A PAC-Bayesian Approach to Generalization Bounds for Graph Neural Networks

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Abstract

In this paper, we derive generalization bounds for the two primary classes of graph neural networks (GNNs), namely graph convolutional networks (GCNs) and message passing GNNs (MPGNNs), via a PAC-Bayesian approach. Our result reveals that the maximum node degree and spectral norm of the weights govern the generalization bounds of both models. We also show that our bound for GCNs is a natural generalization of the results developed in (Neyshabur et al., 2017) for fully-connected and convolutional neural networks. For message passing GNNs, our PAC-Bayes bound improves over the Rademacher complexity based bound in (Garg et al., 2020), showing a tighter dependency on the maximum node degree and the maximum hidden dimension. The key ingredients of our proofs are a perturbation analysis of GNNs and the generalization of PAC-Bayes analysis to non-homogeneous GNNs. We perform an empirical study on several real-world graph datasets and verify that our PAC-Bayes bound is tighter than others.

1 Introduction

Graph neural networks (GNNs) (Gori et al., 2005; Scarselli et al., 2008; Bronstein et al., 2017; Battaglia et al., 2018) have become very popular recently due to their ability to learn powerful representations from graph-structured data, and have achieved state-of-the-art results in a variety of application domains such as social networks (Hamilton et al., 2017), quantum chemistry (Gilmer et al., 2017), computer vision (Monti et al., 2017), reinforcement learning (Sanchez-Gonzalez et al., 2018), robotics (Casas et al., 2019), and physics (Henrion et al., 2017). Given a graph along with node/edge features, GNNs learn node/edge representations by propagating information on the graph via local computations shared across the nodes/edges. Based on the specific form of local computation employed, GNNs can be divided into two categories: graph convolution based GNNs (Bruna et al., 2013; Duvenaud et al., 2015; Kipf & Welling, 2016) and message passing based GNNs (Li et al., 2015; Dai et al., 2016; Gilmer et al., 2017). The former generalizes the convolution operator from regular graphs (e.g., grids) to ones with arbitrary topology, whereas the latter mimics message passing algorithms and parameterizes the shared functions via neural networks.

Due to the tremendous empirical success of GNNs, there is increasing interest in understanding their theoretical properties. For example, some recent works study their expressiveness (Maron et al., 2018; Xu et al., 2018; Chen et al., 2019), that is, what class of functions can be represented by GNNs. However, only few works investigate why GNNs generalize so well to unseen graphs. They are either restricted to a specific model variant (Verma & Zhang, 2019; Du et al., 2019; Garg et al., 2020) or have loose dependencies on graph statistics (Scarselli et al., 2018).

On the other hand, GNNs have close ties to standard feedforward neural networks, e.g., multi-layer perceptrons (MLPs) and convolutional neural networks (CNNs). In particular, if each i.i.d. sample is viewed as a node, then the whole dataset becomes a graph without edges. Therefore, GNNs can be seen as generalizations of MLPs/CNNs since they model not only the regularities within a sample

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but also the dependencies among samples as defined in the graph. It is therefore natural to ask if we can generalize the recent advancements on generalization bounds for MLPs/CNNs (Harvey et al., 2017; Neyshabur et al., 2017; Bartlett et al., 2017; Dziugaite & Roy, 2017; Arora et al., 2018, 2019) to GNNs, and how would graph structures affect the generalization bounds?

In this paper, we answer the above questions by proving generalization bounds for the two primary classes of GNNs, i.e., graph convolutional networks (GCNs) (Kipf & Welling, 2016) and message-passing GNNs (MPGNNs) (Dai et al., 2016; Jin et al., 2018).

Our generalization bound for GCNs shows an intimate relationship with the bounds for MLPs/CNNs with ReLU activations (Neyshabur et al., 2017; Bartlett et al., 2017). In particular, they share the same term, i.e., the product of the spectral norms of the learned weights at each layer multiplied by a factor that is additive across layers. The bound for GCNs has an additional multiplicative factor \( d^{(l-1)/2} \) where \( d - 1 \) is the maximum node degree and \( l \) is the network depth. Since MLPs/CNNs are special GNNs operating on graphs without edges (i.e., \( d - 1 = 0 \)), the bound for GCNs coincides with the ones for MLPs/CNNs with ReLU activations (Neyshabur et al., 2017) on such degenerated graphs. Therefore, our result is a natural generalization of the existing results for MLPs/CNNs.

Our generalization bound for message passing GNNs reveals that the governing terms of the bound are similar to the ones of GCNs, i.e., the geometric series of the learned weights and the multiplicative factor \( d^{-l} \). The geometric series appears due to the weight sharing across message passing steps, thus corresponding to the product term across layers in GCNs. The term \( d^{-l} \) encodes the key graph statistics. Our bound improves the dependency on the maximum node degree and the maximum hidden dimension compared to the recent Rademacher complexity based bound (Garg et al., 2020). Moreover, we compute the bound values on four real-world graph datasets (e.g., social networks and protein structures) and verify that our bounds are tighter.

In terms of the proof techniques, our analysis follows the PAC-Bayes framework in the seminal work of (Neyshabur et al., 2017) for MLPs/CNNs with ReLU activations. However, we make two distinctive contributions which are customized for GNNs. First, a naive adaptation of the perturbation analysis in (Neyshabur et al., 2017) does not work for GNNs since ReLU is not 1-Lipschitz under the spectral norm, i.e., \( \| \text{ReLU}(X) \|_2 \leq \|X\|_2 \) does not hold for some real matrix \( X \). Instead, we construct the recursion on certain node representations of GNNs like the one with maximum \( \ell_2 \) norm, so that we can perform perturbation analysis with vector 2-norm. Second, in contrast to (Neyshabur et al., 2017) which only handles the homogeneous networks, i.e., \( f(ax) = af(x) \) when \( a \geq 0 \), we properly construct a quantity of the learned weights which 1) provides a way to satisfy the constraints of the previous perturbation analysis and 2) induces a finite covering on the range of the quantity so that the PAC-Bayes bound holds for all possible weights. This generalizes the analysis to non-homogeneous GNNs like typical MPGNNs.

The rest of the paper is organized as follows. In Section 2, we introduce background material necessary for our analysis. We then present our generalization bounds and the comparison to existing results in Section 3. We also provide an empirical study to support our theoretical arguments in Section 4. At last, we discuss the extensions, limitations and some open problems.

2 Background

In this section, we first explain our analysis setup including notation and assumptions. We then describe the two representative GNN models in detail. Finally, we review the PAC-Bayes analysis.

2.1 Analysis Setup

In the following analysis, we consider the \( K \)-class graph classification problem which is common in the GNN literature, where given a graph sample \( z \), we would like to classify it into one of the predefined \( K \) classes. We will discuss extensions to other problems like graph regression in Section 5. Each graph sample \( z \) is a triplet of an adjacency matrix \( A \), node features \( X \in \mathbb{R}^{n \times h_0} \) and output label \( y \in \mathbb{R}^{1 \times K} \), i.e., \( z = (A, X, y) \), where \( n \) is the number of nodes and \( h_0 \) is the input feature dimension. We start our discussion by defining our notations. Let \( N_+^k \) be the first \( k \) positive integers, i.e., \( N_+^k = \{1, 2, \ldots, k\} \), \( \| \cdot \|_p \) the vector \( p \)-norm and \( \| \cdot \|_\| \) the operator norm induced by the vector \( p \)-norm. Further, \( \| \cdot \|_F \) denotes the Frobenius norm of a matrix, \( e \) the base of the natural logarithm function \( \log \), \( A[i, j] \) the \((i, j)\)-th element of matrix \( A \) and \( A[i, :] \) the \( i \)-th row. We use parenthesis
therefore, to avoid the ambiguity, e.g., \((AB)[i, j]\) means the \((i, j)\)-th element of the product matrix \(AB\). We then introduce some terminologies from statistical learning theory and define the sample space as \(Z\), \(z = (A, X, y) \in Z\) where \(X \in \mathcal{X}\) (node feature space) and \(A \in \mathcal{G}\) (graph space), data distribution \(D, z \overset{i.i.d.}{\sim} D\), hypothesis (or model) \(f_w\) where \(f_w \in \mathcal{H}\) (hypothesis class), and training set \(S\) with size \(m, S = \{z_1, \ldots, z_m\}\). We make the following assumptions which also appear in the literature:

A1 Data, i.e., triplets \((A, X, y)\), are i.i.d. samples drawn from some unknown distribution \(D\).

A2 The maximum hidden dimension across all layers is \(h\).

A3 Node feature of any graph is contained in a \(\ell_2\)-ball with radius \(B\). Specifically, we have \(\forall i \in \mathbb{N}^+_n\), the \(i\)-th node feature \(X[i, :] \in \mathcal{X}_{B,h_0} = \{x \in \mathbb{R}^{h_0} | \sum_{j=1}^{h_0} x_j^2 \leq B^2\}\).

A4 We only consider simple graphs (i.e., undirected, no loops\(^1\), and no multi-edges) with maximum node degree as \(d - 1\).

Note that it is straightforward to estimate \(B\) and \(d\) empirically on real-world graph data.

### 2.2 Graph Neural Networks (GNNs)

In this part, we describe the details of the GNN models and the loss function we used for the graph classification problem. The essential idea of GNNs is to propagate information over the graph so that the learned representations capture the dependencies among nodes/edges. We now review two classes of GNNs, GCNs and MPGNNs, which have different mechanisms for propagating information. We choose them since they are the most popular variants and represent two common types of neural networks, i.e., feedforward (GCNs) and recurrent (MPGNNs) neural networks. We discuss the extension of our analysis to other GNN variants in Section 5. For ease of notation, we define the model to be \(f_w \in \mathcal{H} : \mathcal{X} \times \mathcal{G} \to \mathbb{R}^K\) where \(w\) is the vectorization of all model parameters.

**GCNs:** Graph convolutional networks (GCNs) (Kipf & Welling, 2016) for the \(K\)-class graph classification problem can be defined as follows,

\[
H_k = \sigma_k \left( \tilde{L}H_{k-1}W_k \right) \quad \text{(k-th Graph Convolution Layer)}
\]

\[
H_l = \frac{1}{n} 1_n H_{l-1} W_l \quad \text{(Readout Layer),}
\]

where \(k \in \mathbb{N}^+_1\), \(H_k \in \mathbb{R}^{n \times h_k}\) are the node representations/states, \(1_n \in \mathbb{R}^{1 \times n}\) is an all-one vector, \(l\) is the number of layers,\(^2\) and \(W_j\) is the weight matrix of the \(j\)-th layer. The initial node state is the observed node feature \(H_0 = X\). For both GCNs and MPGNNs, we consider \(l > 1\) since otherwise the model degenerates to a linear transformation which does not leverage the graph and is trivial to analyze. Due to assumption A2, \(W_j\) is of size at most \(h \times h\), i.e., \(h_k \leq h\), \(\forall k \in \mathbb{N}^+_1\). The graph Laplacian \(\tilde{L}\) is defined as, \(\tilde{A} = I + A, \tilde{L} = D^{-\frac{1}{2}} \tilde{A} D^{-\frac{1}{2}}\) where \(D\) is the degree matrix of \(A\). Note that the maximum eigenvalue of \(\tilde{L}\) is \(1\) in this case. We absorb the bias into the weight by appending constant \(1\) to the node feature. Typically, GCNs use ReLU as the non-linearity, i.e., \(\sigma_t(x) = \max(0, x), \forall i = 1, \ldots, l - 1\). We use the common mean-readout to obtain the graph representation where \(H_{l-1} \in \mathbb{R}^{n \times h_{l-1}}, W_l \in \mathbb{R}^{h_{l-1} \times K}\), and \(H_l \in \mathbb{R}^{1 \times K}\).

**MPGNNs:** There are multiple variants of message passing GNNs, e.g., (Li et al., 2015; Dai et al., 2016; Gilmer et al., 2017), which share the same algorithmic framework but instantiate a few components differently, e.g., the node state update function. We choose the same class of models as in (Garg et al., 2020) which are popular in the literature (Dai et al., 2016; Jin et al., 2018) in order to

\(^1\)Here loop means an edge that connects a vertex to itself, a.k.a., self-loop.

\(^2\)We count the readout function as a layer to be consistent with the existing analysis of MLPs/CNNs.
fairly compare bounds. This MPGNN model can be written in matrix forms as follows,

\[ M_k = g(C_{out}^T H_{k-1}) \quad (k\text{-th step Message Computation}) \]
\[ \hat{M}_k = C_{in} M_k \quad (k\text{-th step Message Aggregation}) \]
\[ H_k = \phi \left( X W_1 + \rho \left( M_k \right) W_2 \right) \quad (k\text{-th step Node State Update}) \]
\[ H_I = \frac{1}{n} \mathbf{1}_n H_{I-1} W_I \quad \text{ (Readout Layer)} , \]

(2)

where \( k \in \mathbb{N}_0^+ \), \( H_k \in \mathbb{R}^{n \times h} \) are node representations/states and \( H_I \in \mathbb{R}^{1 \times K} \) is the output representation. Here we initialize \( H_0 = \mathbf{0} \). W.l.o.g., we assume \( \forall k \in \mathbb{N}_0^+ \), \( H_k \in \mathbb{R}^{n \times h} \) and \( M_k \in \mathbb{R}^{n \times h} \) since \( h \) is the maximum hidden dimension. \( C_{in} \in \mathbb{R}^{n \times c} \) and \( C_{out} \in \mathbb{R}^{n \times c} \) (\( c \) is the number of edges) are the incidence matrices corresponding to incoming and outgoing nodes respectively. Specifically, rows and columns of \( C_{in} \) and \( C_{out} \) correspond to nodes and edges respectively. \( C_{in}[i,j] = 1 \) indicates that the incoming node of the \( j \)-th edge is the \( i \)-th node. Similarly, \( C_{out}[i,j] = 1 \) indicates that the outgoing node of the \( j \)-th edge is the \( i \)-th node. \( g, \phi, \rho \) are non-linear mappings, e.g., ReLU and Tanh. Technically speaking, \( g : \mathbb{R}^h \rightarrow \mathbb{R}^h \), \( \phi : \mathbb{R}^h \rightarrow \mathbb{R}^h \), and \( \rho : \mathbb{R}^h \rightarrow \mathbb{R}^h \) operate on vector-states of individual node/edge. However, since we share these functions across nodes/edges, we can naturally generalize them to matrix-states, e.g., \( \bar{\phi}(X)[i,:) = \phi(X[i,:]) \). By doing so, the same function could be applied to matrices with varying size of the first dimension. For simplicity, we use \( g, \phi, \rho \) to denote such generalization to matrices. We denote the Lipschitz constants of \( g, \phi, \rho \) under the vector 2-norm as \( C_g, C_{\phi}, C_{\rho} \) respectively. We also assume \( g(0) = 0 \), \( \phi(0) = 0 \), and \( \rho(0) = 0 \) and define the percolation complexity as \( C = C_g C_{\phi} C_{\rho} ||W_2||_2 \) following (Garg et al., 2020).

**Multiclass Margin Loss:** We use the multi-class \( \gamma \)-margin loss following (Bartlett et al., 2017; Neyshabur et al., 2017). The generalization error is defined as,

\[ L_{D,\gamma}(f_w) = \mathbb{P}_{z \sim D} \left( f_w(X, A)[y] \leq \gamma + \max_{j \neq y} f_w(X, A)[j] \right) , \]

(3)

where \( \gamma > 0 \) and \( f_w(X, A) \) is the \( l \)-th layer representations, i.e., \( H_l = f_w(X, A) \). Accordingly, we can define the empirical error as,

\[ L_{S,\gamma}(f_w) = \frac{1}{m} \sum_{i \in S} \mathbf{1} \left( f_w(X, A)[y] \leq \gamma + \max_{j \neq y} f_w(X, A)[j] \right) . \]

(4)

### 2.3 Background of PAC-Bayes Analysis

PAC-Bayes (McAllester, 1999, 2003; Langford & Shawe-Taylor, 2003) takes a Bayesian view of the probably approximately correct (PAC) learning theory (Valiant, 1984). In particular, it assumes that we have a prior distribution \( P \) over the hypothesis class \( \mathcal{H} \) and obtain a posterior distribution \( Q \) over the same support through the learning process on the training set. Therefore, instead of having a deterministic model/hypothesis as in common learning formulations, we have a distribution of models. Under this Bayesian view, we define the generalization error and the empirical error as,

\[ L_{S,\gamma}(Q) = \mathbb{E}_{w \sim Q} [L_{S,\gamma}(f_w)] , \quad L_{D,\gamma}(Q) = \mathbb{E}_{w \sim Q} [L_{D,\gamma}(f_w)] . \]

Since many interesting models like neural networks are deterministic and the exact form of the posterior \( Q \) induced by the learning process and the prior \( P \) is typically unknown, it is unclear how one can perform PAC-Bayes analysis. Fortunately, we can exploit the following result from the PAC-Bayes theory.

