HyperGraphConv: Hypergraph Convolutional Networks for Semi-Supervised Classification

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Abstract

Graph-based semi-supervised learning (SSL) is an important learning problem where the goal is to assign labels to initially unlabeled nodes in a graph. Graph Convolutional Networks (GCNs) have recently been shown to be effective for graph-based SSL problems. GCNs inherently assume existence of pairwise relationships in the graph-structured data. However, in many real-world problems, relationships go beyond pairwise connections and hence are more complex. Hypergraphs provide a natural modeling tool to capture such complex relationships. In this work, we explore the use of GCNs for hypergraph-based SSL. In particular, we propose HyperGCN, an SSL method which uses a layer-wise propagation rule for convolutional neural networks operating directly on hypergraphs. To the best of our knowledge, this is the first principled adaptation of GCNs to hypergraphs. HyperGCN is able to encode both the hypergraph structure and hyper-node features in an effective manner. Through detailed experimentation, we demonstrate HyperGCN’s effectiveness at hypergraph-based SSL. We have made HyperGCN’s source code available for reproducible research.

Introduction

Graph-based semi-supervised learning (SSL) is an important learning problem where the goal is to assign labels to initially unlabeled nodes in a graph (Chapelle, Scholkopf, and Zien 2010; Zhu et al. 2009; Subramanya and Talukdar 2014). Graph-based SSL is motivated by the fact that in many real-world problems, labeling of data typically requires expensive human labor whereas unlabeled data is far easier to obtain. A classical use case for graph-based SSL is web categorisation, in which manually labeled web pages are easier to obtain. A classical use case for graph-based SSL is web categorisation, in which manually labeled web pages is large.

In conventional graph-based SSL problems, the loss function is defined as a weighted sum of the supervised loss over labeled data and a regulariser for the graph structure.

$$\mathcal{L} = \mathcal{L}_0 + \lambda \mathcal{L}_{reg}$$

Here, $\mathcal{L}_0$ denotes the supervised loss w.r.t. the labeled part of the graph and $\mathcal{L}_{reg}$ is an explicit graph-based regulariser that smooths the label information over the graph (with $\lambda$ being the weighting factor). A popularly used graph-based regulariser is the graph Laplacian regulariser which relies on the prior assumption that connected nodes in the graph are likely to share the same label (the cluster assumption (Chapelle, Weston, and Scholkopf 2003)). This assumption might restrict modeling capacity, as graph edges need not encode node similarity, but could instead contain other information such as pointwise mutual semantic information (Zhuang and Ma 2018), or knowledge graph relationship information (Wang, Ye, and Gupta 2018).

To avoid this restriction, recent works have encoded both the labeled and graph data using a convolutional neural network (Atwood and Towsley 2016; Kipf and Welling 2017). This allows the network to be trained on a supervised loss function $\mathcal{L} = \mathcal{L}_0$ for all graph nodes, thereby, avoiding an explicit graph-based regulariser in the loss function. Specifically, graph convolutional networks (GCNs) (Kipf and Welling 2017) naturally integrate the graph structure (e.g., citation networks) and the feature attributes of nodes (e.g., bag-of-words features). GCNs have achieved state-of-the-art performance on benchmark graph-based semi-supervised node classification datasets. Even though GCNs are able to incorporate arbitrary relationships between nodes (and not just similarity), they are still limited by pairwise relationships in the graph.

However, in many real-world problems, relationships go beyond pairwise associations. In many naturally occurring graphs, we observe complex relationships involving more than two nodes, e.g., co-authorship, co-citation, email communication, etc. Hypergraphs provide a flexible and natural modeling tool to model such complex relationships. A hypergraph is a generalisation of a simple graph in which an edge (a.k.a., hyperedge) can connect any number of nodes. While simple graph edges connect pairs of nodes (pairwise relationships), hyperedges can connect an arbitrary number of nodes (and thus capture complex relationships). For example, in a co-authorship network modeled as a hypergraph, each node represents a paper and each hyperedge represents an author and connects all papers co-authored by the author. Because of the obvious existence of such complex relationships in many real-world networks, the problem of learning with hypergraphs assumes significance (Zhou, Huang, and Scholkopf 2007; Hein et al. 2013;
In this work, we consider the problem of hypergraph-based semi supervised classification. As in simple graphs, only a small portion of the nodes in the hypergraph are labeled, and the objective is to assign labels to rest of the nodes while utilising the hypergraph structure. While a few methods for hypergraph-based SSL using non-neural methods have been proposed (Zhou, Huang, and Schölkopf 2007; Hein et al. 2013; Zhang et al. 2017), GCNs for hypergraphs is still unexplored and we fill this gap in the paper and make the following contributions:

- We propose HyperGCN, a novel graph convolutional network (GCN) for hypergraph-based semi-supervised classification. To the best of our knowledge, this is the first GCN-based method for hypergraphs.
- In contrast to previous non-neural methods, HyperGCN is able to effectively incorporate and revise features on the nodes of the hypergraph.
- Through extensive experiments on multiple real-world datasets, we demonstrate HyperGCN’s effectiveness compared to other state-of-the-art baselines.

We have released HyperGCN’s source code and all the datasets used in the paper (as supplementary material).

Related work

In this section, we briefly review related work in deep learning on graphs and learning on hypergraphs.

Deep learning on graphs: Geometric deep learning (Bronstein et al. 2017) is an umbrella phrase for emerging techniques attempting to generalise (structured) deep neural network models to non-Euclidean domains such as graphs and manifolds. The earliest attempts to generalise neural networks to graphs embed each node in an Euclidean space with a recurrent neural network (RNN) and use those embeddings as features for classification or regression of nodes or graphs (Gori, Monfardini, and Scarselli 2005; Scarselli et al. 2009).

