PCA (GPCA)

Standard PCA learns c-dimensional projections $Y \in \mathbb{R}^{n \times c}$ of feature matrix $X \in \mathbb{R}^{n \times d}$ on an orthonormal basis $W \in \mathbb{R}^{d \times c}$, aiming to minimize the reconstruction error $\|X - YW^T\|_F^2$. GPCA extends this formalism to graph-structured data by additionally assuming either smoothing bases (Jiang et al., 2013) or smoothing projections (Zhang & Zhao, 2012) over the graph. In this work we consider the latter case where low-dimensional projections are smoothing over the input graph G, with its symmetrically normalized Laplacian matrix defined as $\tilde{L} = I - \tilde{A}_{\text{sym}}$. The objective formulation of GPCA is then given as

$$\min_{Y,W} \|X - YW^T\|_F^2 + \alpha \operatorname{Tr}(Y^T \tilde{L}Y)$$
 (3)

s.t.
$$W^TW = I$$
 (4)

where α is a hyperparameter that balances reconstruction error and the variation of the projections over the graph. Note that the first part of Eq. (3), along with the constraint, corresponds to the objective of the original PCA, while the second part is a graph regularization term that aims to "smooth" the new representations Y over the graph structure. As such, GPCA becomes the standard PCA when $\alpha=0$.

Similar to PCA, the problem (3-4) is non-convex but has a closed-form solution (Zhang & Zhao, 2012). Surprisingly, as we show, it has a close connection with the graph convolution formulation in Eq. (2). In the following, we give the GPCA solution and then detail its connection to graph convolution in the next subsection.

Theorem 3.1. GPCA with formulation shown in (3-4) has the optimal solution (Y^*, W^*) following

$$W^* = (\mathbf{w}_1, \mathbf{w}_2, ..., \mathbf{w}_c)$$
$$Y^* = (I + \alpha \tilde{L})^{-1} X W^*$$

where $\mathbf{w}_1, \mathbf{w}_2, ..., \mathbf{w}_c$ are the eigenvectors corresponding to the largest c eigenvalues of the matrix $X^T(I + \alpha \tilde{L})^{-1}X$.

Proof. We give the proof in two steps.

Step 1: For a fixed W, Solve optimal Y^* as a function of W: When fixing W as constant, the problem becomes quadratic and convex. There is a unique solution, given by first-order optimal condition. Let \mathcal{L} denote the objective function as given in (3). Its gradient can be calculated as

$$\frac{\partial \mathcal{L}}{\partial Y} = 2(I + \alpha \tilde{L})Y - 2XW . \tag{5}$$

Setting (5) to 0 leads to the solution $Y^* = (I + \alpha \tilde{L})^{-1}XW$.

Step 2: Replace Y with Y*, Solve optimal W*: Replacing Y in objective \mathcal{L} with $Y^* = (I + \alpha \tilde{L})^{-1}XW$, we reduce the optimization to

$$\begin{split} \min_{W,W^TW=I} & \|X-(I+\alpha\tilde{L})^{-1}XWW^T\|_F^2 + \\ & \alpha \operatorname{Tr} \left[W^TX^T(I+\alpha\tilde{L})^{-1}\tilde{L}(I+\alpha\tilde{L})^{-1}XW\right]. \end{split} \tag{6}$$

Based on the cyclic property of (Tr)ace, we can simplify as

$$\max_{W,W^TW=I} \quad \text{Tr}\left[W^T X^T (I + \alpha \tilde{L})^{-1} X W\right]. \tag{7}$$

Based on the spectral theorem of PSD matrices, the optimal solution W^* of problem (7) is the combination of eigenvectors, associated with the largest c eigenvalues of the graph-revised covariance matrix $X^T(I + \alpha \tilde{L})^{-1}X$. \square

3.3. Connection btwn. Graph Convolution and GPCA

Let $\Phi_{\alpha} := I + \alpha \tilde{L}$. The closed-form solution of GPCA requires the inverse of the (sparse) matrix Φ_{α} . A much economical way of doing exact inverse along with finding the largest eigenvectors is to use Cholesky factorization, which is summarized in (Zhang & Zhao, 2012).