**Theorem 2.1.** (McAllester, 2003) (Two-sided) Let \( P \) be a prior distribution over \( \mathcal{H} \) and let \( \delta \in (0, 1) \). Then, with probability \( 1 - \delta \) over the choice of an i.i.d. size-\( m \) training set \( S \) according to \( D \), for all distributions \( Q \) over \( \mathcal{H} \) and any \( \gamma > 0 \), we have

\[ L_{D,\gamma}(Q) \leq L_{S,\gamma}(Q) + \sqrt{\frac{D_{\text{KL}}(Q||P) + \ln \frac{2m}{\delta}}{2(m-1)}} . \]

\(^3\)For undirected graphs, we convert each edge into two directed edges.
Here $D_{KL}$ is the KL-divergence. The nice thing about this result is that the inequality holds for all possible prior $P$ and posterior $Q$ distributions. Hence, we have the freedom to construct specific priors and posteriors so that we can work out the bound. Moreover, McAllester (2003); Neyshabur et al. (2017) provide a general recipe to construct the posterior such that for a large class of models, including deterministic ones, the PAC-Bayes bound can be computed. Taking a neural network as an example, we can choose a prior distribution with some known density, e.g., a fixed Gaussian, over the initial weights. After the learning process, we can add random perturbations to the learned weights from another known distribution as long as the KL-divergence permits an analytical form. This converts the deterministic model into a distribution of models while still obtaining a tractable KL divergence. Leveraging Theorem 2.1 and the above recipe, Neyshabur et al. (2017) obtained the following result which holds for a large class of deterministic models.

**Lemma 2.2.** (Neyshabur et al., 2017) Let $f_w(x) : \mathcal{X} \rightarrow \mathbb{R}^K$ be any model with parameters $w$, and let $P$ be any distribution on the parameters that is independent of the training data. For any $w$, we construct a posterior $Q(w + u)$ by adding any random perturbation $u$ to $w$, s.t., $P(\max_{x \in \mathcal{X}} |f_{w+u}(x) - f_w(x)|_\infty < \frac{\gamma}{4}) > \frac{1}{2}$. Then, for any $\gamma, \delta > 0$, with probability at least $1 - \delta$ over an i.i.d. size-$m$ training set $S$ according to $D$, for any $w$, we have:

$$L_{D,0}(f_w) \leq L_{S,\gamma}(f_w) + \sqrt{\frac{2D_{KL}(Q(w + u)||P)}{2(m - 1)}}.$$ 

This lemma guarantees that, as long as the change of the output brought by the perturbations is small with a large probability, one can obtain the corresponding generalization bound.

## 3 Generalization Bounds

In this section, we present the main results: generalization bounds of GCNs and MPGNNs using a PAC-Bayesian approach. We then relate them to existing generalization bounds of GNNs and draw connections to the bounds of MLPs/CNNs. We summarize the key ideas of the proof in the main text and defer the details to the appendix.

### 3.1 PAC-Bayes Bounds of GCNs

As discussed above, in order to apply Lemma 2.2, we must ensure that the change of the output brought by the weight perturbations is small with a large probability. In the following lemma, we bound this change using the product of the spectral norms of learned weights at each layer and a term depending on some statistics of the graph.

**Lemma 3.1.** (GCN Perturbation Bound) For any $B > 0, l > 1$, let $f_w \in \mathcal{H} : \mathcal{X} \times \mathcal{G} \rightarrow \mathbb{R}^K$ be a $l$-layer GCN. Then for any $w$, and $x \in \mathcal{X}_{B,b}$, and any perturbation $u = \text{vec}([U_i]_{i=1}^l)$ such that $\forall i \in \mathbb{N}_l^+, \|U_i\|_2 \leq \frac{\sqrt{\gamma}}{2}\|W_i\|_2$, the change in the output of GCN is bounded as,

$$|f_{w+u}(X, A) - f_w(X, A)|_2 \leq eBd^{\frac{l-1}{2}} \left( \prod_{i=1}^l \|W_i\|_2 \right) \sum_{k=1}^l \|U_k\|_2 \|W_k\|_2.$$ 

The key idea of the proof is to decompose the change of the network output into two terms which depend on two quantities of GNNs respectively: the maximum change of node representations $\max_i \|H'_{i-1}[i, :] - H_{i-1}[i, :]\|_2$ and the maximum node representation $\max_i \|H_{i-1}[i, :]\|_2$. Here the superscript prime denotes the perturbed model. These two terms can be bounded by an induction on the layer index. From this lemma, we can see that the most important graph statistic for the stability of GCNs is the maximum node degree, i.e., $d - 1$. Armed with Lemma 3.1 and Lemma 2.2, we now present the PAC-Bayes generalization bound of GCNs as Theorem 3.2.

**Theorem 3.2.** (GCN Generalization Bound) For any $B > 0, l > 1$, let $f_w \in \mathcal{H} : \mathcal{X} \times \mathcal{G} \rightarrow \mathbb{R}^K$ be a $l$-layer GCN. Then for any $\delta, \gamma > 0$, with probability at least $1 - \delta$ over the choice of an i.i.d. training set $S$ according to $D$, for any $w$, we have:

$$L_{D,0}(f_w) \leq L_{S,\gamma}(f_w) + \sqrt{\frac{2D_{KL}(Q(w + u)||P)}{2(m - 1)}} + eBd^{\frac{l-1}{2}} \left( \prod_{i=1}^l \|W_i\|_2 \right) \sum_{k=1}^l \|U_k\|_2 \|W_k\|_2.$$ 

The constants slightly differ from the original paper since we use a two-sided version of Theorem 2.1.
size-m training set $S$ according to $D$, for any $w$, we have,

$$L_{D,0}(f_w) \leq L_{S, \gamma}(f_w) + O\left(\sqrt{\frac{B^2d^{-1}l^2h \log( lh) \prod_{i=1}^{l} \left\| W_i \right\|_2^2 \sum_{i=1}^{l} (\left\| W_i \right\|_F^2 \left\| W_i \right\|_2^2 + \log \frac{ml}{\gamma^2m})}{\gamma^2m}}\right).$$

Since it is easy to show GCNs are homogeneous, the proof of Theorem 3.2 follows the one for MLPs/CNNs with ReLU activations in (Neyshabur et al., 2017). In particular, we choose the prior distribution $P$ and the perturbation distribution to be zero-mean Gaussians with the same diagonal variance $\sigma$. The key steps of the proof are: 1) constructing a quantity of learned weights $\beta = (\prod_{i=1}^{l} \left\| W_i \right\|_2)^{1/l}$; 2) fixing any $\beta$, considering all $\beta$ that are in the range $|\beta - \beta| \leq \beta / l$ and choosing $\sigma$ which depends on $\beta$ so that one can apply Lemma 3.1 and 2.2 to obtain the PAC-Bayes bound; 3) taking a union bound of the result in the 2nd step by considering multiple choices of $\beta$ so that all possible values of $\beta$ (corresponding to all possible weight $w$) are covered. Although Lemma 2.2 and 3.1 have their own constraints on the random perturbation, above steps provide a way to set the variance $\sigma$ which satisfies these constraints and the independence w.r.t. learned weights. The latter is important since $\sigma$ is also the variance of the prior $P$ which should not depend on data.

### 3.2 PAC-Bayes Bounds of MPGNNs

For MPGNNs, we again need to perform a perturbation analysis to make sure that the change of the network output brought by the perturbations on weights is small with a large probability. Following the same strategy adopted in proving Lemma 3.1, we prove the following Lemma.

**Lemma 3.3.** (MPGNN Perturbation Bound) For any $B > 0, l > 1$, let $f_w \in \mathcal{H} : \mathcal{X} \times \mathcal{G} \rightarrow \mathbb{R}^K$ be a $l$-step MPGNN. Then for any $w$, and $x \in \mathcal{X}_{B, ho}$, and any perturbation $u = \text{vec}\{U_1, U_2, U_1\}$ such that $\eta = \max \left(\frac{\|U_1\|_2}{\|W_1\|_2}, \frac{\|U_2\|_2}{\|W_2\|_2}, \frac{\|U_1\|_2}{\|W_1\|_2}\right) \leq \frac{1}{l}$, the change in the output of MPGNN is bounded as,

$$|f_{w+u}(X, A) - f_w(X, A)|_2 \leq \epsilon B l \eta \|W_1\|_2 \|W_2\|_2 C_f \frac{(dC)^l - 1}{dC - 1},$$

where $C = C_\phi C_\rho C_\eta \|W_2\|_2$.

The proof again involves decomposing the change into two terms which depend on two quantities respectively: the maximum change of node representations $\max_i |H_{-l[i; :]} - H_{-l[i; :]}|$ and the maximum node representation $\max_i |H_{-l[i; :]}|_2$. Then we perform an induction on the layer index to obtain their bounds individually. Due to the weight sharing across steps, we have a form of geometric series $((dC)^l - 1)/(dC - 1)$ rather than the product of spectral norms of each layer as in GCNs. Technically speaking, the above lemma only works with $dC \neq 1$. We refer the reader to the appendix for the special case of $dC = 1$. We now provide the generalization bound for MPGNNs.

**Theorem 3.4.** (MPGNN Generalization Bound) For any $B > 0, l > 1$, let $f_w \in \mathcal{H} : \mathcal{X} \times \mathcal{G} \rightarrow \mathbb{R}^K$ be a $l$-step MPGNN. Then for any $\delta, \gamma > 0$, with probability at least $1 - \delta$ over the choice of an i.i.d. size-$m$ training set $S$ according to $D$, for any $w$, we have,

$$L_{D,0}(f_w) \leq L_{S, \gamma}(f_w) + O\left(\sqrt{\frac{B^2 \left(\max \left(\zeta^{-(l+1)}, (\lambda \xi)^{(l+1)/l}\right)\right)^2 l^2h \log( lh) \|w\|_2^2 \log \frac{ml}{\gamma^2m})}{\gamma^2m}}\right),$$

where $\zeta = \min \left(\|W_1\|_2, \|W_2\|_2, \|W_1\|_2, \|W_2\|_2\right), |w|_2^2 = \|W_1\|_F^2 + \|W_2\|_F^2 + \|W_1\|_2^2, C = C_\phi C_\rho C_\eta \|W_2\|_2$, $\lambda = \|W_1\|_2 \|W_1\|_2$, and $\xi = C_\phi \frac{(dC)^l - 1}{dC - 1}$.

The proof also contains three steps: 1) since MPGNNs are typically non-homogeneous, e.g., when any of $\phi, \rho$, and $g$ is a bounded non-linearity like Sigmoid or Tanh, we design a special quantity of learned weights $\beta = \max(\zeta^{-(l+1)}, (\lambda \xi)^{(l+1)/l})$. 2) fixing any $\beta$, considering all $\beta$ that are in the range $|\beta - \beta| \leq \beta / (l + 1)$ and choosing $\sigma$ which depends on $\beta$ so that one can apply Lemma 3.3 and 2.2 to work out the PAC-Bayes bound; 3) taking a union bound of the previous result by considering
Table 1: Comparison of generalization bounds for GNNs. "-" means inapplicable. $i$ is the network depth. Here $C = C_0 C_{\phi} C_{B} \lVert W_2 \rVert_2$, $\xi = C_{\phi} (\frac{dC}{dl})^{-1} - 1$, $\zeta = \min (\lVert W_1 \rVert_2, \lVert W_2 \rVert_2, \lVert W_1 \rVert_2)$, and $\lambda = \lVert W_1 \rVert_2 \lVert W_2 \rVert_2$. More details about the comparison can be found in Appendix A.5.

| Statistics                      | Max Node Degree $d - 1$ | Max Hidden Dim $h$ | Spectral Norm of Learned Weights |
|--------------------------------|------------------------|-------------------|---------------------------------|
| VC-Dimension                   | $O(d - 1)$             | $O(h^4)$          | $O(h)$                          |
| Rademacher Complexity          | $O\left(\frac{d - 1}{\log(d^2 - 3)}\right)$ | $O\left(h \sqrt{\log h}\right)$ | $O\left(\lambda \xi \sqrt{\log \left(\lVert W_2 \rVert_2 \lambda^2\right)}\right)$ |
| Garg et al. (2020)             | $O\left(d^{-1}\right)$ | $O\left(\frac{\lambda^2}{\sqrt{\log h}}\right)$ | $O\left(\lambda^2 \xi \lambda^2 h \sqrt{\log \left(\lVert W_2 \rVert_2 \lambda^2\right)}\right)$ |
| Ours                           | $O\left(h \sqrt{\log h}\right)$ | $O\left(h \sqrt{\log h}\right)$ | $O\left(h \xi \lambda \sqrt{\log \left(\lVert W_2 \rVert_2 \lambda^2\right)}\right)$ |

multiple choices of $\beta$ so that all possible values of $\beta$ are covered. The case with $dC = 1$ is again included in the appendix. The first step is non-trivial since we do not have the nice construction as in the homogeneous case, i.e., normalizing the weights so that the spectral norms of weights across layers are the same while the network output is unchanged. Moreover, the quantity is vital to the whole proof framework since it determines whether one can 1) satisfy the constraints on the random perturbation (so that Lemma 2.2 and 3.3 are applicable) and 2) simultaneously induce a finite covering on its range (so that the bound holds for any $w$). Since it highly depends on the form of the perturbation bound and the network architecture, there seems to be no general recipe on how to construct such a quantity.

3.3 Comparison with Other Bounds

In this section, we compare our generalization bounds with the ones in the GNN literature and draw connections with existing MLPs/CNNs bounds.

3.3.1 Comparison with Existing GNN Generalization Bounds

We compare against the VC-dimension based bound in (Scarselli et al., 2018) and the most recent Rademacher complexity based bound in (Garg et al., 2020). Our results are not directly comparable to (Du et al., 2019) since they consider a “infinite-wide” class of GNNs constructed based on the neural tangent kernel (Jacot et al., 2018), whereas we focus on commonly-used GNNs. Comparisons to (Verma & Zhang, 2019) are also difficult since: 1) they only show the bound for one graph convolutional layer, i.e., it does not depend on the network depth $l$; and 2) their bound scales as $O\left(\lambda_{\max}^2 \sqrt{T} / \min \right)$, where $T$ is the number of SGD steps and $\lambda_{\max}$ is the maximum absolute eigenvalue of Laplacian $L = D - A$. Therefore, for certain graphs\(^5\), the generalization gap is monotonically increasing with $T$, which cannot explain the generalization phenomenon. We compare different bounds by examining their dependency on three terms: the maximum node degree, the spectral norm of the learned weights, and the maximum hidden dimension. We summarize the overall comparison in Table 1 and leave the details about how we convert bounds into our context to Appendix A.5.

Max Node Degree $(d - 1)$: The Rademacher complexity bound scales as $O\left(d - 1 \sqrt{\log(d^2 - 3)}\right)$ whereas ours scales as $O(d^{-1})^6$. Many real-world graphs such as social networks tend to have large hubs (Barabási et al., 2016), which lead to very large node degrees. Thus, our bound would be significantly better in these scenarios.

Max Hidden Dimension $h$: Our bound scales as $O(\sqrt{h \log h})$ which is tighter than the Rademacher complexity bound $O(h \sqrt{\log h})$ and the VC-dimension bound $O(h^4)$.

Spectral Norm of Learned Weights: As shown in Table 1, we cannot compare the dependencies on the spectral norm of learned weights without knowing the actual values of the learned weights. Therefore, we perform an empirical study in Section 4.

\(^5\)Since $\lambda_{\max} = \max_{i} \langle v^T (D - A) v \rangle / \langle v^T v \rangle$, we have $\lambda_{\max} \geq (D - A)[i, i]$ by choosing $v = e_i$, i.e., the $i$-th standard basis. We can pick any node $i$ which has more than 1 neighbor to make $\lambda_{\max} > 1$.

\(^6\)Our bound actually scales as $O\left(d^{-1}(l-2)/l\right)$ which is upper bounded by $O\left(d^{-1}\right)$.
Figure 1: Bound evaluations on real-world datasets. The maximum node degrees (i.e., \( d - 1 \)) of four datasets from left to right are: 25 (PROTEINS), 88 (IMDB-M), 135 (IMDB-B), and 491 (COLLAB).

3.3.2 Connections with Existing Bounds of MLPs/CNNs

As described above, MLPs/CNNs can be viewed as special cases of GNNs. In particular, we have two ways to show the inclusion relationship. First, we can treat each i.i.d. sample as a node and the whole dataset as a graph without edges. Then conventional tasks (e.g., classification) become node-level tasks (e.g., node classification) on this graph. Second, we can treat each i.i.d. sample as a single-node graph. Then conventional tasks (e.g., classification) becomes graph-level tasks (e.g., graph classification). Since we focus on the graph classification, we adopt the second view. In particular, MLPs/CNNs with ReLU activations are equivalent to GCNs with the graph Laplacian \( \tilde{L} = I \) (hence \( d = 1 \)). We leave the details of this conversion to Appendix A.6. We restate the PAC-Bayes bound for MLPs/CNNs with ReLU activations in (Neyshabur et al., 2017) as follows,

\[
L_{\mathcal{D},0}(f_w) \leq L_{S,\gamma}(f_w) + O \left( \sqrt{B^2 h \log(lh) \prod_{i=1}^{l} \left( \frac{\Vert W_i \Vert_2}{\Vert W_i \Vert_2} \right)} \right) / \gamma^2 m \cdot \log \frac{ml}{\delta}.
\]

Comparing it with our bound for GCNs in Theorem 3.2, it is clear that we only add a factor \( d^{l-1} \) to the first term inside the square root which is due to the underlying graph structure of the data. If we apply GCNs to single-node graphs, the two bounds coincide since \( d = 1 \). Therefore, our Theorem 3.2 directly generalizes the result in (Neyshabur et al., 2017) to GCNs, which is a strictly larger class of models than MLPs/CNNs with ReLU activations.