A CNN-like deep neural neural network on graphs was later formulated in the spectral domain in a pioneering work (Bruna et al. 2014) by a mathematically sound definition of convolution on graph employing the analogy between the classical Fourier transforms and projections onto the eigen basis of the graph Laplacian operator (Hammond, Vandergheynst, and Gribonval 2011). Initial works proposed to learn smooth spectral multipliers of the graph Laplacian, although at high computational cost (Bruna et al. 2014; Henaff, Bruna, and LeCun 2015). To resolve the computational bottleneck and avoid the expensive computation of eigenvectors, the ChebNet framework (Defferrard, Bresson, and Vandergheynst 2016) learns Chebyshev polynomials of the graph Laplacian (hence the name ChebNet). The graph convolutional network (GCN) (Kipf and Welling 2017) is a simplified ChebNet framework that uses simple filters operating on 1-hop local neighborhoods of the graph.

A second formulation of convolution on graph is in the spatial domain (or equivalently in the vertex domain) where the localisation property is provided by construction. The first formulation of a spatial CNN-like neural network on graph generalised standard molecular feature extraction methods based on circular fingerprints (Duvenaud et al. 2015). Subsequently, all of the above types (RNN, spectral CNN, spatial CNN on graph) were unified into a single message passing neural network (MPNN) framework (Gilmer et al. 2017) and a variant of MPNN has been shown to achieve state-of-the-art results on an important molecular property prediction benchmark.

The reader is referred to a comprehensive literature review (Bronstein et al. 2017) and a survey (Hamilton, Ying, and Leskovec 2017) on this topic of deep learning on graphs. To the best of our knowledge all the methods for deep learning on graphs existing in literature assume existence of pairwise relationships between nodes. Below, we give an overview of related research in learning on hypergraphs where relationships go beyond pairwise.

Learning on hypergraphs: The seminal work of (Zhou, Huang, and Schölkopf 2007) generalised the powerful methodology of spectral clustering to hypergraphs and further inspired algorithms for hypergraph embedding and semi-supervised classification of hypernodes. The methods in the work, however, essentially constructed a simple graph starting with the structure of the initial hypergraph. There are two standard ways of approximating hypergraphs using simple graphs and they are clique and star expansions (Agarwal, Branson, and Belongie 2014). Another line of work uses mathematically appealing tensor methods (Shashua, Zass, and Hazan 2006; Bulò and Pelillo 2009; Kolda and Bader 2009), but they are limited to k-uniform hypergraphs.

Recent developments, however, work for arbitrary hypergraphs and fully exploit the hypergraph structure. For example, methods using a family of regularisation functionals on the total variation on hypergraphs have shown to be superior to methods based on the clique expansion for semi-supervised classification (Hein et al. 2013). In a follow-up work, confidence intervals and a simpler subgradient based approach for semi-supervised classification has been shown to be more effective (Zhang et al. 2017).

The clique expansion approximation, nonetheless, has been shown to be effective for multi-view, multi-relational transductive learning (Satchidanand, Ananthapadmanaban, and Ravindr (2015) and for learning on partial-order hypergraphs (Feng et al. 2018) which have partially ordering relationships among the hypernodes in each hyperedge (such relationships commonly exist for example in users ratings on movies and monthly income of customers).

Graph-based semi-supervised learning: In graph-based semi-supervised learning, researchers have shown that using unlabeled data in training can improve learning accuracy significantly. Heavily influential books in this line of work include (Chapelle, Scholkopf, and Zien 2010; Zhu et al. 2009; Subramanya and Talukdar 2014).

GCN on a heterogenous graph: GCN-like neural networks have been recently scaled for web-scale recommender systems (Ying et al. 2018). The PinSAGE framework (Ying et al. 2018) is currently being deployed at Pinterest to gen-
erate high-quality item recommendations. The graph is a bipartite star graph consisting of user pins on one side of the partition and boards on the other side. It should be pointed out that the Pinterest heterogeneous data consisting of user pins and boards can also be modeled using hypergraphs. Each board contains a collection of pins that a Pinterest user deems are thematically similar and hence these pins are involved in a higher-order relationship (hyperedge). PinSAGE can handle unseen nodes at test time but our work assumes all the nodes are present in training.

Background: Graph Convolutional Network

In this section, we briefly present how a graph convolution network (GCN) can be used for semi-supervised node classification. The symbols used throughout this paper and the supplementary are provided in Table 1.

Let $G = (V,E)$, with $N = |V|$, be a simple undirected graph with the adjacency matrix $A \in \mathbb{R}^{N \times N}$, and data matrix $X \in \mathbb{R}^{N \times p}$. The data matrix has $p$-dimensional real-valued vector representations for each node in the graph.

Graph convolution as a linear function of the graph Laplacian

The basic formulation of GCN (Kipf and Welling 2017) stems from the convolution theorem (Mallat 1999) and it can be shown that the convolution $C$ of a real-valued graph signal $S \in \mathbb{R}^N$ and a filter signal $F \in \mathbb{R}^N$ is approximately:

$$C \approx \left( w_0 + w_1 \tilde{L} \right) S,$$

where $w_0$ and $w_1$ are the learned weights, and $\tilde{L} = \frac{2L}{\lambda_N} - I$ is the scaled graph Laplacian, $\lambda_N$ is the largest eigenvalue of the symmetrically normalised graph Laplacian $L = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$ where $D = \text{diag}(d_1, \cdots, d_N)$ is the diagonal degree matrix with elements $d_i = \sum_{j=1,j \neq i}^N A_{ij}$. The filter $F$ depends on the structure of the graph (the graph Laplacian $L$). The detailed derivation from the convolution theorem uses existing tools from graph signal processing (Shuman et al. 2013; Hammond, Vanderheynst, and Gribonval 2011; Bronstein et al. 2017) and is provided in the supplementary material. The key point here is that the convolution of two graph signals is a linear function of the graph Laplacian $L$.

With further simplifications, it can be shown that the output of graph convolution for $p$ different graph signals contained in the data matrix $X \in \mathbb{R}^{N \times p}$ with the learned weight matrix $\Theta \in \mathbb{R}^{p \times r}$ with $r$ hidden units is

$$A X \Theta$$

where $\tilde{A} = \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}}$, $\tilde{A} = A + I$, and $\tilde{D}_{ii} = \sum_{j=1}^N \tilde{A}_{ij}$. The proof of the above graph convolution involves a renormalisation trick (Kipf and Welling 2017) and is also provided in the supplementary material.