Here we take an approximation of the inverse of Φ_{α} . The normalized Laplacian matrix \tilde{L} has absolute eigenvalues bounded by 1, thus, all its positive powers have bounded operator norm. When $\alpha \leq 1$, Φ_{α}^{-1} can be decomposed as

$$(I + \alpha \tilde{L})^{-1} = I - \alpha \tilde{L} + \dots + (-\alpha)^k \tilde{L}^k + \dots$$
 (8)

The first-order truncated form of Eq. (8) is

$$(I + \alpha \tilde{L})^{-1} \approx I - \alpha \tilde{L} = (1 - \alpha)I + \alpha \tilde{A}_{\text{sym}}$$
. (9)

When $\alpha = 1$, the first-order approximation of Y^* follows

$$Y^* \approx \tilde{A}_{sym} X W^* \ . \tag{10}$$

This (approximate) solution to GPCA matches the graph convolution operation in Eq. (2), with W^* plugged in as the eigenvectors of the matrix $X^T \Phi_{\alpha}^{-1} X$.

To restate the key contribution of this paper: The graph convolution can be viewed as the first-order approximation of GPCA with $\alpha=1.1$

4. GPCANET and GCN Initialization

4.1. GPCANET

The connection between deep learning and PCA is previously explored in PCANet (Chan et al., 2015).GPCANET leverages an analogous connection between graph convolution and GPCA as established in the previous section.

The architecture of our (unsupervised) GPCANET exactly follows GCN, with weight of l-th layer calculated as the leading eigenvectors of $H^{(l-1)}{}^T\Phi_{\alpha}^{-1}H^{(l-1)}$, where $H^{(l)}$ is the representation of l-th layer, and Φ_{α} can be approximated by Eq. (9). In principle, GPCANET can be viewed as the stacking of multiple GPCA layers (followed by nonlinear activation). The steps of the algorithm is given in Alg. 1.

Algorithm 1 GPCANET

- 1: **Input:** graph G, features X, GPCA hyper-param. α , #layers L, hidden sizes $d_1,...,d_L$, activation σ
- 2: Output: node embeddings $H^{(L)}$
- 3: Initialize $H^{(0)} = X$.
- 4: for l=1 to L do
- 5: Center $H^{(l-1)}$ by subtracting mean of row vectors
- 6: $W^{(l)} \leftarrow d_l$ top eigenvectors of $H^{(l-1)}{}^T \Phi_{\alpha}^{-1} H^{(l-1)}$
- 7: $H^{(l)} \leftarrow \sigma(\Phi_{\alpha}^{-1}H^{(l-1)}W^{(l)})$
- 8: end for

4.2. GPCA Initialization

As the leading eigenvectors capture the largest variation in data, PCA initialization has been shown (Krähenbühl et al., 2016) to serve as an information-preserving initialization. Similarly, we propose GPCA initialization for the GCN model at all layers. Precisely, we initialize the parameters of a GCN at layer l with the $W^{(l)}$ in line 6 of Alg. 1.

5. Experiments

5.1. Setup

We focus on the semi-supervised node classification (SSNC) problem and use 3 widely-used benchmark datasets: Cora, CiteSeer, and PubMed (Sen et al., 2008). Same dataset splits are used as Kipf & Wellinng (2017). For baseline, we only use GCN, as experiments are conducted to verify the established connection between GCN and GPCA instead of achieving the state-of-the-art performance for SSNC. For both GCN and logistic classifier of GPCA, we

 $^{^{1}}$ When α < 1, Eq. (9) shows the connection between GPCA and graph convolution with 1-step residual.

fix the dropout rate to 0.5. Hidden representation size is fixed as 128 for all models. We use the Adam optimizer with learning rate fixed at 0.005 and weight decay $5e^{-4}$. GCN is fixed with 2 layers, which achieves the best performance over all datasets. For GPCA and GPCANET, we experiment with several hyperparameters: smoothing hyper-parameter α , number of layers (only for GPCANET), and whether to use approximation for matrix inverse (recall Eq. (8)). All experiments use the maximum training epoch as 1000.