4 Experiments

In this section, we perform an empirical comparison between our bound and the Rademacher complexity bound for MPGNNs. We experiment on 6 synthetic datasets of random graphs (corresponding to 6 random graph models), 3 social network datasets (COLLAB, IMDB-BINARY, IMDB-MULTI), and a bioinformatics dataset PROTEINS from (Yanardag & Vishwanathan, 2015). In particular, we create synthetic datasets by generating random graphs from the Erdős–Rényi model and the stochastic block model with different settings (i.e., number of blocks and edge probabilities). All datasets focus on graph classifications. We repeat all experiments 3 times with different random initializations and report the means and the standard deviations. Constants are considered in the bound computation. More details of the experimental setup, dataset statistics, and the bound computation are provided in Appendix A.7.

As shown in Fig. 1 and Fig. 2, our bound is mostly tighter than the Rademacher complexity bound with varying message passing steps \( l \) on both synthetic and real-world datasets. Generally, the larger the maximum node degree is, the more our bound improves over the Rademacher complexity bound (c.f., PROTEINS vs. COLLAB). This could be attributed to the better dependency on \( d \) of our bound. For graphs with large node degrees (e.g., social networks like Twitter have influential users with lots of followers), the gap could be more significant. Moreover, with the number of steps/layers increasing, our bound also improves more in most cases. It may not be clear to read from the figures

\[\text{Note that it may not be obvious from the figure as the y axis is in log domain. Please refer to the appendix where the actual bound values are listed in the table.}\]
Figure 2: Bound evaluations on synthetic datasets. The maximum node degrees (i.e., $d-1$) of datasets from left to right are: 25 (ER-1), 48 (ER-2), 69 (ER-3), 87 (ER-4), 25 (SBM-1), and 36 (SBM-2). ‘ER-X’ and ‘SBM-X’ denote the Erdős–Rényi model and the stochastic block model with the ‘X’-th setting respectively. Please refer to the appendix for more details.

since the y-axis is in the log domain and its range differ from figure to figure. We also provide the numerical values of the bound evaluations in the appendix for an exact comparison. The number of steps is chosen to be no larger than 10 as GNNs are generally shown to perform well with just a few steps/layers (Kipf & Welling, 2016; Jin et al., 2018). We found $dC > 1$ and the geometric series $((dC)^{l-1} - 1)/(dC - 1) \gg 1$ on all datasets which imply learned GNNs are not contraction mappings (i.e., $dC < 1$). This also explains why both bounds becomes larger with more steps. At last, we can see that bound values are much larger than 1 which indicates both bounds are still vacuous, similarly to the cases for regular neural networks in (Bartlett et al., 2017; Neyshabur et al., 2017).

5 Discussion

In this paper, we present generalization bounds for two primary classes of GNNs, i.e., GCNs and MPGNNs. We show that the maximum node degree and the spectral norms of learned weights govern the bound for both models. Our results for GCNs generalize the bounds for MLPs/CNNs in (Neyshabur et al., 2017), while our results for MPGNNs improve over the state-of-the-art Rademacher complexity bound in (Garg et al., 2020). Our PAC-Bayes analysis can be generalized to other graph problems such as node classification and link prediction since our perturbation analysis bounds the maximum change of any node representation. Other loss functions (e.g., ones for regression) could also work in our analysis as long as they are bounded.

However, we are far from being able to explain the practical behaviors of GNNs. Our bound values are still vacuous as shown in the experiments. Our perturbation analysis is in the worst-case sense which may be loose for most cases. We introduce Gaussian posterior in the PAC-Bayes framework to obtain an analytical form of the KL divergence. Nevertheless, the actual posterior induced by the prior and the learning process may likely to be non-Gaussian. We also do not explicitly consider the optimization algorithm in the analysis which clearly has an impact on the learned weights.
This work leads to a few interesting open problems for future work: (1) Is the maximum node degree the only graph statistic that has an impact on the generalization ability of GNNs? Investigating other graph statistics may provide more insights on the behavior of GNNs and inspire the development of novel models and algorithms. (2) Would the analysis still work for other interesting GNN architectures, such as those with attention (Veličković et al., 2017) and learnable spectral filters (Liao et al., 2019)? (3) Can recent advancements for MLPs/CNNs, e.g., the compression technique in (Arora et al., 2018) and data-dependent prior of (Parrado-Hernández et al., 2012), help further improve the bounds for GNNs? (4) What is the impact of the optimization algorithms like SGD on the generalization ability of GNNs? Would graph structures play a role in the analysis of optimization?

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A Appendix

We summarize the notations used throughout the paper in Table 2. In the following sections, we provide proofs of all results in the main text and the additional details.

| Symbol | Meaning |
|--------|---------|
| $\mathbb{R}$ | the set of real numbers |
| $\mathbb{R}^{m \times n}$ | the set of $m \times n$ real matrices |
| $\mathbb{N}^+_k$ | the set of first $k$ positive numbers |
| $\| \cdot \|_p$ | the vector $p$-norm |
| $\| \cdot \|_F$ | the Frobenius norm |
| $X[i,j]$ | the $(i,j)$-th element of matrix $X$ |
| $X[i,:]$ | the $i$-th row of matrix $X$ |
| $X[:,i]$ | the $i$-th column of matrix $X$ |
| $\mathbf{1}_n$ | a all-one vector with size $n$ |
| $A$ | an adjacency matrix |
| $\tilde{A}$ | an adjacency matrix plus the identity matrix |
| $B$ | the radius of the $\ell_2$-ball where an input node feature lies |
| $C_{\text{in}}$ | an incidence matrix of incoming nodes |
| $C_{\text{out}}$ | an incidence matrix of outgoing nodes |
| $\phi, \rho, g$ | non-linearities in MPGNN |
| $C_{\phi}, C_{\rho}, C_{g}$ | Lipschitz constants of $\phi, \rho, g$ under the vector 2-norm |
| $\mathcal{C}$ | the percolation complexity |
| $D$ | the degree matrix |
| $\mathcal{D}$ | the unknown data distribution |
| $d$ | the maximum node degree plus one |
| $e$ | the Euler’s number |
| $f_w$ | a model parameterized by vector $w$ |
| $\mathcal{G}$ | the space of graph |
| $h$ | the maximum hidden dimension |
| $H$ | a node representation matrix |
| $\mathcal{H}$ | the hypothesis/model class |
| $I$ | the identity matrix |
| $l$ | the number of graph convolution layers / message passing steps |
| $L$ | the loss function |
| $\tilde{L}$ | the Laplacian matrix |
| $m$ | the number of training samples |
| $P, E$ | probability and expectation of a random variable |
| $P$ | the prior distribution over hypothesis class |
| $Q$ | the posterior distribution over hypothesis class |
| $S$ | a set of training samples |
| $W$ | a weight matrix |
| $X$ | a node feature matrix where each row corresponds to a node |
| $\mathcal{X}$ | the space of node feature |
| $y$ | the graph class label |
| $\gamma$ | the margin parameter |
| $z$ | a data triplet $(A, X, y)$ |
| $Z$ | the space of data triplet |
| $\log$ | the natural logarithm |

Table 2: Summary of important notations.

A.1 PAC Bayes Results

For completeness, we provide the proofs of the standard PAC-Bayes results as below.
Lemma A.1. For non-negative continuous random variables $X$, we have

$$E[X] = \int_0^\infty P(X \geq \nu) d\nu.$$  

Proof.

$$E[X] = \int_0^\infty X P(X) dX = \int_0^\infty \int_0^X 1 d\nu P(X) dX = \int_0^\infty \int_0^\nu P(X) d\nu dX = \int_0^\infty P(X \geq \nu) d\nu$$

Lemma A.2. [2-side] Let $X$ be a random variable satisfying $P(X \geq \epsilon) \leq e^{-2m\epsilon^2}$ and $P(X \leq -\epsilon) \leq e^{-2m\epsilon^2}$ where $m \geq 1$ and $\epsilon > 0$, we have

$$E[e^{2(m-1)X^2}] \leq 2m.$$  

Proof. If $m = 1$, the inequality holds trivially. Let us now consider $m > 1$.

$$E[e^{2(m-1)X^2}] = \int_0^\infty P(e^{2(m-1)X^2} \geq \nu) d\nu \quad \text{(Lemma A.1)}$$

$$= \int_0^\infty P(X^2 \geq \frac{\log \nu}{2(m-1)}) d\nu = \int_0^\infty P(X \geq \sqrt{\frac{\log \nu}{2(m-1)}}) d\nu + \int_0^\infty P(X \leq -\sqrt{\frac{\log \nu}{2(m-1)}}) d\nu \quad (5)$$

$$\int_0^\infty P(X \geq \sqrt{\frac{\log \nu}{2(m-1)}}) d\nu = \int_0^1 P(X \geq \sqrt{\frac{\log \nu}{2(m-1)}}) d\nu + \int_1^\infty P(X \geq \sqrt{\frac{\log \nu}{2(m-1)}}) d\nu \leq 1 + \int_1^\infty e^{-2m\frac{\log \nu}{2(m-1)}} d\nu$$

$$= 1 + \left[-\frac{\log \nu}{m-1}\right]_1^\infty = m$$

Similarly, we can show that

$$\int_0^\infty P(X \leq -\sqrt{\frac{\log \nu}{2(m-1)}}) d\nu \leq m$$

Combining Eq. (5) and Eq. (6), we finish the proof. 

14
Theorem 2.1. (Two-side) Let $P$ be a prior distribution over $\mathcal{H}$ and let $\delta \in (0, 1)$. Then, with probability $1 - \delta$ over the choice of an i.i.d. training set $S$ according to $\mathcal{D}$, for all distributions $Q$ over $\mathcal{H}$ and any $\gamma > 0$, we have

$$L_{\mathcal{D}, \gamma}(Q) \leq L_{S, \gamma}(Q) + \sqrt{\frac{D_{\text{KL}}(Q||P) + \log \frac{2m}{\delta}}{2(m - 1)}}$$

Proof. Let $\Delta(h) = L_{\mathcal{D}, \gamma}(h) - L_{S, \gamma}(h)$. For any function $f(h)$, we have

$$\mathbb{E}_{h \sim Q}[f(h)] = \mathbb{E}_{h \sim Q}[\log e^{f(h)}] = \mathbb{E}_{h \sim Q}[\log e^{f(h)} + \log \frac{Q}{P} + \log \frac{P}{Q}] = D_{\text{KL}}(Q||P) + \mathbb{E}_{h \sim Q} \left[ \log \left( \frac{P}{Q} e^{f(h)} \right) \right] \leq D_{\text{KL}}(Q||P) + \mathbb{E}_{h \sim Q} \left[ e^{2(m-1)\Delta(h)^2} \right].$$

(Jensen’s inequality)

$$= D_{\text{KL}}(Q||P) + \mathbb{E}_{h \sim P} \left[ e^{f(h)} \right].$$

(8)

Let $f(h) = 2(m - 1)\Delta(h)^2$. We have

$$2(m - 1)\mathbb{E}_{h \sim Q}[\Delta(h)^2] \leq 2(m - 1)\mathbb{E}_{h \sim Q}[\Delta(h)^2] \leq D_{\text{KL}}(Q||P) + \mathbb{E}_{h \sim P} \left[ e^{2(m-1)\Delta(h)^2} \right].$$

(Jensen’s inequality)

(9)

Since $L_{\mathcal{D}}(h) \in [0, 1]$, based on Hoeffding’s inequality, for any $\epsilon > 0$, we have

$$\mathbb{P}(\Delta(h) \geq \epsilon) \leq e^{-2m\epsilon^2}$$

$$\mathbb{P}(\Delta(h) \leq -\epsilon) \leq e^{-2m\epsilon^2}$$

Hence, based on Lemma A.2, we have

$$\mathbb{E}_S e^{2(m-1)\Delta(h)^2} \leq 2m \implies \mathbb{E}_{h \sim P} \left[ \mathbb{E}_S e^{2(m-1)\Delta(h)^2} \right] \leq 2m$$

$$\iff \mathbb{E}_{h \sim P} \left[ \mathbb{E}_S e^{2(m-1)\Delta(h)^2} \right] \leq 2m$$

Based on Markov’s inequality, we have

$$\mathbb{P} \left( \mathbb{E}_{h \sim P} e^{2(m-1)\Delta(h)^2} \geq \frac{2m}{\delta} \right) \leq \frac{\delta \mathbb{E}_S \left[ \mathbb{E}_{h \sim P} e^{2(m-1)\Delta(h)^2} \right]}{2m} \leq \delta.$$

(10)

Combining Eq. (9) and Eq. (10), with probability $1 - \delta$, we have

$$\mathbb{E}_{h \sim Q}[\Delta(h)^2] \leq \frac{D_{\text{KL}}(Q||P) + \log \frac{2m}{\delta}}{2(m - 1)}$$

(11)

which proves the theorem. □

Lemma 2.2. Let $f_w(x) : \mathcal{X} \to \mathbb{R}^k$ be any model with parameters $w$, and $P$ be any distribution on the parameters that is independent of the training data. For any $w$, we construct a posterior $Q(w + u)$ by adding any random perturbation $u$ to $w$, s.t., $\mathbb{P}(\max_{x \in \mathcal{X}} |f_{w + u}(x) - f_w(x)|_\infty < \frac{\epsilon}{2}) > \frac{1}{2}$. Then, for any $\gamma, \delta > 0$, with probability at least $1 - \delta$ over an i.i.d. size-$m$ training set $S$ according to $\mathcal{D}$, for any $w$, we have:

$$L_{\mathcal{D}, 0}(f_w) \leq L_{S, \gamma}(f_w) + \sqrt{\frac{2D_{\text{KL}}(Q(w + u)||P) + \log \frac{2m}{\delta}}{2(m - 1)}}$$
Proof. Let \( \tilde{w} = w + u \). Let \( \mathcal{C} \) be the set of perturbation with the following property,

\[
\mathcal{C} = \left\{ w : \max_{x \in \mathcal{X}} |f_w(x) - f_{\hat{w}}(x)|_{\infty} < \frac{\gamma}{4} \right\}.
\]  

(12)

\( \tilde{w} = w + u \) (\( w \) is deterministic and \( u \) is stochastic) is distributed according to \( Q(\tilde{w}) \). We now construct a new posterior \( \tilde{Q} \) as follows,

\[
\tilde{Q}(\tilde{w}) = \begin{cases} \frac{1}{2} Q(\tilde{w}) & \tilde{w} \in \mathcal{C} \\ 0 & \tilde{w} \in \bar{\mathcal{C}}. \end{cases}
\]  

(13)

Here \( Z = \int_{\tilde{w} \in \mathcal{C}} dQ(\tilde{w}) = \mathbb{P}_{\tilde{w} \sim \tilde{Q}} (\tilde{w} \in \mathcal{C}) \) and \( \bar{\mathcal{C}} \) is the complement set of \( \mathcal{C} \). We know from the assumption that \( Z > \frac{1}{4} \). Therefore, for any \( \tilde{w} \sim \tilde{Q} \), we have

\[
\max_{i \in N^+, j \in N^+, x \in \mathcal{X}} |f_{\tilde{w}}(x)[i] - f_{\hat{w}}(x)[j] - |f_w(x)[i] - f_{\hat{w}}(x)[j]| \\
\leq \max_{i \in N^+, j \in N^+, x \in \mathcal{X}} |f_{\tilde{w}}(x)[i] - f_{\hat{w}}(x)[j] - f_w(x)[i] + f_w(x)[j]| \\
\leq \max_{i \in N^+, j \in N^+, x \in \mathcal{X}} |f_{\tilde{w}}(x)[i] - f_w(x)[i]| + \max_{j \in N^+, x \in \mathcal{X}} |f_{\hat{w}}(x)[j] - f_w(x)[j]| \\
\leq \frac{\gamma}{4} + \frac{\gamma}{4} = \frac{\gamma}{2}
\]  

(14)

Recall that

\[
L_D(f_w, 0) = \mathbb{P}_{z \sim \mathcal{D}} \left( f_w(x)[y] \leq \max_{j \neq y} f_w(x)[j] \right) \\
L_D(f_{\hat{w}}, \frac{\gamma}{2}) = \mathbb{P}_{z \sim \mathcal{D}} \left( f_{\hat{w}}(x)[y] \leq \frac{\gamma}{2} + \max_{j \neq y} f_{\hat{w}}(x)[j] \right).
\]

Denoting \( j_1^* = \arg \max_{j \neq y} f_{\hat{w}}(x)[j] \) and \( j_2^* = \arg \max_{j \neq y} f_w(x)[j] \), from Eq. (14), we have

\[
\left| f_{\hat{w}}(x)[y] - f_{\hat{w}}(x)[j_2^*] - f_{\hat{w}}(x)[j_1^*] \right| \leq \frac{\gamma}{2} \\
\Rightarrow f_{\hat{w}}(x)[y] - f_{\hat{w}}(x)[j_2^*] < f_w(x)[y] - f_{\hat{w}}(x)[j_2^*] + \frac{\gamma}{2}
\]  

(15)

Note that since \( f_{\hat{w}}(x)[j_1^*] \geq f_{\hat{w}}(x)[j_2^*] \), we have

\[
f_{\hat{w}}(x)[y] - f_{\hat{w}}(x)[j_2^*] \leq f_{\hat{w}}(x)[y] - f_{\hat{w}}(x)[j_2^*] \\
\leq f_w(x)[y] - f_{\hat{w}}(x)[j_2^*] + \frac{\gamma}{2} \quad \text{(Eq. (15))}
\]

Therefore, we have

\[
f_w(x)[y] - f_w(x)[j_2^*] \leq 0 \Rightarrow f_{\hat{w}}(x)[y] - f_{\hat{w}}(x)[j_1^*] \leq \frac{\gamma}{2},
\]

which indicates \( \mathbb{P}_{z \sim \mathcal{D}} (f_w(x)[y] \leq f_w(x)[j_2^*]) \leq \mathbb{P}_{z \sim \mathcal{D}} (f_{\hat{w}}(x)[y] \leq f_{\hat{w}}(x)[j_1^*] + \frac{\gamma}{2}) \), or equivalently

\[
L_{D,0}(f_w) \leq L_{D,\frac{\gamma}{2}}(f_{\hat{w}}).
\]  

(16)

Note that this holds for any perturbation \( \tilde{w} \sim \tilde{Q} \).