GCN (Kipf and Welling 2017)

GCN is conditioned on both the adjacency matrix $A$ (underlying graph structure) and the data matrix $X$ (input features). This allows us to relax certain assumptions typically made in graph-based SSL; for example, the cluster assumption (Chapelle, Weston, and Schölkopf 2003) made by the explicit Laplacian-based regularisation methods. This setting is especially powerful in scenarios where the adjacency matrix contains information not present in the data (such as citation links between documents in a citation network or relations in a knowledge graph). The forward model for a simple two-layer GCN takes the following simple form:

$$Z = f_{GCN}(X, A) = \text{softmax} \left( \tilde{A} \text{ReLU} \left( \tilde{A} X \Theta^{(0)} \right) \Theta^{(1)} \right),$$

where $\Theta^{(0)} \in \mathbb{R}^{p \times h}$ is an input-to-hidden weight matrix for a hidden layer with $h$ hidden units and $\Theta^{(1)} \in \mathbb{R}^{h \times r}$ is a hidden-to-output weight matrix. The softmax activation function is defined as $\text{softmax}(x_i) = \frac{\exp(x_i)}{\sum_{j=1}^N \exp(x_j)}$ and applied row-wise.

GCN training for semi-supervised learning:

For semi-supervised multi-class classification with $q$ classes, we minimise the cross-entropy error over the set of labeled examples, $\mathcal{V}_L$.

$$\mathcal{L} = - \sum_{i \in \mathcal{V}_L} \sum_{j=1}^q Y_{ij} \ln Z_{ij}.$$  

The weights of the graph convolutional network, viz. $\Theta^{(0)}$ and $\Theta^{(1)}$, are trained using gradient descent.

HyperGCN: Hypergraph Convolutional Network for Semi-supervised Classification

We consider semi-supervised hypernode classification on an undirected hypergraph $H = (V,E)$ with $|V| = n$, $|E| = m$ and a small set $\mathcal{V}_L$ of labeled hypernodes. The structure of the hypergraph is encoded in a binary incidence matrix $H \in \{0,1\}^{n \times m}$ which is defined as follows.

$$H_{ve} = \begin{cases} 1 & v \in e, \\ 0 & v \notin e \end{cases}.$$
The data matrix $X$ associated with a feature vector $x$ are likely to share the same label (Zhang et al. 2017). Suppose in the same hyperedge are similar and hence the hypernodes in the same hyperedge are similar and hence all the hypernodes in the set $V \setminus V_2$. 

**Overview:** The crucial working principle here is that the hypernodes in the same hyperedge are similar and hence are likely to share the same label (Zhang et al. 2017). Suppose we use $\{ h_v : v \in V \}$ to denote some representation of the hypernodes in $V$, then, for any $e \in E$, the function $\max_{i,j \in e} ||h_i - h_j||^2$ will be “small” only if vectors corresponding to the hypernodes in $e$ are “close” to each other. Therefore, $\sum_{e \in E} \max_{i,j \in e} ||h_i - h_j||^2$ as a regulariser is likely to achieve the objective of the hypernodes in the same hyperedge having similar representations. However, instead of using it as an explicit regulariser, we can achieve the same goal by using GCN over an appropriately defined Laplacian of the hypergraph. In other words, we use the notion of hypergraph Laplacian as an implicit regulariser which achieves this objective.

Fortunately, a hypergraph Laplacian with the same underlying motivation as stated above was proposed in (Chan et al. 2018; Louis 2015). We present this Laplacian first. Then we run GCN over the simple graph associated with this hypergraph Laplacian. We call the resulting method HyperGCN.

One epoch of HyperGCN is pictorially shown in Figure 1.

**Hypergraph Laplacian**

As shown in Equation 2, the key element for a GCN is the graph Laplacian of the given graph $G$. Thus, in order to develop a GCN-based SSL method for hypergraphs, we first need to define a Laplacian for hypergraphs. There can be many natural ways of extending the notion of graph Laplacians to hypergraphs. One such way, proposed by (Chan et al. 2018) (see also (Louis 2015)), is a non-linear function $L : \mathbb{R}^n \rightarrow \mathbb{R}^n$ (the Laplacian matrix for graphs can be viewed as a linear function $L : \mathbb{R}^n \rightarrow \mathbb{R}^n$).

**Definition 1** (Hypergraph Laplacian (Chan et al. 2018; Louis 2015)). Given a real-valued signal $S \in \mathbb{R}^n$ defined on the hypernodes, $L(S)$ is computed as follows.

For each hyperedge $e \in E$, let $(i_e, j_e) := \arg\max_{i,j \in e} |S_i - S_j|$, breaking ties randomly. 

A weighted graph $G_S$ on the vertex set $V$ is constructed by adding edges $\{i_e, j_e\} : e \in E$ with weights $w(\{i_e, j_e\}) := w(e)$ to $G_S$, where $w(e)$ is the weight of the hyperedge $e$. Next, to each vertex $v$, self-loops of sufficient weight are added such that the degree of the vertex in $G_S$ is equal to $d_v$. Let $A_S$ denote the weighted adjacency matrix of the graph $G_S$.

3. The symmetrically normalised hypergraph Laplacian is defined as follows.

$$L(S) := (I - D^{-\frac{1}{2}} A_S D^{-\frac{1}{2}})S. \quad (6)$$

**HyperGCN**

By following the Laplacian construction steps outlined in Section 2, we end up with the simple graph $G_S$ with normalized adjacency matrix $A_S$. We now perform GCN over this simple graph $G_S$. The graph convolution operation in Equation (4), when applied to a hypernode $v \in V$ in the simple graph $G_S$, can be rewritten in the neural message-passing framework (Gilmer et al. 2017) using the iterative equation shown below.

$$h_v^{(\tau + 1)} = \sigma \left( (\Theta^{(\tau)})^T \sum_{u \in N(v)} ([A_S^{(\tau)}]_{v,u} \cdot h_u^{(\tau)}) \right), \quad (7)$$