5.2. GPCA vs. GCN

Having proved the mathematical similarity between GPCA and graph convolution of GCN, a perhaps naïve conjecture is that the (unsupervised) GPCA can generate a comparable representation to (supervised) GCN for node classification tasks. To test this conjecture, we perform GPCA with different α to obtain node representations and then pass those to a logistic classifier. We find that, by selecting a suitable α , GPCA achieves similar performance to 2-layer GCN for all 3 benchmark datasets. We run each experiment 5 times and report mean in Table 1.

Table 1. Performance of GPCA with Exact (GPCA-E) and Approximated (GPCA-A) matrix inverse over benchmark datasets, comparied with GCN.

	CORA	CITESEER	PUBMED
2-LAYER GCN	82.1	69.3	77.7
GPCA-E ($\alpha = 0.5$)	69.3	64.2	71.8
GPCA-E ($\alpha = 1.0$)	73.6	67.1	74.5
GPCA-E ($\alpha = 5.0$)	79.7	70.2	<u>77.3</u>
GPCA-E ($\alpha = 10.0$)	<u>81.3</u>	70.7	77.1
GPCA-A ($\alpha = 0.5$)	72.3	66.1	73.2
GPCA-A ($\alpha = 1.0$)	76.0	67.8	74.9
GPCA-A ($\alpha = 5.0$)	80.1	70.1	<u>77.5</u>
GPCA-A ($\alpha = 10.0$)	<u>81.2</u>	70.5	76.8

Surprisingly, the simple parameter-free GPCA paired with logistic classifier performs similar to the end-to-end supervised multi-layer GCN model. We find that a larger α is preferable for all datasets, graph-regularizing the representations more heavily. This is intuitive as all these datasets exhibit strong label homophily. What is more, GPCA with the fast first-order approximation of matrix inverse performs as well as when exact matrix inverse is used, also making GPCA a computationally competitive alternative to GCN.

5.3. Stacking GPCA: GPCANET

Compared to GPCA that only has a single linear layer, GP-CANET has a deeper architecture like GCN along with non-linear activation function. We have empirically observed that adding nonlinear activation does not make a difference so we ignore it for simplicity. For all benchmark datasets, the best performance of GPCANET with different number of layers match the best performance of GPCA with different number.

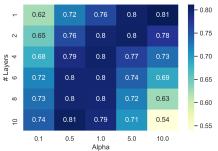


Figure 1. Performance (avg'ed over 5 runs) of GPCANET with different number of layers and different α on Cora dataset. Similar results hold for CiteSeer and PubMed.

ent α . Due to limited space we instead report GPCANET's performance w.r.t. varying layers and α in Fig. 1. This suggests that increasing the number of layers has the same effect as increasing α , in other words, a stronger graph smoothing is also achieved by a deeper model.

5.4. GPCA Initialization

As GPCANET shares exact architecture with GCN, it can be used to initialize GCN. To show the effectiveness of GPCANET-based initialization, we compare the standard Xavier (Glorot & Bengio, 2010) vs. GPCA initialization for GCN with different number of layers (maximum training epoch set to 100). Results in Table 2 suggest that GPCA-initialization works better than the standard, and the improvement increases as the number of layers goes up.

Table 2. Performance (avg'ed over 5 runs) of GCN w.r.t. varying number of layers (L) and initialization methods, on Cora (CR), CiteSeer (CS), and PubMed (PM).

DATASET	2L	4L	7L	10L	15L
CR XAIVER	82.5	81.7	79.4	79.4	35.8
CR GPCA-INIT	82.6	82.0	80.9	79.9	78.1
CS XAIVER	68.9	67.8	63.7	63.6	25.6
CS GPCA-INIT	69.1	67.8	66.3	66.3	64.8
PM XAIVER	77.6	76.0 75.7	76.5	77.0	69.4
PM GPCA-INIT	77.6		76.8	77.5	73.0

6. Conclusion

We showed the mathematical connection between graph-regularized PCA and graph convolution. Capitalizing on the discovered connection, we proposed (1) a new *parameter-free* graph neural network model, called GPCANET, by stacking multiple GPCA layers—its projection matrices analogous to GCN parameters are directly computed from data as matrix eigenvectors, and (2) a scheme where we initialize GCN with those data-driven projection matrices. Experiments show that GPCANET achieves similar performance to GCN on benchmark datasets, and our initialization scheme enables a more robust deep GCN.

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