Again, recall that

\[
L_{D,\frac{\gamma}{2}}(f_{\hat{w}}) = \mathbb{P}_{z \sim \mathcal{D}} \left( f_{\hat{w}}(x)[y] \leq \frac{\gamma}{2} + \max_{j \neq y} f_{\hat{w}}(x)[j] \right) \\
L_{D,\gamma}(f_w) = \mathbb{P}_{z \sim \mathcal{D}} \left( f_w(x)[y] \leq \gamma + \max_{j \neq y} f_w(x)[j] \right)
\]
From Eq. (14), we have
\[
\left| f_\hat{w}(x)[y] - f_\hat{w}(x)[j_1^*] - f_w(x)[y] + f_w(x)[j_1^*] \right| < \frac{\gamma}{2}
\]
\[
\Rightarrow f_w(x)[y] - f_w(x)[j_1^*] < f_\hat{w}(x)[y] - f_\hat{w}(x)[j_1^*] + \frac{\gamma}{2}
\] (Eq. (17))

Note that since \( f_w(x)[j_1^*] \geq f_w(x)[j_1^*] \), we have
\[
f_w(x)[y] - f_w(x)[j_2^*] \leq f_w(x)[y] - f_w(x)[j_1^*]
\]
\[
\leq f_\hat{w}(x)[y] - f_\hat{w}(x)[j_1^*] + \frac{\gamma}{2}
\] (Eq. (17))

Therefore, we have
\[
f_\hat{w}(x)[y] - f_\hat{w}(x)[j_1^*] \leq \frac{\gamma}{2} \Rightarrow f_w(x)[y] - f_w(x)[j_2^*] \leq \gamma,
\]
which indicates \( L_{D, \hat{Z}}(f_\hat{w}) \leq L_{D, \gamma}(f_w) \). Therefore, from the perspective of the empirical estimation of the probability, for any \( \hat{w} \sim \hat{Q} \), we almost surely have
\[
L_{S, \hat{Z}}(f_\hat{w}) \leq L_{S, \gamma}(f_w).
\] (18)

Now with probability at least \( 1 - \beta \), we have
\[
L_{D, 0}(f_w) \leq \mathbb{E}_{\hat{w} \sim \hat{Q}} \left[ L_{D, \hat{Z}}(f_\hat{w}) \right] \quad (\text{Eq. (16)})
\]
\[
\leq \mathbb{E}_{\hat{w} \sim \hat{Q}} \left[ L_{S, \hat{Z}}(f_\hat{w}) \right] + \sqrt{\frac{\text{D}_\text{KL}(\hat{Q} \| P) + \log \frac{2m}{\delta}}{2(m - 1)}} \quad (\text{Theorem 2.1})
\]
\[
\leq L_{S, \gamma}(f_w) + \sqrt{\frac{\text{D}_\text{KL}(\hat{Q} \| P) + \log \frac{2m}{\delta}}{2(m - 1)}} \quad (\text{Eq. (18)})
\] (19)

Note that
\[
\text{D}_\text{KL}(Q \| P) = \int_{\hat{w} \in \hat{C}} Q \log \frac{Q}{P} d\hat{w} + \int_{\hat{w} \in \hat{C}} Q \log \frac{Q}{P} d\hat{w}
\]
\[
= \int_{\hat{w} \in \hat{C}} QZ \log \frac{Q}{ZP} d\hat{w} + \int_{\hat{w} \in \hat{C}} Q \log Z d\hat{w}
\]
\[
+ \int_{\hat{w} \in \hat{C}} Q(1 - Z) \log \frac{Q}{(1 - Z)P} d\hat{w} + \int_{\hat{w} \in \hat{C}} Q \log(1 - Z) d\hat{w}
\]
\[
= Z \text{D}_\text{KL}(\hat{Q} \| P) + (1 - Z) \text{D}_\text{KL}(\hat{Q} \| P) - H(Z),
\] (20)

where \( \hat{Q} \) denotes the normalized density of \( Q \) restricted to \( \hat{C} \). \( H(Z) \) is the entropy of a Bernoulli random variable with parameter \( Z \). Since we know \( \frac{1}{2} \leq Z \leq 1 \) from the beginning, \( 0 \leq H(Z) \leq \log 2 \), and \( \text{D}_\text{KL} \) is nonnegative, from Eq. (20), we have
\[
\text{D}_\text{KL}(\hat{Q} \| P) = \frac{1}{Z} [\text{D}_\text{KL}(Q \| P) + H(Z) - (1 - Z) \text{D}_\text{KL}(\hat{Q} \| P)]
\]
\[
\leq \frac{1}{Z} [\text{D}_\text{KL}(Q \| P) + H(Z)]
\]
\[
\leq 2 \text{D}_\text{KL}(Q \| P) + 2 \log 2.
\] (21)

Combining Eq. (19) and Eq. (21), we have
\[
L_{D, 0}(f_w) \leq L_{S, \gamma}(f_w) + \sqrt{\frac{\text{D}_\text{KL}(Q \| P) + \frac{1}{2} \log \frac{8m}{\delta}}{m - 1}},
\] (22)

which finishes the proof.
A.2 Graph Results

In this part, we provide a result on the graph Laplacian used by GCNs along with the proof. It is used in the perturbation analysis of GCNs.

**Lemma A.3.** Let $A$ be the binary adjacency matrix of an arbitrary simple graph $G = (V, E)$ and $\tilde{A} = A + I$. We define the graph Laplacian $L = D^{-1/2} \tilde{A} D^{-1/2}$ where $D$ is the degree matrix of $\tilde{A}$. Then we have $\|L\|_1 = \|L\|_\infty \leq \sqrt{d}$, $\|L\|_2 \leq 1$, and $\|L\|_F \leq \sqrt{r}$ where $r$ is the rank of $L$ and $d - 1$ is the maximum node degree of $G$.

**Proof.** First, $\tilde{A}$ is symmetric and element-wise nonnegative. Denoting $n = |V|$, we have $\tilde{A} \in \mathbb{R}^{n \times n}$, $D_i = \sum_{j=1}^{n} \tilde{A}[i, j]$, and $1 \leq D_i \leq d, \forall i \in \mathbb{N}_+^n$. It is easy to show that $L[i, j] = \tilde{A}[i, j] / \sqrt{D_i D_j}$.

For the infinity norm and 1-norm, we have $\|L\|_1 = \|L^T\|_\infty = \|L\|_\infty$. Moreover,

$$\|L\|_\infty = \max_{i \in \mathbb{N}_+^n} \sum_{j=1}^{n} |L[i, j]|$$

$$= \max_{i \in \mathbb{N}_+^n} \sum_{j=1}^{n} \frac{\tilde{A}[i, j]}{\sqrt{D_i D_j}}$$

$$\leq \max_{i \in \mathbb{N}_+^n} \frac{1}{\sqrt{D_i}} \sum_{j=1}^{n} \tilde{A}[i, j]$$

$$= \max_{i \in \mathbb{N}_+^n} \sqrt{D_i}$$

(23)

For the spectral norm, based on the definition, we have

$$\|L\|_2 = \sup_{x \neq 0} \frac{|Lx|_2}{|x|_2} = \sigma_{\text{max}},$$

(24)

where $\sigma_{\text{max}}$ is the maximum singular value of $L$. Since $L$ is symmetric, we have $\sigma_i = |\lambda_i|$ where $\lambda_i$ is the $i$-th eigenvalue of $L$. Hence, $\sigma_{\text{max}} = \max_i |\lambda_i|$. From Rayleigh quotient and Courant–Fischer minimax theorem, we have

$$\|L\|_2 = \max_i |\lambda_i| = \max_{x \neq 0} \frac{|x^\top Lx|}{|x|_2}$$

$$= \max_{x \neq 0} \left| \sum_{i=1}^{n} \sum_{j=1}^{n} L[i, j] x_i x_j \right|$$

$$= \max_{x \neq 0} \left| \sum_{i=1}^{n} \sum_{j=1}^{n} \tilde{A}[i, j] x_i x_j / \sqrt{D_i D_j} \right|$$

$$= \max_{x \neq 0} \left| \sum_{(i, j) \in E} \frac{x_i x_j / \sqrt{D_i D_j}}{\sum_{i=1}^{n} x_i^2} \right|$$

$$\leq \max_{x \neq 0} \left| \frac{1}{2} \sum_{(i, j) \in E} \frac{x_i^2 D_i + x_j^2 D_j}{\sum_{i=1}^{n} x_i^2} \right|$$

$$= \max_{x \neq 0} \left| \frac{\sum_{(i, j) \in E} x_i^2 / D_i}{\sum_{i=1}^{n} x_i^2} \right| = \max_{x \neq 0} \frac{\sum_{i=1}^{n} x_i^2}{\sum_{i=1}^{n} x_i^2} = 1,$$

(25)

where $E$ is the union of the set of edges $E$ in the original graph and the set of self-loops. For Frobenius norm, we have $\|L\|_F \leq \sqrt{r} \|L\|_2 \leq \sqrt{r}$ where $r$ is the rank of $L$. \qed
A.3 GCN Results

In this part, we provide the proofs of the main results regarding GCNs.

**Lemma 3.1. (GCN Perturbation Bound)** For any $B > 0$, $l > 1$, let $f_w \in \mathcal{H} : \mathcal{X} \times \mathcal{G} \to \mathbb{R}^K$ be a $l$-layer GCN. Then for any $w$, and $x \in \mathcal{X}_{\mathcal{H}, h_0}$, and any perturbation $u = \text{vec}\{U_i\}_{i=1}^l$ such that $\forall i \in \mathcal{N}_i^l, \|U_i\|_2 \leq \frac{B}{l} \|W_i\|_2$, the change in the output of GCN is bounded as,

$$|f_{w+u}(X, A) - f_w(X, A)|_2 \leq eBd^{\frac{l+2}{2}} \left(\prod_{i=1}^l \|W_i\|_2\right) \sum_{i=1}^l \|U_k\|_2$$

**Proof.** We first perform the recursive perturbation analysis on node representations of all layers except the last one, i.e., the readout layer. Then we derive the bound for the graph representation of the last readout layer.

**Perturbation Analysis on Node Representations.** In GCN, for any layer $j < l$ besides the last readout one, the node representations are,

$$f_{w_j}^j(X, A) = H_j = \sigma_j \left(\tilde{L}H_{j-1}W_j\right).$$

(26)

We add perturbation $u$ to the weights $w$, i.e., for the $j$-th layer, the perturbed weights are $W_j + U_j$. For the ease of notation, we use the superscript of prime to denote the perturbed node representations, e.g., $H'_j = f_{w_j + u}^j(X, A)$. Let $\Delta_j = f_{w_j + u}^j(X, A) - f_{w}^j(X, A) = H'_j - H_j$. Note that $\Delta_j \in \mathbb{R}^{n \times h_j}$. Let $\Psi_j = \max_i |\Delta_j[i, :]|_2 = \max_i |H'_j[i, :] - H_j[i, :]|_2$ and $\Phi_j = \max_i |H_j[i, :]|_2$. We denote the $u^*_j = \arg \max_i |\Delta_j[i, :]|_2$ and $v^*_j = \arg \max_i |H_j[i, :]|_2$.

**Upper Bound on the Max Node Representation** For any layer $j < l$, we can derive an upper bound on the maximum (w.r.t. $\ell_2$ norm) node representation as follows,

$$\Phi_j = \max_i |H_j[i, :]|_2 = \|\tilde{L}[v^*_j, :]W_j\|_2$$

(27)

$$\leq \|\tilde{L}[v^*_j, :]\|_2 \|W_j\|_2 \leq \sum_{k \in \mathcal{N}_v^j} \tilde{L}[v^*_j, k] H_{j-1}[k, :] \|W_j\|_2$$

(28)

$$\leq \sum_{k \in \mathcal{N}_v^j} \tilde{L}[v^*_j, k] \Phi_{j-1} \|W_j\|_2$$

where in the last inequality we use the fact $\Phi_0 = \max_i |X[i, :]|_2 \leq B$ based on the assumption $A3$. $\mathcal{N}_v^j$ is the set of neighboring nodes (including itself) of node $v^*_j$. In the third from the last inequality, we use the Lemma A.3 to derive the following fact that $\forall i,$

$$\sum_{k \in \mathcal{N}_i^l} \tilde{L}[i, k] = \sum_{k \in \mathcal{N}_i} \tilde{L}[i, k] \leq \|\tilde{L}\|_\infty \leq \sqrt{d}.$$
Upper Bound on the Max Change of Node Representation. For any layer $j < l$, we can derive an upper bound on the maximum (w.r.t. $L_2$ norm) change between the representations with and without the weight perturbation for any node as follows,

$$
\Psi_j = \max |H'_j[i, :] - H_j[i, :]|_2 = \sigma_j \left( \tilde{L} H'_{j-1}(W_j + U_j) \right)[u_j^*, :] - \sigma_j \left( \tilde{L} H_{j-1}W_j \right)[u_j^*, :]
\leq \left| \left( \tilde{L} H'_{j-1}(W_j + U_j) \right)[u_j^*, :] - \left( \tilde{L} H_{j-1}W_j \right)[u_j^*, :] \right|_2
\leq \left| \left( \tilde{L} H'_j - \tilde{L} H_{j-1} \right)[u_j^*, :] \right|_2 (W_j + U_j) + \left| \left( \tilde{L} H_{j-1} \right)[u_j^*, :] \right|_2 W_j
\leq \left| \left( \sum_{k \in \mathcal{N}_{u_j}} \tilde{L}[u_j^*, k] (H'_{j-1}[k, :] - H_{j-1}[k, :) \right) (W_j + U_j) + \left| \sum_{k \in \mathcal{N}_{u_j}} \tilde{L}[u_j^*, k] H_{j-1}[k, :]) W_j \right|_2
\leq \sum_{k \in \mathcal{N}_{u_j}} \tilde{L}[u_j^*, k] \Psi_{j-1} ||W_j + U_j||_2 + \sum_{k \in \mathcal{N}_{u_j}} \tilde{L}[u_j^*, k] \Phi_{j-1} ||U_j||_2
\leq \sqrt{d} \Psi_{j-1} ||W_j + U_j||_2 + \sqrt{d} \Phi_{j-1} ||U_j||_2,
$$

(29)

where in the second from the last inequality we use the fact $\forall k$, $|H'_{j-1}[k, :] - H_{j-1}[k, :]|_2 \leq \Psi_{j-1}$ and $\forall k$, $|H_{j-1}[k, :]|_2 \leq \Phi_{j-1}$. In the last inequality, we again use the fact in Eq. (28). We can simplify the notations in Eq. (29) as $\Psi_j \leq a_{j-1} \Psi_{j-1} + b_{j-1}$ where $a_{j-1} = \sqrt{d}||W_j + U_j||_2$ and $b_{j-1} = \sqrt{d} \Phi_{j-1} ||U_j||_2$. Since $\Delta_0 = X - X = 0$, we have $\Psi_0 = 0$. It is straightforward to work out the recursion as,

$$
\Psi_j \leq \sum_{k=0}^{j-1} \frac{d^{k}}{k+1} \Phi_k ||U_{k+1}||_2 \left( \prod_{i=k+2}^{j} ||W_i + U_i||_2 \right)
\leq \sum_{k=0}^{j-1} \frac{d^{k}}{k+1} \left( \frac{d^{k} B \prod_{i=1}^{k} ||W_i||_2}{||U_{k+1}||_2} \right) \left( \prod_{i=k+2}^{j} \frac{1}{1 + \frac{1}{7}} \right) ||W_i||_2
\leq B \sum_{k=0}^{j-1} \frac{d^{k}}{k+1} \left( \prod_{i=1}^{k} ||W_i||_2 \right) \frac{||U_{k+1}||_2}{||W_{k+1}||_2} \left( \prod_{i=k+2}^{j} \frac{1}{1 + \frac{1}{7}} \right) ||W_i||_2
\leq B d^{j} \left( \prod_{i=1}^{j} ||W_i||_2 \right) \sum_{k=0}^{j-1} \frac{||U_{k+1}||_2}{||W_{k+1}||_2} \left( 1 + \frac{1}{7} \right)^{j-k-1}
\leq B d^{j} \left( \prod_{i=1}^{j} ||W_i||_2 \right) \sum_{k=1}^{j} \frac{||U_k||_2}{||W_k||_2} \left( 1 + \frac{1}{7} \right)^{j-k}
$$