Here, $\tau$ is epoch number, $h_v^{(\tau + 1)}$ is the new hidden layer representation of node $v$, $\sigma$ is a non-linear activation function, $\Theta$ is a matrix of learned weights, $N(u)$ is the set of neighbours of $u$, $[A_S^{(\tau)}]_{v,u}$ is the weight on the edge $\{v, u\}$ after normalisation, and $h_v^{(\tau)}$ is the previous hidden layer representation of the neighbour $u$. We note that along with the

The problem of breaking ties in choosing $i_e$ (resp. $j_e$) is a non-trivial problem as shown in (Chan et al. 2017). Breaking ties randomly was proposed in (Louis 2015), but (Chan et al. 2018) showed that this might not work for all applications (see Chan et al. 2018 for more details). (Chan et al. 2018) gave a way to break ties, and gave a proof of correctness for their tie-breaking rule for the problems they studied. We chose to break ties randomly because of its simplicity and its efficiency.
embeddings of the hypernodes, the adjacency matrix is also re-estimated in each epoch.

Figure 1 shows a hypernode \( v \) with five hyperedges incident on it. We consider exactly one representative simple edge for each hyperedge \( e \in E \) given by \((i_e, j_e)\) where \((i_e, j_e) = \arg \max_{i,j:|e|=1} ||(h^\tau)^T (h^\tau_i - h^\tau_j)||_2 \) for epoch \( \tau \). Because of this consideration, the hypernode \( v \) may not be a part of all representative simple edges (only three shown in figure). We then use traditional Graph Convolution Operation (7) on node \( v \) considering only the simple edges incident on it. Note that we apply the operation on each hypernode \( v \in V \) in each epoch \( \tau \) of training until there is no change in hidden representations or weights.

Connection to total variation on hypergraphs: Our HyperGCN model can be seen as performing implicit regularisation based on the total variation on hypergraphs (Hein et al. 2013). In that prior work, explicit regularisation and only the hypergraph structure is used for node classification in the SSL setting. HyperGCN, on the other hand, use both the hypergraph structure and can also exploit any available features on the hypernodes, e.g., text attributes for documents.

Improving HyperGCN with mediators

One peculiar aspect of the hypergraph Laplacian discussed is that each hyperedge \( e \) is represented by a single pairwise simple edge \( \{i_e, j_e\} \) (with this simple edge potentially changing from epoch to epoch). This hypergraph Laplacian ignores the hypernodes in \( K_e := \{ k \in e : k \neq i_e, k \neq j_e \} \) in the given epoch. Recently, it has been shown that a generalised hypergraph Laplacian in which the hypernodes in \( K_e \) act as “mediators” (Chan and Liang 2018) satisfies all the properties satisfied by the Laplacian given by (Chan et al. 2018) (which we discussed briefly above). The two Laplacians are pictorially compared in Figure 2. Note that if the hyperedge is of size 2, we connect \( i_e \) and \( j_e \) with an edge. We also run a GCN on the simple graph associated with the hypergraph Laplacian with mediators (Chan and Liang 2018) (right in Figure 2).

Formal details: Closely following the notations of (Chan and Liang 2018), we denote \( \{e\} := e \cup \{0\} \) where 0 is a special index that does not refer to any hypernode. Mathematically, each hyperedge \( e \in E \) is equipped with non-negative constants \( \beta^e_j : j \in \{e\} \) such that \( \sum_{j \in \{e\}} \beta^e_j = 1 \). Now, \( \beta^e_0 = 1 \) refers to the Laplacian of (Louis 2015; Chan et al. 2018). We compare \( \beta^e_0 = 1 \) (left) and \( \beta^e_j = \frac{1}{|e|} \) (right) in figure 2. \( \beta^e_j = \frac{1}{|e|} \) means that every hypernode in a hyperedge is equally important as the mediators. It does not have anything to do with the weights on the edges. We use weights \( \frac{1}{|e|} \) for all edges for normalisation.

We call the method which runs GCN using the left Laplacian in Figure 2 as HyperGCN(\( \beta^e_0 = 1 \)) and the method that runs GCN using the right Laplacian (with mediators) as HyperGCN (\( \beta^e_j = \frac{1}{|e|}, \forall j \in e \)).

Experiments

We compared HyperGCN against two baselines:

- **Zhang et al. ICML 2017**: We used the confidence interval and subgradient method approach of (Zhang et al. 2017) as the main baseline for all our experiments for real-world datasets. We note that this method has consistently been shown to be superior to the primal dual hybrid gradient (PDHG) of (Hein et al. 2013) and also (Zhou, Huang, and Schölkopf 2007). Hence, we did not use these other previous methods as baselines, and directly compared HyperGCN against Zhang et al. ICML 2017.

- **GCN on clique expansion**: A fairly straightforward way to approximate the given hypergraph with a simple graph is by introducing pairwise connections (edges) between all pairs of hypernodes in each hyperedge (Zhou, Huang, and Schölkopf 2007). This approximation is commonly known as the clique expansion of the hypergraph (Agarwal, Branson, and Belongie 2006), because it expands each hyperedge of size \( s \) into an \( s \)-clique. The (weighted) adjacency of the clique expansion (CE) is then given by \( A_{CE} = HH^T - D_V \) where \( D_V \in \mathbb{R}^{n \times n} \) is a diagonal matrix of node degrees (Zhou, Huang, and Schölkopf 2007). We use \( A_{CE} \) in Equation 4 for the GCN on the clique expansion of the given hypergraph.
Table 2: Summary of the document classification datasets used in the experiments in the experiments.

|                      | cora (co-authorship) | cora (co-citation) | citeseer (co-citation) |
|----------------------|----------------------|--------------------|------------------------|
| number of hypernodes, $|V| | 2708 | 2708 | 3312 |
| number of hyperedges, $|E| | 1072 | 1579 | 1079 |
| number of features (vocabulary size) | 1433 | 1433 | 3703 |
| number of classes, $|q| | 7 | 7 | 6 |

| $|V_L|$ | Zhang et al. ICML 17 | GCN on clique expansion | HyperGCN ($\beta^e_j = 1$) | HyperGCN ($\beta^e_j = \frac{1}{|\mathcal{P}|}$, $\forall j \in e$) |
|------|----------------------|------------------------|-----------------------------|------------------------------------------------|-----------------------------|
| 21   | 76.66 ± 0.70         | 60.74 ± 7.3            | 62.89 ± 6.5                 | 55.43 ± 7.6                                      |
| 42   | 67.72 ± 0.60         | 45.23 ± 5.0            | 50.26 ± 4.8                 | 43.86 ± 4.8                                      |
| 63   | 63.1 ± 0.58          | 39.91 ± 3.9            | 44.69 ± 3.6                 | 38.96 ± 3.4                                      |
| 84   | 62.89 ± 0.57         | 36.02 ± 3.1            | 41.13 ± 3.0                 | 35.12 ± 1.9                                      |
| 98   | 58.55 ± 0.53         | 34.08 ± 2.4            | 39.01 ± 2.4                 | 33.83 ± 1.8                                      |

| $|V_L|$ | Zhang et al. ICML 17 | GCN on clique expansion | HyperGCN ($\beta^e_j = 1$) | HyperGCN ($\beta^e_j = \frac{1}{|\mathcal{P}|}$, $\forall j \in e$) |
|------|----------------------|------------------------|-----------------------------|------------------------------------------------|-----------------------------|
| 119  | 57.38 ± 0.53         | 33.42 ± 1.7            | 37.97 ± 2.4                 | 31.50 ± 1.9                                      |
| 140  | 55.45 ± 0.55         | 31.90 ± 1.9            | 36.2 ± 2.2                  | 30.08 ± 1.8                                      |
| 161  | 53.78 ± 0.52         | 31.2 ± 1.6             | 34.9 ± 1.8                  | 29.17 ± 1.7                                      |
| 182  | 52.43 ± 0.33         | 29.8 ± 1.8             | 33.37 ± 1.7                 | 29.09 ± 1.6                                      |
| 203  | 51.44 ± 0.32         | 28.9 ± 1.5             | 32.78 ± 1.6                 | 29.08 ± 1.4                                      |

Table 3: Mean test error ± standard deviation (lower is better) over 100 trials on cora co-authorship hypergraph for different values of $|V_L|$. We randomly sampled the same number of labeled hypernodes from each class and hence we chose each $|V_L|$ to be divisible by $q$ and close to a multiple of 20.

Note HyperGCN($\beta^e_j = 1$) has each hyperedge converted to a pairwise edge while HyperGCN($\beta^e_j = \frac{1}{|\mathcal{P}|}$, $\forall j \in e$) has each hyperedge of size $s > 2$ converted to a subgraph of $2s – 4$ edges as opposed to $^*C_2$ for GCN on clique expansion.

We conducted experiments on three real-world datasets. Two datasets have co-citation relationships, i.e., all documents cited by a document are connected by a hyperedge; and one dataset has co-authorship relationships, i.e., all documents co-authored by an author are in one hyperedge. Co-citation and co-authorship relationships, clearly, are natural occurrences of higher order relationships in the real world. For example, all references of a document (co-citation) or all occurrences of higher order relationships in the real world.

Co-authorship data: We used the author data^2 to get the co-authorship hypergraph for cora.

Co-citation data: We used citeseer and cora^3 for co-citation relationships.

We removed hyperedges which had exactly one hypernode as our focus in this work is on hyperedges with two or more hypernodes. The task for each dataset is to predict the topic to which a document belongs (multi-class classification). Each hypernode (document) is represented by bag-of-words features. The datasets are summarised in Table 2.

We trained HyperGCN (with both Laplacians) and GCN on clique expansion for full 200 epochs and used the same set of hyperparameters as in (Kipf and Welling 2017). We report the mean test error and standard deviation over 100 trials for each value of $|V_L|$. Note that we randomly sample the same number of labeled examples from each class for all the models in all the datasets. As a result, we have $|V_L|$ numbers divisible by the number of classes for each dataset.

**Discussion of results**

The results on the co-authorship data are shown in Table 3 while the results on the two co-citation datasets are shown in Tables 4 and 5. Firstly, we observe that HyperGCN($\beta^e_j = 1$) performs better than the state-of-the-art non-neural baseline (Zhang et al. 2017). We believe this is because of the powerful feature extraction capability of neural methods. The non-neural baseline uses only the hypergraph structure and does not take into account the text-attribute bag-of-word features for learning. We also observe that HyperGCN($\beta^e_j = 0$) does not do better than GCN on clique expansion because, in line with our intuition, only two hypernodes viz. $i_e, j_e$ of each hyperedge $e$ (and not all) contribute to a pairwise edge in a given epoch. Clique expansion constructs a clique for each hyperedge and hence takes into account all the hypernodes in hyperedge in each epoch of training. However, we observe that HyperGCN ($\beta^e_j = \frac{1}{|\mathcal{P}|}$, $\forall j \in e$) is able to outperform GCN on clique expansion for all but one value of $|V_L|$ for co-authorship and for small values of $|V_L|$ in all the datasets. Because GCN on clique expansion connects all the hypernodes in a hyperedge with pairwise relationships it does feature mixing (Li, Han, and Wu 2018) of too many nodes potentially belonging to different labels. Intuitively, HyperGCN ($\beta^e_j = \frac{1}{|\mathcal{P}|}$, $\forall j \in e$) mixes the features (Li, Han, and Wu 2018) of all the hypernodes in $K_e$ with those of $i_e$ and $j_e$ separately. Hence, the issue of connecting too many nodes potentially belonging to different labels is less pronounced. Finally, we observe that for larger values of $|V_L|$, GCN on clique expansion is able to learn and extract effec-

^2https://people.cs.umass.edu/mccallum/data.html
^3https://linqs.soe.ucsc.edu/data
Table 4: Results of the different models on cora co-citation hypergraph. We observe that HyperGCN($\beta_e = \frac{1}{|e|}$, $\forall j \in e$) outperforms the baselines for small number of labeled points ($|V_L| \approx 20$, 40) and is competitive with GCN on clique expansion for increasing supervision.