(31)
**Final Bound on the Readout Layer** Now let us consider the average readout function in the last layer, i.e., the \( l \)-th layer. Based on Eq. (27) and Eq. (31), we can bound the change of GCN’s output with and without the weight perturbation as follows,

\[
|\Delta l|_2 = \left| \frac{1}{n} \mathbf{1}_n H_{l-1}^T (W_l + U_l) - \frac{1}{n} \mathbf{1}_n H_{l-1} W_l \right|_2
\]

\[
= \left| \frac{1}{n} \mathbf{1}_n \Delta_{l-1}(W_l + U_l) + \frac{1}{n} \mathbf{1}_n H_{l-1} U_l \right|_2
\]

\[
\leq \frac{1}{n} \left| \mathbf{1}_n \Delta_{l-1}(W_l + U_l) \right|_2 + \frac{1}{n} \left| \mathbf{1}_n H_{l-1} U_l \right|_2
\]

\[
\leq \frac{1}{n} \| W_l + U_l \|_2 \left| \mathbf{1}_n \Delta_{l-1} \right|_2 + \frac{1}{n} \| U_l \|_2 \left| \mathbf{1}_n H_{l-1} \right|_2
\]

\[
= \frac{1}{n} \| W_l + U_l \|_2 \left\{ \sum_{i=1}^{n} \left| \Delta_{l-1}[i, \cdot] \right|_2 \right\} + \frac{1}{n} \| U_l \|_2 \left\{ \sum_{i=1}^{n} \left| H_{l-1}[i, \cdot] \right|_2 \right\}
\]

\[
\leq \frac{1}{n} \| W_l + U_l \|_2 \left( \sum_{i=1}^{n} \left| \Delta_{l-1}[i, \cdot] \right|_2 \right) + \frac{1}{n} \| U_l \|_2 \left( \sum_{i=1}^{n} \left| H_{l-1}[i, \cdot] \right|_2 \right)
\]

\[
\leq \frac{1}{n} \| W_l + U_l \|_2 \Phi_{l-1} + \| U_l \|_2 \Phi_{l-1}
\]

\[
\leq \| W_l + U_l \|_2 B d^{\frac{l-1}{2}} \left( \prod_{i=1}^{l-1} \| W_i \|_2 \right) \sum_{k=1}^{l-1} \| U_k \|_2 \left( 1 + \frac{1}{7} \right)^{l-1-k} + \| U_l \|_2 \prod_{i=1}^{l-1} \| W_i \|_2
\]

\[
= B d^{\frac{l-1}{2}} \left( \prod_{i=1}^{l-1} \| W_i \|_2 \right) \left( \sum_{k=1}^{l-1} \| U_k \|_2 \left( 1 + \frac{1}{7} \right)^{l-1-k} + \| U_l \|_2 \prod_{i=1}^{l-1} \| W_i \|_2 \right)
\]

\[
\leq B d^{\frac{l-1}{2}} \left( \prod_{i=1}^{l-1} \| W_i \|_2 \right) \left[ \left( 1 + \frac{1}{7} \right) \sum_{k=1}^{l-1} \| U_k \|_2 \left( 1 + \frac{1}{7} \right)^{l-1-k} + \| U_l \|_2 \| W_l \|_2 \right]
\]

\[
\leq B d^{\frac{l-1}{2}} \left( \prod_{i=1}^{l-1} \| W_i \|_2 \right) \left[ \left( 1 + \frac{1}{7} \right)^l \sum_{k=1}^{l-1} \| U_k \|_2 \left( 1 + \frac{1}{7} \right)^{-k} + \| U_l \|_2 \| W_l \|_2 \right]
\]

\[
\leq \epsilon B d^{\frac{l-1}{2}} \left( \prod_{i=1}^{l-1} \| W_i \|_2 \right) \left[ \sum_{k=1}^{l-1} \| U_k \|_2 \| W_k \|_2 \right] \left( 1 + \frac{1}{7} \right)^l \leq \epsilon
\]

which proves the lemma. □

**Theorem 3.2. (GCN Generalization Bound)** For any \( B > 0, l > 1 \), let \( f_w \in \mathcal{H} \subset \mathcal{X} \times \mathcal{G} \to \mathbb{R}^K \) be a \( l \)-layer GCN. Then for any \( \delta, \gamma > 0 \), with probability at least \( 1 - \delta \) over the choice of an i.i.d. size-\( m \) training set \( S \) according to \( \mathcal{D} \), for any \( w \), we have,

\[
L_{D,0}(f_w) \leq L_{S,\gamma}(f_w) + O \left( \frac{B^2 d^{\frac{l-1}{2}} \log(\eta h)}{\gamma^2 m} \right)
\]

**Proof.** Let \( \beta = \left( \prod_{i=1}^{l} \| W_i \|_2 \right)^{1/l} \). We normalize the weights as \( \tilde{W}_i = \frac{\beta}{\| W_i \|_2} W_i \). Due to the homogeneity of ReLU, i.e., \( a \phi(x) = \phi(ax) \), \( \forall a \geq 0 \), we have \( f_w = \tilde{f}_w \). We can also verify that \( \prod_{i=1}^{l} \| W_i \|_2 = \prod_{i=1}^{l} \| \tilde{W}_i \|_2 \) and \( \| W_i \|_F \| W_i \|_2 = \| \tilde{W}_i \|_F \| \tilde{W}_i \|_2 \), i.e., the terms appear in the bound stay the same after applying the normalization. Therefore, w.l.o.g., we assume that the norm is equal across layers, i.e., \( \forall i, \| W_i \|_2 = \beta \).
Consider the prior \( P = \mathcal{N}(0, \sigma^2 I) \) and the random perturbation \( u \sim \mathcal{N}(0, \sigma^2 I) \). Note that the \( \sigma \) of the prior and the perturbation are the same and will be set according to \( \beta \). More precisely, we will set the \( \sigma \) based on some approximation \( \bar{\beta} \) of \( \beta \) since the prior \( P \) cannot depend on any learned weights directly. The approximation \( \bar{\beta} \) is chosen to be a cover set which covers the meaningful range of \( \beta \). For now, let us assume that we have a fix \( \bar{\beta} \) and consider \( \beta \) which satisfies \( |\beta - \bar{\beta}| \leq \frac{1}{l} \beta \). Note that this also implies

\[
|\beta - \bar{\beta}| \leq \frac{1}{l} \beta \Rightarrow \left( 1 - \frac{1}{l} \right) \beta \leq \bar{\beta} \leq \left( 1 + \frac{1}{l} \right) \beta \\
\Rightarrow \left( 1 - \frac{1}{l} \right)^{l-1} \beta^{l-1} \leq \bar{\beta}^{l-1} \leq \left( 1 + \frac{1}{l} \right)^{l-1} \beta^{l-1} \\
\Rightarrow \frac{1}{e} \beta^{l-1} \leq \bar{\beta}^{l-1} \leq e \beta^{l-1}
\] (33)

From Tropp (2012), for \( U_i \in \mathbb{R}^{h \times h} \) and \( U_i \sim \mathcal{N}(0, \sigma^2 I) \), we have,

\[
\mathbb{P} ( \|U_i\|_2 \geq t ) \leq 2he^{-t^2/2h\sigma^2}.
\] (34)

Taking a union bound, we have

\[
\mathbb{P} ( \|U_i\|_2 < t \land \cdots \land \|U_i\|_2 < t ) = 1 - \mathbb{P} ( \exists i, \|U_i\|_2 \geq t ) = 1 - \sum_{i=1}^{l} \mathbb{P} ( \|U_i\|_2 \geq t ) \\
\geq 1 - \sum_{i=1}^{l} 2he^{-t^2/2h\sigma^2} \\
\geq 1 - 2lhe^{-t^2/2h\sigma^2}.
\] (35)

Setting \( 2lhe^{-t^2/2h\sigma^2} = \frac{1}{2} \), we have \( t = \sigma \sqrt{2h \log(4lh)} \). This implies that the probability that the spectral norm of the perturbation of any layer is no larger than \( \sigma \sqrt{2h \log(4lh)} \) holds with probability at least \( \frac{1}{2} \). Plugging this bound into Lemma 3.1, we have with probability at least \( \frac{1}{2} \),

\[
|f_{w+u}(X, A) - f_w(X, A)|_2 \leq eBd^{1/l^2} \left( \prod_{i=1}^{l} \|W_i\|_2 \right) \sum_{k=1}^{l} \|U_k\|_2 / \|W_k\|_2 \\
= eBd^{1/l^2} \frac{l}{\beta} \sum_{k=1}^{l} \|U_k\|_2 / \|W_k\|_2 \\
\leq eBd^{1/l^2} \frac{\beta^{-1}l\sigma}{\sqrt{2h \log(4lh)}} \\
\leq e^2Bd^{1/l^2} \frac{\beta^{-1}l\sigma\sqrt{2h \log(4lh)}}{\sqrt{2h \log(4lh)}} \leq \frac{\gamma}{4},
\] (36)

where we can set \( \sigma = \frac{\gamma}{4eBd^{1/l^2} \beta^{-1}l\sqrt{2h \log(4lh)}} \) to get the last inequality. Note that Lemma 3.1 also requires \( \forall i \in \mathbb{N}_+, \|U_i\|_2 \leq \frac{1}{l} \|W_i\|_2 \). The requirement is satisfied if \( \sigma \leq \frac{\beta}{l\sqrt{2h \log(4lh)}} \) which in turn can be satisfied if

\[
\frac{\gamma}{4eBd^{1/l^2} \beta^{-1}l\sqrt{2h \log(4lh)}} \leq \frac{\beta}{l\sqrt{2h \log(4lh)}},
\] (37)

since the chosen value of \( \sigma \) satisfies \( \sigma \leq \frac{\gamma}{4eBd^{1/l^2} \beta^{-1}l\sqrt{2h \log(4lh)}} \). Note that Eq. (37) is equivalent to \( \frac{\gamma}{4eBd^{1/l^2}} \leq \beta^l \). We will see how to satisfy this condition later.
We now compute the KL term in the PAC-Bayes bound in Lemma 2.2.

\[
\begin{align*}
\text{KL}(Q\|P) &= \frac{|w|^2}{2\sigma^2} = \frac{42^4 B^2 d^{-1} \beta^2 l^2 h \log(4l|)}{2\gamma^2} \sum_{i=1}^{l} \|W_i\|_F^2, \\
&\leq O \left( \frac{B^2 d^{-1} \beta^2 l^2 h \log(lh)}{\gamma^2} \sum_{i=1}^{l} \|W_i\|_F^2 \right) \\
&\leq O \left( B^2 d^{-1} l^2 h \log(lh) \prod_{i=1}^{l} \|W_i\|_2^2 \sum_{i=1}^{l} \|W_i\|_F^2 \right). 
\end{align*}
\]

From Lemma 2.2, fixing any \(\tilde{\beta}\), with probability \(1 - \delta\) and for all \(w\) such that \(|\beta - \tilde{\beta}| \leq \frac{1}{l} \beta\), we have,

\[
L_{D,0}(f_w) \leq L_{S,\gamma}(f_w) + O \left( \frac{B^2 d^{-1} l^2 h \log(lh) \prod_{i=1}^{l} \|W_i\|_2^2 \sum_{i=1}^{l} \|W_i\|_F^2 + \log \frac{m}{\delta}}{\gamma^2 m} \right). 
\]

Finally, we need to consider multiple choices of \(\tilde{\beta}\) so that for any \(\beta\), we can bound the generalization error like Eq. (39). First, we only need to consider values of \(\beta\) in the following range,

\[
\frac{1}{\sqrt{d}} \left( \frac{\gamma \sqrt{d}}{2B} \right)^{1/l} \leq \beta \leq \frac{1}{\sqrt{d}} \left( \frac{\gamma \sqrt{md}}{2B} \right)^{1/l},
\]

since otherwise the bound holds trivially as \(L_{D,0}(f_w) \leq 1\) by definition. Note that the lower bound in Eq. (40) ensures that Eq. (37) holds which in turn justifies the applicability of Lemma 3.1. If \(\beta < \frac{1}{\sqrt{d}} \left( \frac{\gamma \sqrt{md}}{2B} \right)^{1/l}\), then for any \((X, A)\) and any \(j \in \mathbb{N}_K^+, |f(X, A)[j]| \leq \frac{\gamma}{2}\). To see this, we have,

\[
|f_w(X, A)[j]| \leq |f_w(X, A)|_2 = \frac{1}{n} |1_n H_{l-1} W_l|_2 \\
\leq \frac{1}{n} |1_n H_{l-1}|_2 \|W_l\|_2 \\
\leq \|W_l\|_2 \max_i \|H_{l-1}[i ,:]\|_2 \\
\leq B d^{l-1} \prod_{i=1}^{l} \|W_i\|_2 = d^{l-1} \beta^l B 
\]

(Use Eq. (27))

\[
= d^{l-1} B \frac{\gamma}{2Bd^{l-1}} \leq \frac{\gamma}{2} 
\]

Therefore, by the definition in Eq. (4), we always have \(L_{S,\gamma}(f_w) = 1\) when \(\beta < \frac{1}{\sqrt{d}} \left( \frac{\gamma \sqrt{md}}{2B} \right)^{1/l}\).

Alternatively, if \(\beta > \frac{1}{\sqrt{d}} \left( \frac{\gamma \sqrt{md}}{2B} \right)^{1/l}\), the term inside the big-O notation in Eq. (39) would be,

\[
\sqrt{\frac{B^2 d^{-1} l^2 h \log(lh) \prod_{i=1}^{l} \|W_i\|_2^2 \sum_{i=1}^{l} \|W_i\|_F^2 + \log \frac{m}{\delta}}{\gamma^2 m}} \\
\geq \sqrt{\frac{l^2 h \log(lh) \sum_{i=1}^{l} \|W_i\|_F^2}{4 \|W_i\|_2^2}} \\
\geq \sqrt{\frac{l^2 h \log(lh)}{4}} \geq 1,
\]

where we use the facts that \(\|W_i\|_F \geq \|W_i\|_2\) and we typically choose \(h \geq 2\) in practice and \(l \geq 2\). Since we only need to consider \(\beta\) in the range of Eq. (40), a sufficient condition to make \(|\beta - \tilde{\beta}| \leq \frac{1}{l} \beta\) hold would be \(|\beta - \tilde{\beta}| \leq \frac{1}{\sqrt{d}} \left( \frac{\gamma \sqrt{md}}{2B} \right)^{1/l}\). Therefore, if we can find a covering of the interval in Eq.
besides the last readout one, the node representations are, \[ \text{(MPGNN Perturbation Bound)} \]

\[ \forall \text{Lemma 3.3}. \]

In this part, we provide the proofs of the main results regarding MPGNNs.

\subsection*{A.4 MPGNNs Results}

\[ (\ref{eq:mpgnn_perturbation_bound}) \]

\[ \text{with } \tilde{\beta} \text{ taking all possible values from the covering, then we can get a bound which holds for all } \beta. \]

We first perform the recursive perturbation analysis on node representations of all steps except the last readout step.

\[ \text{Proof.} \]

\[ \text{where the incidence matrices } C_{in}, C_{out} \in \mathbb{R}^{n \times c} \text{ (recall } c \text{ is the number of edges).} \]

Moreover, since each edge only connects one incoming and one outgoing node, we have,

\[ \sum_{k=1}^{c} C_{in}[i, k] \leq \max_{i} \sum_{k=1}^{c} C_{in}[i, k] = \|C_{in}\|_{\infty} \leq d \]

\[ \sum_{l=1}^{n} C_{out}[t, k] \leq \max_{k} \sum_{l=1}^{n} C_{out}[t, k] = \|C_{out}\|_{1} \leq 1 \]

\[ (46) \]

(40) with radius \( \frac{1}{\sqrt{d}} \left( \frac{\sqrt{n}}{2d} \right)^{1/d} \) and make sure bounds like Eq. (39) holds while \( \tilde{\beta} \) takes all possible values from the covering, then we can get a bound which holds for all \( \beta \). It is clear that we only need to consider a covering \( C \) with size \( |C| = \frac{1}{2} \left( \frac{m}{d} - 1 \right) \). Therefore, denoting the event of Eq. (39) with \( \tilde{\beta} \) taking the \( i \)-th value of the covering as \( E_i \), we have,

\[ \mathbb{P}(E_1 \& \cdots \& E_{|C|}) = 1 - \mathbb{P}(\bar{E}_1) \geq 1 - \sum_{i=1}^{|C|} \mathbb{P}(\bar{E}_i) \geq 1 - |C|\delta. \]

Note \( \bar{E}_i \) denotes the complement of \( E_i \). Hence, with probability \( 1 - \delta \) and for all \( w \), we have,

\[ L_{D,0}(f_w) \leq \left( \frac{B^2d^{-1/2}\log(lh) \prod_{i=1}^{l} \|W_l\|_2^2 \sum_{i=1}^{l} \|W_l\|_F^2 + \log \frac{m|C|}{\delta}}{\gamma^2 m} \right), \]

which proves the theorem.