Table 5: Results of the different models on citeseer co-citation hypergraph. We observe that HyperGCN($\beta_j = \frac{1}{|j|}$, $\forall j \in e$) outperforms the baselines for small number of labeled points ($|V_L| \approx 20$, 40) and is competitive with GCN on clique expansion for increasing supervision.

tive features for classification (esp. in co-citation networks).

In summary, we conclude that HyperGCN, is a principled approach to hypergraph-based SSL. Further, HyperGCN($\beta_j = \frac{1}{|j|}$, $\forall j \in e$) is an effective method with very minimal supervision ($|V_L| \approx 20$, 40) for semi-supervised hypernode classification over hypergraphs. It outperforms GCN on clique expansion almost consistently for the cora co-authorship hypergraph and is competitive with GCN on clique expansion for larger values of $|V_L|$ for all the datasets (observed in all the Tables).

Experiments on datasets with categorical attributes

A standard practice in hypergraph-based SSL research is constructing hypergraphs from categorical data (Zhou, Huang, and Schölkopf 2007; Hein et al. 2013; Zhang et al. 2017). Instances with the same value of a categorical attribute are connected by a hyperedge. We have pushed the results of our approach on hypergraphs constructed from categorical data to the supplementary.

Limitations and future work

We have introduced HyperGCN, a novel neural approach for hypergraph-based semi-supervised classification. To the best of our knowledge, this is the first GCN-based method for hypergraphs. HyperGCN is capable of encoding both hypergraph structure and hypernode features in an effective manner for improved semi-supervised classification.

There are at least a couple of ways in which our work could be extended. For example, approaches that use self-training and co-training with random walk (Li, Han, and Wu 2018), pointwise mutual semantic information (Zhuang and Ma 2018), and attention (Velicković et al. 2018) have improved results on graph-based semi-supervised learning tasks. HyperGCN may be augmented with such approaches for even more improved performance. On the hypergraph side, our HyperGCN model currently is designed for undirected hypergraphs. Extending the model for directed hypergraphs (where the direction captures a casual relationship) (Zhang et al. 2017), and partial-order hypergraphs (Feng et al. 2018) can be an interesting avenue for further research. Investigating the recently proposed p-Laplacians for sub-modular hypergraphs (Li and Milenkovic 2018) is also an interesting direction.

The proposed HyperGCN framework inherently assumes the presence of both training and test data (transductive in nature). In real world scenarios however, test data may not be readily available, because the hypergraph maybe constantly expanding with new hypernodes and hyperedges (new documents in a co-citation graph, or new authors in a co-authorship graph, or new boards and pins in the Pinterest graph (Ying et al. 2018)). Such scenarios require the model to be able to learn only from a training set of hypernodes and generalise well to any augmentation of the graph (an inductive scheme). We leave extending this framework for inductive settings for future work.

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**Supplementary material**

We show how the graph convolutional network (GCN) (Kipf and Welling 2017) has its roots from the convolution theorem (Mallat 1999).

**Graph signal processing**

We now briefly review essential concepts of graph signal processing that are important in the construction of ChebNet and graph convolutional networks. We need convolutions on graphs defined in the spectral domain. Similar to regular 1-D or 2-D signals, real-valued graph signals can be efficiently analysed via harmonic analysis and processed in the spectral domain (Shuman et al. 2013). To define spectral convolution, we note that the convolution theorem (Mallat 1999) generalises from classical discrete signal processing to take into account arbitrary graphs (Sandryhaila and Moura 2013).

Informally, the convolution theorem says the convolution of two signals in one domain (say time domain) equals point-wise multiplication of the signals in the other domain (frequency domain). More formally, given a graph signal, $S : V \rightarrow \mathbb{R}$, $S \in \mathbb{R}^N$, and a filter signal, $F : V \rightarrow \mathbb{R}$, $F \in \mathbb{R}^N$, both of which are defined in the vertex domain (time domain), the convolution of the two signals, $C = S \ast F$, satisfies

$$\hat{C} = \hat{S} \circ \hat{F}$$

where $\hat{S}$, $\hat{F}$, $\hat{C}$ are the graph signals in the spectral domain (frequency domain) corresponding, respectively, to $S$, $F$ and $S \ast F$.

An essential operator for computing graph signals in the spectral domain is the symmetrically normalised graph Laplacian operator of $G$, defined as

$$L = I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$$

where $D = \text{diag}(d_1, \ldots, d_N)$ is the diagonal degree matrix with elements $d_i = \sum_{j=1, j \neq i} A_{ij}$. As the above graph Laplacian operator, $L$, is a real symmetric and positive semidefinite matrix, it admits spectral eigen decomposition of the form $L = U \Lambda U^T$, where, $U = [u_1, \cdots, u_N]$ forms an orthonormal basis of eigenvectors and $\Lambda = \text{diag}(\lambda_1, \cdots, \lambda_N)$ is the diagonal matrix of the corresponding eigenvalues with $0 = \lambda_1 \leq \cdots \leq \lambda_N \leq 2$.

The eigenvectors form a Fourier basis and the eigenvalues carry a notion of frequencies as in classical Fourier analysis. The graph Fourier transform of a graph signal $S = (S_1, \cdots, S_N) \in \mathbb{R}^N$, is thus defined as $\hat{S} = U^T S$ and the inverse graph Fourier transform turns out to be $S = U \hat{S}$, which is the same as,

$$S_i = \sum_{j=1}^N \hat{S}(\lambda_j)u_j(i) \quad \text{for} \quad i \in V = \{1, \cdots, N\}$$

The convolution theorem generalised to graph signals 8 can thus be rewritten as $U^T C = \hat{S} \circ \hat{F}$. It follows that $C = U(\hat{S} \circ \hat{F})$, which is the same as

$$C_i = \sum_{j=1}^N \hat{S}(\lambda_j)\hat{F}(\lambda_j)u_j(i) \quad \text{for} \quad i \in V = \{1, \cdots, N\}$$

**ChebNet convolution**

We could use a non-parametric filter $\hat{F}(\lambda_j) = \theta_j$ for $j \in \{1, \cdots, N\}$ but there are two limitations: (i) they are not localised in space (ii) their learning complexity is $O(N)$. The two limitations above contrast with contrast with with traditional CNNs where the filters are localised in space and the learning complexity is independent of the input size. It is proposed by (Defferrard, Bresson, and Vandergheynst 2016) to use a polynomial filter to overcome the limitations. A polynomial filter is defined as:

$$\hat{F}(\lambda_j) = \sum_{k=0}^{K} w_k \lambda_j^k \quad \text{for} \quad j \in \{1, \cdots, N\}$$

Using 12 in 11, we get

$$C_i = \sum_{j=1}^N \hat{S}(\lambda_j) \left( \sum_{k=0}^{K} w_k \lambda_j^k \right) u_j(i) \quad \text{for} \quad i \in V = \{1, \cdots, N\}$$

From the definition of an eigenvalue, we have $Lu_j = \lambda_j u_j$ and hence $L^k u_j = \lambda_j^k u_j$ for a positive integer $k$ and for $j \in \{1, \cdots, N\}$. Therefore,

$$C_i = \sum_{j=1}^N \hat{S}(\lambda_j) \left( \sum_{k=0}^{K} w_k L_j^k \right) u_j(i) = \left( \sum_{k=0}^{K} w_k L_j^k \right) \sum_{j=1}^N \hat{S}(\lambda_j) u_j(i)$$

$$= \left( \sum_{k=0}^{K} w_k L_j^k \right) S_i$$

Hence,

$$C = \left( \sum_{k=0}^{K} w_k L^k \right) S$$

The graph convolution provided by Eq. 14 uses the monomial basis $1, x, \cdots, x^K$ to learn filter weights. Monomial bases are not optimal for training and not stable under perturbations because they do not form an orthogonal basis. It is proposed by (Defferrard, Bresson, and Vandergheynst 2016) to use the orthogonal Chebychev polynomials (Hammond, Vandergheynst, and Gribonval 2011) (and hence the name ChebNet) to recursively compute the powers of the graph Laplacian.

A Chebychev polynomial $T_k(x)$ of order $k$ can be computed recursively by the stable recurrence relation $T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$ with $T_0 = 1$ and $T_1 = x$. These polynomials form an orthogonal basis in $[-1, 1]$. Note that the eigenvalues of the symmetrically normalised graph Laplacian lie in the range $[0, 2]$. Through appropriate scaling
of eigenvalues from $[0, 2]$ to $[-1, 1]$ i.e. $\tilde{\lambda}_j = \frac{2\lambda_j}{\sqrt{\lambda_N}} - 1$ for $j = \{1, \cdots, N\}$, where $\lambda_N$ is the largest eigenvalue, the filter in 12 can be parametrised as the truncated expansion

$$F(\lambda_j) = \sum_{k=0}^{K} w_k T_k(\tilde{\lambda}_j) \quad \text{for } j = \{1, \cdots, N\} \quad (15)$$

From Eq. 13, it follows that

$$C = \left( \sum_{k=0}^{K} w_k T_k(\tilde{\lambda}) \right) S \quad \text{where } \tilde{\lambda} = \frac{2L}{\lambda_N} - I \quad (16)$$

**Graph convolutional network (GCN): first-order approximation of ChebNet**

The spectral convolution of 16 is $K$-localised since it is a $K^{th}$-order polynomial in the Laplacian i.e. it depends only on nodes that are at most $K$ hops away. (Kipf and Welling 2017) simplify 16 to $K=1$ i.e. they use simple filters operating on 1-hop neighbourhoods of the graph.

More formally,

$$C = \left( w_0 + w_1 \tilde{\lambda} \right) S \quad (17)$$

and also,

$$F(\lambda_j) = w_0 + w_1 \tilde{\lambda}_j \quad \text{for } j = \{1, \cdots, N\} \quad (18)$$

The main motivation here is that 17 is not limited to the explicit parameterisation given by the Chebyshev polynomials. Intuitively such a model cannot overfit on local neighbourhood structures for graphs with very wide node degree distributions, common in real-world graph datasets such as citation networks, social networks, and knowledge graphs.

In this formulation, (Kipf and Welling 2017) further approximate $\lambda_N \approx 2$, as the neural network parameters can adapt to the change in scale during training. To address overfitting issues and to minimise the number of matrix multiplications, they set $w_0 = -w_1 = \theta$. 17 now reduces to

$$C = \theta(I - \tilde{\lambda})S = \theta(2I - L)S = \theta(I + D^{-\frac{1}{2}}AD^{-\frac{1}{2}})S \quad (19)$$

The filter parameter $\theta$ is shared over the whole graph and successive application of a filter of this form $K$ times then effectively convolves the $K^{th}$-order neighbourhood of a node, where $K$ is the number of convolutional layers (depth) of the neural network model. We note that the eigenvalues of $L$ are in $[0, 2]$ and hence the eigenvalues of $2I - L = I + D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ are also in the range $[0, 2]$. Repeated application of this operator can therefore lead to numerical instabilities and exploding/vanishing gradients. To alleviate this problem, a *renormalisation trick* can be used (Kipf and Welling 2017):

$$I + D^{-\frac{1}{2}}AD^{-\frac{1}{2}} \to \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} \quad (20)$$

with $\tilde{A} = A + I$ and $\tilde{D}_{ii} = \sum_{j=1}^{N} \tilde{A}_{ij}$. Generalising the above to $p$ signals contained in the matrix $X \in \mathbb{R}^{N \times p}$ (also called the data matrix), and $r$ filter maps contained in the matrix $\Theta \in \mathbb{R}^{p \times r}$, the output convolved signal matrix will be:

$$\tilde{A}X\Theta \quad \text{where } \tilde{A} = D^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} \quad (21)$$

**GCNs for graph-based semi-supervised node classification**

The GCN is conditioned on both the adjacency matrix $A$ (underlying graph structure) and the data matrix $X$ (input features). This allows us to relax certain assumptions typically made in graph-based SSL, for example, the cluster assumption (Chapelle, Weston, and Schölkopf 2003) made by the explicit Laplacian-based regularisation methods. This setting is especially powerful in scenarios where the adjacency matrix contains information not present in the data (such as citation links between documents in a citation network or relations in a knowledge graph). The forward model for a simple two-layer GCN takes the following simple form:

$$Z = f_{GCN}(X, A) = \text{softmax} \left( \tilde{A} \text{ReLU} \left( \tilde{A}X\Theta^{(0)} \right) \Theta^{(1)} \right) \quad (22)$$

where $\Theta^{(0)} \in \mathbb{R}^{p \times h}$ is an input-to-hidden weight matrix for a hidden layer with $h$ hidden units and $\Theta^{(1)} \in \mathbb{R}^{h \times r}$ is a hidden-to-output weight matrix. The softmax activation function defined as $\text{softmax}(x_i) = \frac{\exp(x_i)}{\sum_i \exp(x_i)}$ is applied row-wise.