\[ (44) \]

\[ (43) \]

\[ (42) \]

\[ (41) \]

\[ (40) \]

\[ (39) \]

\[ (38) \]

\[ (37) \]

\[ (36) \]

\[ (35) \]

\[ (34) \]

\[ (33) \]

\[ (32) \]

\[ (31) \]

\[ (30) \]

\[ (29) \]

\[ (28) \]

\[ (27) \]

\[ (26) \]

\[ (25) \]

\[ (24) \]

\[ (23) \]

\[ (22) \]

\[ (21) \]

\[ (20) \]

\[ (19) \]

\[ (18) \]

\[ (17) \]

\[ (16) \]

\[ (15) \]

\[ (14) \]

\[ (13) \]

\[ (12) \]

\[ (11) \]

\[ (10) \]

\[ (9) \]

\[ (8) \]

\[ (7) \]

\[ (6) \]

\[ (5) \]

\[ (4) \]

\[ (3) \]

\[ (2) \]

\[ (1) \]
We add perturbation \( u \) to the weights \( w \), i.e., the perturbed weights are \( W_1 + U_1, W_2 + U_2 \) and \( W_l + U_l \). For the ease of notation, we use the superscript of prime to denote the perturbed node representations, e.g., \( H'_j = f_{w+u}(X, A) \). Let \( \Delta_j = f_{w}(X, A) - f_{w+u}(X, A) = H'_j - H_j \). Note that \( \Delta_j \in \mathbb{R}^{n \times h_j} \). Let \( \Psi_j = \max_i |\Delta_j[i,:]|_2 = \max_i |H'_j[i,:] - H_j[i,:]|_2 \) and \( \Phi_j = \max_i |H_j[i,:]|_2 \). We denote the \( \kappa = C \|B\|_{W_1} \|W_2\|_2 \) and \( \tau = dC \) throughout the proof where \( C = C_{\phi}C_{\rho}C_g \). We denote the upper bound on the max change of node representation as follows,

**Upper Bound on the Max Change of Node Representation.** For any step \( j < l \), we can derive an upper bound on the \( \ell_2 \) norm of the aggregated message of any node \( i \) as follows,

\[
\|M_j[i,:]|_2 = \left| \sum_{k=1}^{c} C_{in}[i,k] \left( g \left( C_{out}^T H_{j-1} \right) \right) [k,:]|_2 \leq \sum_{k=1}^{c} C_{in}[i,k] \left| g \left( C_{out}^T [k,:] H_{j-1} \right) \right|_2 \leq \sum_{k=1}^{c} C_{in}[i,k] C_g \left| C_{out}^T [k,:] H_{j-1} \right|_2 = \sum_{k=1}^{c} C_{in}[i,k] C_g \left( \sum_{t=1}^{n} C_{out}[t,k] \| H_{j-1}[t,:]|_2 \right) \leq \sum_{k=1}^{c} C_{in}[i,k] C_g \left( \sum_{t=1}^{n} C_{out}[t,k] \Phi_{j-1} \right) \leq dC_g \Phi_{j-1}. \tag{47} \]

Then we can derive an upper bound on the maximum (w.r.t. \( \ell_2 \) norm) node representation as follows,

\[
\Phi_j = \max_i |H_j[i,:]|_2 = |\phi \left( XW_1 + \rho \left( M_j \right) W_2 \right) [v_j^*,,:]|_2 = |\phi \left( XW_1 + \rho \left( M_j \right) W_2 \right) [v_j^*,,:]|_2 \leq C_{\phi} \left| \phi \left( XW_1 + \rho \left( M_j \right) W_2 \right) [v_j^*,,:]\right|_2 = C_{\phi} \left| \phi \left( XW_1 \right) [v_j^*,,:]\right|_2 + C_{\phi} \left| \phi \left( \rho \left( M_j \right) W_2 \right) [v_j^*,,:]\right|_2 = C_{\phi} \left| X[v_j^*,,:] W_1 \right|_2 + C_{\phi} \left| \phi \left( \rho \left( M_j \right) W_2 \right) [v_j^*,,:]\right|_2 \leq C_{\phi} \left| X[v_j^*,,:] W_1 \right|_2 \|W_1\|_2 + C_{\phi} \left| \phi \left( \rho \left( M_j \right) W_2 \right) [v_j^*,,:]\right|_2 \|W_2\|_2 \leq C_{\phi} B \|W_1\|_2 + C_{\phi} \| \rho \left( M_j \right) [v_j^*,,:]\|_2 \|W_2\|_2 \leq C_{\phi} B \|W_1\|_2 + dC_{\phi} C_{\rho} C_g \Phi_{j-1} \|W_2\|_2 = \kappa + \tau \Phi_{j-1} \leq \tau \Phi_0 + \sum_{i=0}^{j-1} \tau^{j-1-i} \kappa \quad \text{(Unroll recursion)} \leq \sum_{i=0}^{j-1} \tau^{j-1-i} \kappa \quad \text{(Use } \Phi_0 = 0) \leq \begin{cases} j \kappa, & \text{if } \tau = 1 \\ \kappa \tau^{j-1}, & \text{otherwise} \end{cases} \tag{48} \]

**Upper Bound on the Max Change of Node Representation.** For any step \( j < l \), we can derive an upper bound on the maximum (w.r.t. \( \ell_2 \) norm) change between the aggregated message with and without the weight perturbation for any node \( i \) as follows,
\begin{align*}
|M'_j[i,:]-M_j[i,:]|_2 & \leq \left|(C_{in} g (C_{out}^T H'_{j-1})) [i,:]- (C_{in} g (C_{out}^T H_{j-1})) [i,:]\right|_2 \\
& = \sum_{k=1}^c C_{in}[i,k] \left(g(C_{out}^T H'_{j-1})- g(C_{out}^T H_{j-1})\right) [k,:]|_2 \\
& \leq \sum_{k=1}^c C_{in}[i,k] \left|g(C_{out}^T H'_{j-1})- g(C_{out}^T H_{j-1})\right|_2 \\
& = \sum_{k=1}^c C_{in}[i,k] C_g \left|g\left(C_{out}^T H'_{j-1}\right) [k,:]- g\left(C_{out}^T H_{j-1}\right) [k,:]\right|_2 \\
& \leq \sum_{k=1}^c C_{in}[i,k] C_g \left|\left(C_{out}^T H'_{j-1}\right) [k,:]- \left(C_{out}^T H_{j-1}\right) [k,:]\right|_2 \\
& \leq d C_g \Psi_{j-1} \tag{49}
\end{align*}

Based on Eq. (49), we can derive an upper bound on the maximum (w.r.t. \ell_2 norm) change between the representations with and without the weight perturbation for any node as follows,

\begin{align*}
\Psi_j &= \max \left|H'_j[i,:]-H_j[i,:]\right|_2 \\
& = \left|\left(\phi \left(X(W_1+U_1)+\rho \left(M'_j\right)\left(W_2+U_2\right)\right)\right) [u'_j,:]- \left(\phi \left(XW_1+\rho \left(M_j\right)W_2\right)\right) [u'_j,:]\right|_2 \\
& = \left|\phi \left(\left(X(W_1+U_1)+\rho \left(M'_j\right)\left(W_2+U_2\right)\right)\right) [u'_j,:]- \phi \left(\left(XW_1+\rho \left(M_j\right)W_2\right)\right) [u'_j,:]\right|_2 \\
& \leq C_\phi \left|\left(X(W_1+U_1)+\rho \left(M'_j\right)\left(W_2+U_2\right)\right) [u'_j,:]- \left(XW_1+\rho \left(M_j\right)W_2\right) [u'_j,:]\right|_2 \\
& \leq C_\phi \left|\left(X[u'_j,:];U_1+\rho \left(M'_j\right)\right) [u'_j,:];(W_2+U_2)-(\rho \left(M_j\right)) [u'_j,:];W_2\right|_2 \\
& = C_\phi \left|\left(X[u'_j,:];U_1+\rho \left(M'_j\right)-\rho \left(M_j\right)\right) [u'_j,:];(W_2+U_2)+\rho \left(M_j\right) [u'_j,:];U_2\right|_2 \\
& \leq C_\phi B \left|\left(U_1\right)_{2}+C_\phi C_p \left[M'_j[u'_j,:];-\left(M_j\right)[u'_j,:];U_2\right]\right|_2+ C_\phi C_p \left|\left(U'_j\right)_{2}\right|_2 + C_\phi C_p \left|\left(U_j\right)_{2}\right|_2 \tag{Use Eq. (47) and (49)} \\
& \leq \kappa \left|\left(U_1\right)_{2} \right|_2 + dC \Psi_{j-1} \left|\left(U_2\right)_{2} \right|_2 + dC \Psi_{j-1} \left|\left(U_2\right)_{2} \right|_2 + \tau \Phi_{j-1} \left|\left(U_2\right)_{2} \right|_2 \\
& \leq \tau \left(1 + \frac{\left|\left(U_2\right)_{2} \right|_2}{\left|\left(U_1\right)_{2} \right|_2} \right) \Psi_{j-1} + \kappa \left|\left(U_1\right)_{2} \right|_2 + \tau \Phi_{j-1} \left|\left(U_2\right)_{2} \right|_2 \tag{50}
\end{align*}

If \( \tau = 1 \), then we have,

\begin{align*}
\Psi_j & \leq \tau \left(1 + \frac{\left|\left(U_2\right)_{2} \right|_2}{\left|\left(U_1\right)_{2} \right|_2} \right) \Psi_{j-1} + \kappa \left|\left(U_1\right)_{2} \right|_2 + \tau \Phi_{j-1} \left|\left(U_2\right)_{2} \right|_2 \\
& \leq \left(1 + \frac{\left|\left(U_2\right)_{2} \right|_2}{\left|\left(U_1\right)_{2} \right|_2} \right) \Psi_{j-1} + \kappa \left(\left|\left(U_1\right)_{2} \right|_2 + \left|\left(U_2\right)_{2} \right|_2 \right) (j-1) \tag{Use Eq. (48)} \\
& \leq (1 + \eta) \Psi_{j-1} + \kappa \eta (1 + (j-1)) \tag{Use \eta = \max \left(\frac{\left|\left(U_1\right)_{2} \right|_2}{\left|\left(U_1\right)_{2} \right|_2}, \frac{\left|\left(U_2\right)_{2} \right|_2}{\left|\left(U_2\right)_{2} \right|_2}, \frac{\left|\left(U_1\right)_{2} \right|_2}{\left|\left(U_1\right)_{2} \right|_2}\right)} \\
& = (1 + \eta) \Psi_{j-1} + \kappa \eta j. \tag{51}
\end{align*}
If \( \tau \neq 1 \), then we have,

\[
\Psi_j \leq \tau \left( 1 + \frac{\|U_1\|_2}{\|W_2\|_2} \right) \Psi_{j-1} + \kappa \frac{\|U_1\|_2}{\|W_1\|_2} + \tau \Phi_{j-1} \frac{\|U_2\|_2}{\|W_2\|_2}
\]

\[
\leq \tau \left( 1 + \frac{\|U_2\|_2}{\|W_2\|_2} \right) \Psi_{j-1} + \kappa \left( \frac{\|U_1\|_2}{\|W_1\|_2} + \tau \frac{\|U_2\|_2}{\|W_2\|_2} \tau^{j-1} - 1 \right) \left( \frac{\|U_2\|_2}{\|W_2\|_2} \right) \frac{\tau^{j-1}}{\tau - 1} \quad \text{(Use Eq. (48))}
\]

\[
\leq \tau (1 + \eta) \Psi_{j-1} + \kappa \eta \left( 1 + \frac{\tau^{j-1} - \tau}{\tau - 1} \right) \quad \text{(Use } \eta = \max \left( \frac{\|U_1\|_2}{\|W_1\|_2}, \frac{\|U_2\|_2}{\|W_2\|_2}, \frac{\|U_l\|_2}{\|W_l\|_2} \right) \text{)}
\]

\[
= \tau (1 + \eta) \Psi_{j-1} + \kappa \eta \left( \frac{\tau^{j-1} - \tau}{\tau - 1} \right). \tag{52}
\]

Recall from Eq. (30), if \( \Psi_j \leq a_j - 1 \Psi_{j-1} + b_j - 1 \) and \( \Psi_0 = 0 \), then \( \Psi_j \leq \sum_{k=0}^{j-1} b_k \left( \prod_{i=k+1}^{j-1} a_i \right) \).

If \( \tau = 1 \), then we have \( a_{j-1} = 1 + \eta, b_{j-1} = \kappa \eta j \) in our case and,

\[
\Psi_j \leq \sum_{k=0}^{j-1} b_k \left( \prod_{i=k+1}^{j-1} a_i \right) = \sum_{k=0}^{j-1} \kappa \eta (k + 1) (1 + \eta)^{j-k-1}
\]

\[
\leq \kappa \eta \left( 1 + \frac{1}{7} \right) \sum_{k=0}^{j-1} (k + 1) \left( 1 + \frac{1}{7} \right)^{j-k-1} \quad \text{(Use } \eta \leq \frac{1}{7} \text{)}
\]

\[
= \kappa \eta \left( 1 + \frac{1}{7} \right)^{j} \left( 1 + \frac{1}{7} \right)^{-1} \frac{1 - (j + 1) \left( 1 + \frac{1}{7} \right)^{-j} + j \left( 1 + \frac{1}{7} \right)^{-j-1}}{(1 - (1 + \frac{1}{7})^{-j})^2}
\]

\[
= \kappa \eta \left( 1 + \frac{1}{7} \right)^{j+1} - (j + 1) \left( 1 + \frac{1}{7} \right) + j
\]

\[
(1 + \frac{1}{7})^{j+1} - (j + 1) \left( 1 + \frac{1}{7} \right) + j
\]

\[
\leq \kappa \eta (l + 1) \left( 1 + \frac{1}{7} \right)^j \tag{53}
\]

If \( \tau \neq 1 \), then we have \( a_{j-1} = \tau (1 + \eta), b_{j-1} = \kappa \eta \left( \frac{\tau^{j-1} - \tau}{\tau - 1} \right) \) in our case and,

\[
\Psi_j \leq \sum_{k=0}^{j-1} b_k \left( \prod_{i=k+1}^{j-1} a_i \right) = \sum_{k=0}^{j-1} \kappa \eta \left( \frac{\tau^{k+1} - 1}{\tau - 1} \right) \tau^{j-k-1} (1 + \eta)^{j-k-1}
\]

\[
\leq \kappa \eta \tau^j \left( 1 + \frac{1}{7} \right) \sum_{k=0}^{j-1} \left( \frac{\tau^{k+1} - 1}{\tau - 1} \right) \tau^{-k-1} \left( 1 + \frac{1}{7} \right)^{j-k-1} \quad \text{(Use } \eta \leq \frac{1}{7} \text{)}
\]

\[
\leq \kappa \eta \tau^{j} \left( 1 + \frac{1}{7} \right) \sum_{k=0}^{j-1} \left( 1 - \tau^{-k-1} \right) \left( 1 + \frac{1}{7} \right)^{-k-1}
\]

\[
\leq \frac{\kappa \eta \tau^j}{\tau - 1} \left( 1 + \frac{1}{7} \right) \sum_{k=1}^{j} (1 - \tau^{-k}) \tag{54}
\]
Final Bound with Readout Function  Now let us consider the readout function. Since the last readout layer produces a vector in $\mathbb{R}^{1 \times C}$, we have,

$$
|\Delta|_2 = \left| \frac{1}{n} \mathbf{1}_n H_{l-1} (W_i + U_l) - \frac{1}{n} \mathbf{1}_n H_{l-1} W_i \right|_2 \\
= \left| \frac{1}{n} \mathbf{1}_n \Delta_{l-1} (W_i + U_l) + \frac{1}{n} \mathbf{1}_n H_{l-1} U_l \right|_2 \\
\leq \frac{1}{n} |\mathbf{1}_n \Delta_{l-1} (W_i + U_l)|_2 + \frac{1}{n} |\mathbf{1}_n H_{l-1} U_l|_2 \\
\leq \frac{1}{n} \|W_i + U_l\|_2 |\mathbf{1}_n \Delta_{l-1}|_2 + \frac{1}{n} \|U_l\|_2 |\mathbf{1}_n H_{l-1}|_2 \\
\leq \|W_i + U_l\|_2 |\Psi_{l-1}| + \|U_l\|_2 |\Phi_{l-1}| \\
(55)
$$

If $\tau = 1$, we have,

$$
|\Delta|_2 \leq \|W_i\|_2 \left( 1 + \frac{1}{7} \right) \kappa (l + 1) \left( 1 + \frac{1}{7} \right)^{l-1} (l + 1) \kappa \|U_l\|_2 \\
\text{(Use Eq. (48), (53))} \\
\leq \|W_i\|_2 \left( 1 + \frac{1}{7} \right)^l \kappa \left( \eta (l + 1) + (l - 1) \|U_l\|_2 \right) \left( 1 + \frac{1}{7} \right)^{l-1} \\
\leq \|W_i\|_2 \kappa (l + 1)^2 \\
(56)
$$

Otherwise, we have,

$$
|\Delta|_2 \leq \|W_i\|_2 \left( 1 + \frac{1}{7} \right)^l \kappa \left( \sum_{k=1}^{l-1} (1 - \tau^{-k}) + \kappa \|U_l\|_2 \right) \left( \frac{1 - 1}{\tau - 1} \right) \\
\text{(Use Eq. (48), (54))} \\
\leq \|W_i\|_2 \frac{\kappa \tau^{l-1}}{\tau - 1} \left( 1 + \frac{1}{7} \right)^l \left( \sum_{k=1}^{l-1} (1 - \tau^{-k}) + \|U_l\|_2 \right) \left( 1 - \tau^{1-l} \right) \\
(57)
$$