**Training** For semi-supervised multi-class classification with $q$ classes, we then evaluate the cross-entropy error over all the set of labeled examples, $\mathcal{V}_L$:

$$\mathcal{L} = - \sum_{i \in \mathcal{V}_L} \sum_{j=1}^{q} Y_{ij} \ln Z_{ij} \quad (23)$$

The weights of the graph convolutional network, viz. $\Theta^{(0)}$ and $\Theta^{(1)}$, are trained using gradient descent. Using efficient sparse-dense matrix multiplications for computing, the computational complexity of evaluating Eq. 22 is $O(|E|phr)$ which is linear in the number of graph edges.

**GCNs as a special form of Laplacian smoothing**

GCNs can be interpreted as a special form of symmetric Laplacian smoothing (Li, Han, and Wu 2018). The Laplacian smoothing (Taubin 1995) on each of the $p$ input channels in the input feature matrix $X \in \mathbb{R}^{N \times p}$ is defined as:

$$x_i = (1 - \gamma)x_i + \gamma \sum_j \frac{A_{ij}}{d_i} x_j \quad i = 1, \cdots, N \quad (24)$$

here $\tilde{A} = A + I$ and $d_i$ is the degree of node $i$. Equivalently the Laplacian smoothing can be written as $\chi = X - \gamma \tilde{D}^{-1}\tilde{L}X = (I - \gamma \tilde{D}^{-1}\tilde{L})X$ where $\tilde{L} = \tilde{D} - \tilde{A}$. Here $0 \leq \gamma \leq 1$ is a parameter which controls the weighting between the feature of the current vertex and those of its neighbours. If we let $\gamma = 1$, and replace the normalised Laplacian $\tilde{D}^{-1}\tilde{L}$ by the symmetrically normalised Laplacian $\tilde{D}^{-\frac{1}{2}}\tilde{L}\tilde{D}^{-\frac{1}{2}}$, then $\chi = (I - \tilde{D}^{-\frac{1}{2}}\tilde{L}\tilde{D}^{-\frac{1}{2}})X = AX$, the same as in the expression 21.

Hence the graph convolution in the GCN is a special form of (symmetric) Laplacian smoothing. The Laplacian
Table 6: Summary of the three UCI datasets used in the experiments in Section 4.5.5.

| property/dataset | mushroom | covertype45 | covertype67 |
|------------------|-----------|-------------|-------------|
| number of hypernodes, | 8124      | 12240       | 37877       |
| number of hyperedges, | 112       | 104         | 125         |
| number of edges in clique expansion | 65,999,376 | 143,008,092 | 1,348,219,153 |
| number of classes, | 2         | 2           | 2           |

Figure 3: Test errors (lower is better) comparing HyperGCN_with_mediators with the non-neural baseline (Zhang et al. 2017) on the UCI datasets. HyperGCN_with_mediators offers superior performance. Comparing against GCN on Clique Expansion is unfair. Please see below for details.

smoothing of Eq. 24 computes the new features of a node as the weighted average of itself and its neighbours. Since nodes in the same cluster tend to be densely connected, the smoothing makes their features similar, which makes the subsequent classification task much easier. Repeated application of Laplacian smoothing many times over leads to over-smoothing - the node features within each connected component of the graph will converge to the same values (Li, Han, and Wu 2018).

Experiments on datasets with categorical attributes

We closely followed the experimental setup of the baseline model (Zhang et al. 2017). We experimented on three different datasets viz., mushroom, covertype45, and covertype67 from the UCI machine learning repository (Dheeru and Karra Taniskidou 2017). Properties of the datasets are summarised in Table 6. The task for each of the three datasets is to predict one of two labels (binary classification) for each unlabeled instance (hypernode). The datasets contain instances with categorical attributes. To construct the hypergraph, we treat each attribute value as a hyperedge, i.e., all instances (hypernodes) with the same attribute value are contained in a hyperedge. Because of this particular definition of a hyperedge clique expansion is destined to produce an almost fully connected graph and hence clique expansion does not have any useful information. So GCN on clique expansion is unfair to compare against.

As in (Zhang et al. 2017), we performed 100 trials for each $|V_L|$ and report the mean accuracy (averaged over the 100 trials). The results are shown in Figure 3. We find that HyperGCN_with_mediators model generally does better than the baselines. We believe that this is because of the powerful feature extraction capability of HyperGCN_with_mediators.

Relevance of SSL: the main reason for performing these experiments, as pointed out in the publicly accessible NIPS reviews of the total variation on hypergraphs (Hein et al. 2013), is to show that the proposed method (the primal-dual hybrid gradient method in their case and the HyperGCN_with_mediators method in our case) has improved results on SSL, even if SSL is not very relevant in the first place.

We do not claim that SSL with HyperGCN_with_mediators is the best way to go about handling these categorical data but we do claim that, given this built hypergraph albeit from non-relational data, it has superior results compared to the previous best non-neural hypergraph-based SSL method (Zhang et al. 2017) in the literature and that is why we have followed their experimental setup.

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4https://papers.nips.cc/paper/4914-the-total-variation-on-hypergraphs-learning-on-hypergraphs-revisited
Multi-class classification with noisy labels

We experimented on a particular subset of 20 news dataset and closely follow the experimental setup of Hein et al. (Hein et al. 2013).