If $\tau > 1$, then $\frac{1 - \tau^{-1}}{\tau - 1} \leq \frac{1 - \tau^{-k}}{\tau - 1}$ when $1 \leq k \leq l - 1$. If $\tau < 1$, we also have $\frac{1 - \tau^{-1}}{\tau - 1} \leq \frac{1 - \tau^{-k}}{\tau - 1}$ when $1 \leq k \leq l - 1$. Therefore, Eq. (57) can be further relaxed as,

$$
|\Delta|_2 \leq \|W_i\|_2 \frac{\kappa \tau^{l-1}}{\tau - 1} \left( 1 + \frac{1}{7} \right)^l \left( \sum_{k=1}^{l-1} (1 - \tau^{-k}) + \|U_l\|_2 \right) \left( 1 - \tau^{1-l} \right) \\
= \|W_i\|_2 \kappa \tau^{l-1} \left( 1 + \frac{1}{7} \right)^l \left( \sum_{k=1}^{l-1} (1 - \tau^{-k}) + \|U_l\|_2 \right) \left( 1 - \tau^{1-l} \right) \\
\leq \|W_i\|_2 \kappa \tau^{l-1} \eta \left( \sum_{k=1}^{l-1} (1 - \tau^{-k}) + \|U_l\|_2 \right) \left( 1 - \tau^{1-l} \right) \\
\leq \|W_i\|_2 \kappa \tau^{l-1} \eta \left( \frac{1 - \tau^{1-l}}{\tau - 1} \right) \left( \text{Use } \frac{\|U_l\|_2}{\|W_i\|_2} \leq \eta \right) \\
= \eta \kappa \|W_i\|_2 \frac{\tau^{l-1} - 1}{\tau - 1}, \\
(58)
$$

Therefore, combining Eq. (56) and Eq. (58), we have,

$$
|\Delta|_2 \leq \begin{cases} 
\eta \kappa \|W_i\|_2, & \text{if } dC = 1 \\
\eta \kappa dC \|W_i\|_2 \frac{\tau^{l-1} - 1}{\tau - 1}, & \text{otherwise}
\end{cases} \\
(59)
$$

which proves the lemma. □
Theorem 3.4. (MPGNN Generalization Bound) For any $B > 0, l > 1$, let $f_w \in \mathcal{H} : \mathcal{X} \times \mathcal{G} \to \mathbb{R}^K$ be a $l$-step MPGNN. Then for any $\delta, \gamma > 0$, with probability at least $1 - \delta$ over the choice of an i.i.d. size-$m$ training set $S$ according to $\mathcal{D}$, for any $w$, we have,

1. If $dC \neq 1$, then

$$L_{\mathcal{D},0}(f_w) \leq L_{\mathcal{S},\gamma}(f_w) + O\left(\sqrt{\frac{B^2 (max (\zeta^{l+1}), (\lambda \xi)^{l+1})^2 \rho \log (lh) \|w\|_2^2 + \log \frac{m l+1}{\xi}}{\gamma^2 m}}\right).$$

2. If $dC = 1$, then

$$L_{\mathcal{D},\delta}(f_w) \leq L_{\mathcal{S},\gamma}(f_w) + O\left(\sqrt{\frac{B^2 \max (\zeta^{-6}, \lambda^3 \xi^3) (l + 1)^4 \rho \log (lh) \|w\|_2^2 + \log \frac{m l+1}{\xi}}{\gamma^2 m}}\right).$$

where $\zeta = \min (\|W_1\|_2, \|W_2\|_2, \|W_I\|_2), \|w\|_2 = \|W_1\|_2^2 + \|W_2\|_2^2 + \|W_I\|_2^2, C = C \phi C \rho C \gamma \|W_2\|_2, \lambda = \|W_1\|_2 \|W_I\|_2$, and $\xi = C \phi^{(dC)^{-1} - 1}.$

Proof. We will derive the results conditioning on the value of $dC$.

General Case $dC \neq 1$ We first consider the general case $dC \neq 1$. To derive the generalization bound, we construct a special statistic of the learned weights $\beta = \max \left(\frac{1}{\lambda}, (\lambda \xi)^{\frac{1}{l}}\right)$. It is clear that $\frac{1}{\xi} \leq \beta, \lambda \xi \leq \beta^l$, and $\lambda \xi / \zeta \leq \beta^{l+1}$. Note that $\frac{1}{\xi} = \max \left(\frac{1}{\|W_1\|_2}, \frac{1}{\|W_2\|_2}, \frac{1}{\|W_I\|_2}\right)$.

Consider the prior $P = \mathcal{N}(0, \sigma^2 I)$ and the random perturbation $u \sim \mathcal{N}(0, \sigma^2 I)$. Note that the $\sigma$ of the prior and the perturbation are the same and will be set according to $\beta$. More precisely, we will set the $\sigma$ based on some approximation $\bar{\beta}$ of $\beta$ since the prior $P$ can not depend on any learned weights directly. The approximation $\bar{\beta}$ is chosen to be a cover set which covers the meaningful range of $\beta$. For now, let us fix any $\beta$ and consider $\beta$ which satisfies $|\beta - \bar{\beta}| \leq \frac{1}{l+1} \beta$. This also implies,

$$|\beta - \bar{\beta}| \leq \frac{1}{l+1} \beta \Rightarrow \left(1 - \frac{1}{l+1}\right) \beta \leq \bar{\beta} \leq \left(1 + \frac{1}{l+1}\right) \beta \Rightarrow \left(1 - \frac{1}{l+1}\right)^{l+1} \beta^{l+1} \leq \bar{\beta}^{l+1} \leq \left(1 + \frac{1}{l+1}\right)^{l+1} \beta^{l+1} \Rightarrow e^{\beta^{l+1}} \leq \bar{\beta}^{l+1} \leq e^{\beta^{l+1}}.$$ (60)

From Tropp (2012), for $U_i \in \mathbb{R}^{h \times h}$ and $U_i \sim \mathcal{N}(0, \sigma^2 I)$, we have,

$$\mathbb{P} (\|U_i\|_2 \geq t) \leq 2he^{-t^2 / 2h\sigma^2}.$$ (61)

Taking a union bound, we have

$$\mathbb{P} (\|U_i\|_2 < t \& \cdots \& \|U_i\|_2 < t) = 1 - \mathbb{P} (\exists i, \|U_i\|_2 \geq t) \geq 1 - \sum_{i=1}^{l} \mathbb{P} (\|U_i\|_2 \geq t) \geq 1 - 2lhe^{-t^2 / 2h\sigma^2}. \quad (62)$$

Setting $2lhe^{-t^2 / 2h\sigma^2} = \frac{1}{2}$, we have $t = \sigma \sqrt{2h \log(4lh)}$. This implies that the probability that the spectral norm of the perturbation of any layer is no larger than $\sigma \sqrt{2h \log(4lh)}$ holds with probability
at least $\frac{1}{2}$. Plugging this bound into Lemma 3.3, we have with probability at least $\frac{1}{2}$,

$$\left| f_{w+w}(X, A) - f_w(X, A) \right|_2 \leq e^t \frac{LC\phi B}{\varnothing} \left| W_1 \right|_2 \left| W_i \right|_2 \frac{(dC)^{l-1} - 1}{dC - 1}$$

$$= etB \frac{\lambda e}{\varnothing}$$

$$= eB \frac{\beta+1}{\varnothing} \leq e^2 B \frac{\beta+1}{\varnothing} \sqrt{2h \log(4h)} \leq \frac{\gamma}{4},$$

(63)

where we can set $\sigma = \frac{42B \beta+1 \sqrt{2h \log(4h)}}{4eB \beta+1}$ to get the last inequality. Note that Lemma 3.3 also requires $\max \left( \frac{\parallel U_j \parallel_2}{\parallel W_j \parallel_2}, \frac{\parallel U_j \parallel_2}{\parallel W_j \parallel_2}, \frac{\parallel U_j \parallel_2}{\parallel W_j \parallel_2} \right) \leq \frac{1}{7}$. The requirement is satisfied if $\sigma \leq \frac{\gamma}{4}eB \beta+1 \sqrt{2h \log(4h)}$ which in turn can be satisfied if

$$\frac{\gamma}{4eB \beta+1 \sqrt{2h \log(4h)}} \leq \frac{1}{\beta \sqrt{2h \log(4h)}},$$

(64)

since the chosen value of $\sigma$ satisfies $\sigma \leq \frac{42B \beta+1 \sqrt{2h \log(4h)}}{4eB \beta+1}$ and $\frac{1}{\beta} \leq \frac{\varnothing}{\gamma}$. Therefore, one sufficient condition to make Eq. (64) hold is $\frac{\gamma}{4eB} \leq \beta$. We will see how to satisfy this condition later.

We now compute the KL term in the PAC-Bayes bound in Lemma 2.2.

$$\text{KL} (Q || P) = \frac{\left| w \right|_2^2}{2\varnothing^2}$$

$$= \frac{42B^2 \beta+1 \gamma^2 \sqrt{2h \log(4h)}}{2\gamma^2} \left( \parallel W_1 \parallel_2^2 + \parallel W_2 \parallel_2^2 + \parallel W_i \parallel_2^2 \right)$$

$$\leq \mathcal{O} \left( \frac{B^2 \beta+1 \gamma^2 \sqrt{2h \log(4h)}}{2\gamma^2} \left( \parallel W_1 \parallel_2^2 + \parallel W_2 \parallel_2^2 + \parallel W_i \parallel_2^2 \right) \right)$$

(65)

From Lemma 2.2, fixing any $\tilde{\beta}$, with probability $1 - \delta$ and for all $w$ such that $|\beta - \tilde{\beta}| \leq \frac{1}{1+1} \tilde{\beta}$, we have,

$$L_{D,0}(f_w) \leq L\sqrt{\gamma}(f_w) + \mathcal{O} \left( \sqrt{\frac{B^2 \beta+1 \gamma^2 \sqrt{2h \log(4h)} \parallel w \parallel_2^2 + \log \frac{\varnothing}{\varnothing}}{\gamma^2 m} \right).$$

(66)

Finally, we need to consider multiple choices of $\tilde{\beta}$ so that for any $\beta$, we can bound the generalization error like Eq. (66). In particular, we only need to consider values of $\beta$ in the following range,

$$\left( \frac{\gamma}{2B} \right)^{\frac{1}{2}} \leq \beta \leq \left( \frac{\gamma \sqrt{m}}{2B} \right)^{\frac{1}{2}},$$

(67)

since otherwise the bound holds trivially as $L_{D,0}(f_w) \leq 1$ by definition. To see this, if $\beta < \frac{\gamma}{2B}$, then for any $(X, A)$ and any $j \in \mathbb{N}_K^+$, we have,

$$\left| f_w(X, A)[j] \right| \leq \left| f_w(X, A) \right|_2 = \frac{1}{n} \parallel H_{l-1} W_i \parallel_2$$

$$\leq \frac{1}{n} \parallel H_{l-1} \parallel_2 \parallel W_i \parallel_2$$

$$\leq \parallel W_i \parallel_2 \max_i \parallel H_{l-1}[i, :]\parallel_2$$

$$\leq B C_0 \parallel W_1 \parallel_2 \parallel W_i \parallel_2 \frac{(dC)^{l-1} - 1}{dC - 1} \quad \text{(Use Eq. (48))}$$

$$\leq B \lambda \xi \quad \text{(Use definition of } \lambda \text{ and } \xi)$$

$$\leq B \beta^l \quad \text{(Use definition of } \beta)$$

$$\leq \frac{\gamma}{2}.$$  

(68)
Therefore, based on the definition in Eq. (4), we always have \( L_{S, \gamma}(f_w) = 1 \) when \( \beta^t < \frac{\gamma}{2B} \). It is hence sufficient to consider \( \beta^t \geq \frac{\gamma}{2B} > \frac{\gamma}{4}\sigma \) which also makes Eq. (64) hold. Alternatively, if \( \beta^t > \frac{\gamma}{2B} \), the term inside the big-O notation in Eq. (66) would be,

\[
\sqrt{B^2 \beta^t l^2 h \log(lh)(|w|^2)} + \log \frac{m}{\delta} \geq \sqrt{\frac{l^2 h \log(lh)(|w|^2)}{\delta}} \geq 1,
\]

(69)

The last inequality uses the fact that we typically choose \( h \geq 2 \) in practice, \( l \geq 2 \) and \(|w|^2 \geq \min \left(\|W_1\|^2, \|W_2\|^2, \|W_3\|^2\right) \geq \sigma^2 \). Since we only need to consider \( \beta \) in the range of Eq. (67), one sufficient condition to ensure \( |\beta - \hat{\beta}| \leq \frac{\gamma}{4 \sigma} \) holds would be \( |\beta - \hat{\beta}| \leq \frac{1}{\sigma^2 + \frac{\gamma}{2B}} \). Therefore, if we can find a covering of the interval in Eq. (67) with radius \( \frac{1}{\sigma^2 + \frac{\gamma}{2B}} \) and make sure bounds like Eq. (66) holds while \( \hat{\beta} \) takes all possible values from the covering, then we can get a bound which holds for all \( \beta \). It is clear that we only need to consider a covering \( C \) with size \( |C| = \frac{(l+1)}{2} (m^{1/2l} - 1) \). Therefore, denoting the event of Eq. (66) with \( \beta \) taking the \( i \)-th value of the covering as \( E_i \), we have

\[
\mathbb{P} (E_1 \& \cdots \& E_{|C|}) = 1 - \mathbb{P} (\exists i, \bar{E}_i) \geq 1 - \sum_{i=1}^{|C|} \mathbb{P} (\bar{E}_i) \geq 1 - |C| \delta,
\]

(70)

where \( \bar{E}_i \) denotes the complement of \( E_i \). Hence, with probability \( 1 - \delta \) and for all \( w \), we have,

\[
L_{D,0}(f_w) \leq L_{S, \gamma}(f_w) + O \left( \sqrt{\frac{B^2 \beta^t l^2 h \log(lh)(|w|^2) + \log \frac{m|C|}{\delta}}{\gamma^2 m}} \right)
\]

\[
= L_{S, \gamma}(f_w) + O \left( \sqrt{\frac{B^2 \beta^t l^2 h \log(lh)(|w|^2) + \log \frac{m(l+1)}{\delta} + \frac{1}{2l} \log m}{\gamma^2 m}} \right)
\]

\[
= L_{S, \gamma}(f_w) + O \left( \frac{B^2 \max \left( \zeta^{-1}, (\lambda \zeta)^2 \right) \log(lh)(|w|^2) + \log \frac{m(l+1)}{\delta}}{\gamma^2 m} \right)
\]

(71)

which proves the theorem for the case of \( dC \neq 1 \).

**Special Case** \( dC = 1 \)  
Now we consider \( dC = 1 \) of which the proof follows the logic of the one for \( dC \neq 1 \). Note that this case happens rarely in practice. We only include it for the completeness of the analysis. We again construct a statistic \( \beta = \max \left( \frac{1}{\zeta}, \sqrt{\lambda C_{\phi}} \right) \). For now, let us fix any \( \tilde{\beta} \) and consider \( \beta \) which satisfies \( |\beta - \tilde{\beta}| \leq \frac{\gamma}{2B} \). This also implies \( \frac{1}{\zeta} \beta^3 \leq \tilde{\beta}^3 \leq e \beta^3 \). Based on Lemma 3.3, we have,

\[
|f_{w+w}(X, A) - f_w(X, A)|_2 \leq e \frac{l}{\zeta} (l+1)^2 C_{\phi} B \|W_1\|_2 \|W_1\|_2
\]

\[
= e \frac{l}{\zeta} (l+1)^2 B \sqrt{\lambda C_{\phi}} \leq eB(l+1)^2 \beta^3 t
\]

\[
\leq e^2 B(l+1)^2 \beta^3 \sqrt{2h \log(4lh)} \leq \frac{\gamma}{4},
\]

(72)

where we can set \( \sigma = \frac{\gamma}{4B(l+1)^2 \beta^3 \sqrt{2h \log(4lh)}} \) to get the last inequality. Note that Lemma 3.3 also requires \( \max \left( \frac{\|W_1\|^2}{\|W_1\|^2}, \frac{\|W_2\|^2}{\|W_2\|^2}, \frac{\|W_3\|^2}{\|W_3\|^2} \right) \leq \frac{1}{\zeta} \). The requirement is satisfied if \( \sigma \leq \frac{\zeta}{\sqrt{2h \log(4lh)}} \) which in turn can be satisfied if

\[
\frac{\gamma}{4eB(l+1)^2 \beta^3 \sqrt{2h \log(4lh)}} \leq \frac{1}{\beta l \sqrt{2h \log(4lh)}},
\]

(73)
since the chosen value of $\sigma$ satisfies $\sigma \leq \frac{1}{4eB(l+1)^2}\beta^2\sqrt{2h\log(4lh)}$ and $\frac{1}{\beta} \leq \zeta$. As shown later, we only need to consider a certain range of values of $\beta$ which naturally satisfy the condition $\frac{1}{\beta} \leq \beta^2$, i.e., the equivalent form of Eq. (73). This assures the applicability of Lemma 3.3. Now we compute the KL divergence,

$$\text{KL}(Q\|P) = \frac{|w|^2}{2\sigma^2} = \frac{42^2B^2\beta^6(l+1)^4h\log(4lh)}{2\gamma^2} \left(\|W_1\|_F^2 + \|W_2\|_F^2 + \|W_i\|_F^2\right)$$

$$\leq O\left(\frac{B^2\beta^6(l+1)^4h\log(4lh)}{\gamma^2} \left(\|W_1\|_F^2 + \|W_2\|_F^2 + \|W_i\|_F^2\right)\right)$$ (74)

In particular, we only need to consider values of $\beta$ in the following range,

$$\sqrt{\frac{\gamma}{2Bl}} \leq \beta \leq \sqrt{\frac{\gamma\sqrt{m}}{2Bl}},$$ (75)

since otherwise the bound holds trivially as $L_{D,0}(f_w) \leq 1$ by definition. To see this, if $\beta < \frac{\gamma}{2Bl}$, then for any $(X, A)$ and any $j \in \mathbb{N}_k^n$, we have,

$$|f_w(X, A)[j]| \leq |f_w(X, A)|_2 = \frac{1}{n}1_nH_{l-1}W_l|_2$$

$$\leq \frac{1}{n}1_nH_{l-1}|2||W_l|_2$$

$$\leq ||W_l||_2 \max_i|H_{l-1}[i, :]|_2$$

$$\leq B(l-1)C_\phi||W_1||_2||W_l||_2$$ (Use Eq. (48))

$$\leq B(l-1)\lambda C_\phi$$ (Use definition of $\lambda$)

$$\leq Bl\beta^2$$ (Use definition of $\beta$)

$$< \frac{\gamma}{2}$$ (76)

Therefore, based on the definition in Eq. (4), we always have $L_{S, \gamma}(f_w) = 1$ when $\beta < \frac{\gamma}{2Bl}$. It it hence sufficient to consider $\beta^2 \geq \frac{\gamma}{2Bl} \geq \frac{\gamma}{4eB(l+1)^2}$ which means the condition in Eq. (73) is indeed satisfied. Alternatively, if $\beta > \sqrt{\frac{\gamma\sqrt{m}}{2Bl}}$, the term inside the big-O notation in Eq. (74) would be,

$$\sqrt{\frac{B^2\beta^4(l+1)^4h\log(4lh)}{\gamma^2m}} \geq \sqrt{\frac{(l+1)^4h\log(4lh)|w|^2}{4l^2}} \geq 1,$$ (77)

where the first inequality hold since $\beta \geq \frac{1}{l}$. The last inequality uses the fact that we typically choose $h \geq 2$ in practice, $l \geq 2$, and $|w|^2 \geq \min(\|W_1\|_F^2, \|W_2\|_F^2, \|W_l\|_F^2) \geq \zeta^2$. Since we only need to consider $\beta$ in the range of Eq. (75), one sufficient condition to ensure $|\beta - \tilde{\beta}| \leq \frac{1}{2}\beta$ always holds would be $|\beta - \tilde{\beta}| \leq \frac{1}{l}\sqrt{\frac{\gamma}{2Bl}}$. Therefore, if we can find a covering of the interval in Eq. (75) with radius $\frac{1}{l}\sqrt{\frac{\gamma}{2Bl}}$ and make sure bounds like Eq. (66) holds while $\tilde{\beta}$ takes all possible values from the covering, then we can get a bound which holds for all $\beta$. It is clear that we only need to consider a covering $C$ with size $|C| = \frac{3}{2}\left(m^{\frac{1}{2}} - 1\right)$. 32
We first restate the Rademacher complexity bound from (Garg et al., 2020) as below:

\[
L_{D,0}(f_w) \leq L_{S,\gamma}(f_w) + \mathcal{O} \left( \frac{B^2 \beta^6 (l + 1)^4 h \log(\|h\|_2^2 + \log \frac{n|C|}{\delta})}{\gamma^2 m} \right)
\]

\[
= L_{S,\gamma}(f_w) + \mathcal{O} \left( \frac{B^2 \beta^6 (l + 1)^4 h \log(\|h\|_2^2 + \log \frac{n}{\delta} + \frac{1}{4} \log m)}{\gamma^2 m} \right)
\]

\[
= L_{S,\gamma}(f_w) + \mathcal{O} \left( \frac{B^2 \max \left( \zeta^{-6}, \lambda^3 C^3 \right) (l + 1)^4 h \log(\|h\|_2^2 + \log \frac{n}{\delta})}{\gamma^2 m} \right) \tag{78}
\]

which proves the theorem for the case of \( d|C| \equiv 1 \).

\[\Box\]

Remark. Note that our proof applies to both homogeneous and non-homogeneous GNNs.

**A.5 Bound Comparison**

In this section, we explain the details of the comparison with Rademacher complexity based generalization bounds of GNNs.

**A.5.1 Rademacher Complexity based Bound**

We first restate the Rademacher complexity bound from (Garg et al., 2020) as below:

\[
L_{D,0}(f_w) \leq L_{S,\gamma}(f_w) + \mathcal{O} \left( \frac{1}{\gamma m} + hB \sqrt{Z} \left( \log \left( B_1 \sqrt{m} \max \left( Z, M \sqrt{h} \max \left( BB_1, \bar{R} B_2 \right) \right) \right) \right) \right) + \mathcal{O} \left( \frac{1}{m} \right) \tag{79}
\]

where \( M = C_\phi \left( \frac{C_\rho C_g d B_0 B_B}{C_\tau C_g d B_0} \right)^{l-1} \), \( Z = C_\phi \left( BB_1 + \bar{R} B_2 \right) \), \( \bar{R} \leq C_\rho C_g d \min \left( b \sqrt{h}, BB_1 M \right) \), \( b \) is the uniform upper bound of \( \phi \) (i.e., \( \forall x \in \mathbb{R}^h, \phi(x) \leq b \)), and \( B_1, B_2, B_I \) are the spectral norms of the weight matrices \( W_1, W_2, W_I \). Note that the numerator of \( M \) has the exponent \( l - 1 \) since we count the readout function in the number of layers/steps, i.e., there are \( l - 1 \) message passing steps in total.
A.5.2 Comparison in Our Context

For typical message passing GNNs presented in the literature, node state update function $\phi$ could be a neural network like MLP or GRU, a ReLU unit, etc. This makes the assumption of the uniform upper bound on $\phi$ impractical, e.g., $b = \infty$ when $\phi$ is ReLU. Therefore, we do not adopt this assumption in our analysis$^8$.

Rademacher Complexity Based Bound Based on the above consideration, we have $\bar{R} \leq C_\rho C_g dB B_1 M$. We further convert some notations in the original bound to the ones in our context.

$$M = C_\phi \frac{(C_\rho C_g dB_2)^l - 1}{C_\rho C_g dB_2 - 1} = \xi \quad (80)$$

$$\bar{R} \leq C_\rho C_g dB B_1 M = C_\rho C_g dB \|W_1\|_2 \xi \quad (81)$$

$$Z = C_\phi (B B_1 + \bar{R} B_2) = B \|W_1\|_2 (C_\phi + d \xi) \quad , \quad (82)$$

where we use the same abbreviations as in Theorem 3.4, $\xi = C_\phi \frac{(d C)^{l-1}}{d C - 1}$, $\lambda = \|W_1\|_2 \|W_l\|_2$, $C = C_\phi C_\rho C_g \|W_2\|_2$.

We need to consider three cases for the big-O term of the original bound in Eq. (79) depending on the outcomes of the two point-wise maximum functions.

Case A If $\max \left( Z, M \sqrt{h} \max (B B_1, \bar{R} B_2) \right) = Z$, then the generalization bound is,

$$O \left( h B_l Z \sqrt{\frac{\log (B_l \sqrt{m} Z)}{m}} \right)$$

$$= O \left( h\|W_l\|_2 B \|W_1\|_2 (C_\phi + d \xi) \sqrt{\frac{\log (\|W_l\|_2 \sqrt{m} B \|W_1\|_2 (C_\phi + d \xi))}{m}} \right)$$

$$= O \left( h B \lambda (C_\phi + d \xi) \sqrt{\frac{\log (\sqrt{m} \lambda \xi \sqrt{B})}{m}} \right). \quad (83)$$

Case B If $\max \left( Z, M \sqrt{h} \max (B B_1, \bar{R} B_2) \right) = M \sqrt{h} \max (B B_1, \bar{R} B_2)$ and $B B_1 = \max (B B_1, \bar{R} B_2)$, then the generalization bound is,

$$O \left( h B_l Z \sqrt{\frac{\log (B_l \sqrt{m} M \sqrt{h} B B_1)}{m}} \right)$$

$$= O \left( h\|W_l\|_2 B \|W_1\|_2 (C_\phi + d \xi) \sqrt{\frac{\log (\|W_l\|_2 \sqrt{m} \xi \sqrt{h} B \|W_1\|_2)}{m}} \right)$$

$$= O \left( h B \lambda (C_\phi + d \xi) \sqrt{\frac{\log (\sqrt{m} \lambda \xi \sqrt{h} B)}{m}} \right). \quad (84)$$

$^8$If we introduce the uniform upper bound on $\phi$ in our analysis, we can also obtain a similar functional dependency in our bound like $\min (b \sqrt{h}, \cdot)$. But as aforementioned, it is somewhat impractical and leads to a more cumbersome bound.
Case C If $\max \left( Z, M \sqrt{h} \max (BB_1, \bar{RB}_2) \right) = M \sqrt{h} \max (BB_1, \bar{RB}_2)$ and $\bar{RB}_2 = \max (BB_1, \bar{RB}_2)$, then the generalization bound is,

$$
O \left( hBZ \left[ \log \left( Bz \sqrt{m} \sqrt{h} \bar{RB}_2 \right) \right] \right) = O \left( h\|W_l\|_2 \|B\|_2 \|W_1\|_2 (C_\phi + dC\xi) \frac{\log \left( \|W_l\|_2 \sqrt{m} \sqrt{h} C_\psi dB \|W_1\|_2 \|W_2\|_2 \right)}{m} \right) = O \left( hB \lambda (C_\phi + dC\xi) \frac{\log \left( \lambda \sqrt{m} \sqrt{h} C_\psi dB \xi^2 \|W_2\|_2 \right)}{m} \right)
$$

(85)

We show the detailed dependencies of the Rademacher complexity based bound under three cases in Table 3. In practice, we found message passing GNNs typically do not behave like a contraction mapping. In other words, we have $dC > 1$ and $\xi \gg 1$ hold for many datasets. Therefore, the case C happens more often in practice, i.e., $\max \left( Z, M \sqrt{h} \max (BB_1, \bar{RB}_2) \right) = M \sqrt{h} \bar{RB}_2$.

PAC Bayes Bound For our PAC-Bayes bound in Theorem 3.4, we also need to consider two cases which correspond to $\max (\zeta^{-1}, (\lambda \xi)^{\frac{1}{2}}) = \zeta^{-1}$ (case A) and $\max (\zeta^{-1}, (\lambda \xi)^{\frac{1}{2}}) = (\lambda \xi)^{\frac{1}{2}}$ (case B) respectively. Here $\zeta = \min (\|W_1\|_2, \|W_2\|_2, \|W_l\|_2)$. We show the detailed dependencies of our bound under three cases in Table 3. Again, in practice, we found $dC > 1$, $\xi \gg 1$ and $\zeta \leq 1$. Therefore, case B occurs more often.

VC-dim Bound (Scarselli et al., 2018) show that the upper bound of the VC-dimension of general GNNs with Sigmoid or Tanh activations is $O(p^4 N^2)$ where $p$ is the total number of parameters and $N$ is the maximum number of nodes. Since $p = O(h^2)$ in our case, the VC-dim bound is $O(h^8 N^2)$. Therefore, the corresponding generalization bound scales as $O(h^4 \sqrt{N} \sqrt{m})$. Note that $N$ is at least $d$ and could be much larger than $d$ for some datasets.

A.6 Connections with Existing Bounds of MLPs/CNNs

ReLU Networks are Special GCNs Since regular feedforward neural networks could be viewed as a special case of GNNs by treating each sample as the node feature of a single-node graph, it is natural to investigate the connections between these two classes of models. In particular, we consider the class of ReLU networks studied in Neyshabur et al. (2017),

$$
H_0 = X \quad \text{(Input Node Feature)}
$$

$$
H_k = \sigma_k (H_{k-1} W_k) \quad \text{(k-th Layer)}
$$

$$
H_l = H_{l-1} W_l \quad \text{(Readout Layer)},
$$

(86)

where $\sigma_k = \text{ReLU}$. It includes two commonly-seen types of deep neural networks, i.e., fully connected networks (or MLPs) and convolutional neural networks (CNNs), as special cases. Comparing Eq. (86) against Eq. (1), it is clear that these ReLU networks can be further viewed as special cases of GCNs which operate on single-node graphs, i.e., $\tilde{L} = I$. 35
Connections of Generalization Bounds

Let us restate the PAC-Bayes bound of ReLU networks in Neyshabur et al. (2017) as below,

$$L_{D,0}(f_w) \leq L_{S,\gamma}(f_w) + O\left(\frac{B^{2l}h \log(lh) \prod_{i=1}^{l} \|W_i\|^2}{\gamma^2 m} + \log \frac{ml}{\delta}\right). \quad (87)$$

Comparing it with the bound in Theorem 3.2, we can find that our bound only adds a factor $d^{l-1}$ to the first term inside the square root of the big-O notation which is brought by the underlying graph structure of the data. If we consider GCNs operating on single-node graphs, i.e., the case where GCNs degenerate to ReLU networks, two bounds coincide since $d = 1$. Therefore, our Theorem 3.2 directly generalizes the result in Neyshabur et al. (2017) to GCNs which is a strictly larger class of models than ReLU networks.

A.7 Experimental Details

Datasets

We create 6 synthetic datasets by generating random graphs from different random graph models. In particular, the first 4 synthetic datasets correspond to the Erdős–Rényi models with different edge probabilities: 1) Erdős–Rényi-1 (ER-1), edge probability = 0.1; 2) Erdős–Rényi-2 (ER-2), edge probability = 0.3; 3) Erdős–Rényi-3 (ER-3), edge probability = 0.5; 4) Erdős–Rényi-4 (ER-4), edge probability = 0.7. The remaining 2 synthetic datasets correspond to the stochastic block model with the following settings: 1) Stochastic-Block-Model-1 (SBM-1), two blocks, sizes = [40, 60], edge probability = [[0.25, 0.13], [0.13, 0.37]]; 2) Stochastic-Block-Model-2 (SBM-2), three blocks, sizes = [25, 25, 50], edge probability = [[0.25, 0.05, 0.02], [0.05, 0.35, 0.07], [0.02, 0.07, 0.40]]. Each synthetic dataset has 200 graphs where the number of nodes of individual graph is 100, the number of classes is 2, and the random train-test split ratio is $90\%/10\%$. For each random graph of individual synthetic dataset, we generate the 16-dimension random Gaussian node feature (normalized to have unit $\ell_2$ norm) and a binary class label following a uniform distribution. We summarize the statistics of the real-world and synthetic datasets in Table 4 and Table 5 respectively.

Experimental Setup

For all MPGNNs used in the experiments, we specify $\phi = \text{ReLU}, \rho = \tanh,$ and $g = \tanh$ which imply $C_\phi = C_\rho = C_g = 1$. For experiments on real-world datasets, we set
and it will play a role when the term involved with
different settings except for one synthetic setting which falls in the scenario “small
datasets). As you can see, our bound is tighter than the Rademacher complexity based one under all
numerical values of the bound evaluations in Table 6 (real-world datasets) and Table 7 (synthetic
Experimental Results where the variables are the same as Eq. (79).

For the Rademacher complexity based bound, we compute the following quantity

\[ \frac{42^2 B^2 \left( \max \left( \zeta^{-l(l+1)}, (\lambda \xi)^{l+1/2} \right) \right)^2 \gamma^2 m}{4 \lambda h \log(4h) \| w \|_2^2} \tag{88} \]

For the Rademacher complexity based bound, we compute the following quantity

\[ 2 \times 4hB_l B Z \sqrt{3 \log \left( \frac{24B_l \sqrt{m} \max \left( \zeta, MB \max \left( BB_1, \hat{R}B_2 \right) \right)}{m} \right)} \gamma^2 m \tag{89} \]

where the variables are the same as Eq. (79).

Experimental Results In addition to the figures shown in the main paper, we also provide the
numerical values of the bound evaluations in Table 6 (real-world datasets) and Table 7 (synthetic
datasets). As you can see, our bound is tighter than the Rademacher complexity based one under all
settings except for one synthetic setting which falls in the scenario “small d (max-node-degree) and
large l (number-of-steps)”. This makes sense since we have a square term on the number of steps l
and it will play a role when the term involved with d is comparable (i.e., when d is small). Again,
all quantities are in the log domain.

\[
\begin{array}{|c|c|c|c|c|c|}
\hline
l = 2 & PROTEINS & IMDB-MULTI & IMDB-BINARY & COLLAB \\
\hline
Rademacher & 11.80 ± 0.18 & 16.66 ± 0.04 & 17.37 ± 0.02 & 21.26 ± 0.07 \\
PAC-Bayes & 8.45 ± 0.28 & 15.26 ± 0.07 & 15.44 ± 0.03 & 19.37 ± 0.17 \\
\hline
l = 4 & & & & \\
Rademacher & 24.04 ± 0.23 & 29.94 ± 0.10 & 31.38 ± 0.09 & 41.03 ± 0.33 \\
PAC-Bayes & 22.10 ± 0.23 & 28.35 ± 0.11 & 29.53 ± 0.08 & 40.31 ± 0.36 \\
\hline
\end{array}
\]

Table 6: Bound (log value) comparisons on real-world datasets.

\[
\begin{array}{|c|c|c|c|c|c|}
\hline
l = 2 & ER-1 & ER-2 & ER-3 & ER-4 & SBM-1 & SBM-2 \\
\hline
Rademacher & 17.37 ± 0.16 & 17.98 ± 0.13 & 18.15 ± 0.15 & 18.35 ± 0.10 & 17.88 ± 0.11 & 17.71 ± 0.09 \\
PAC-Bayes & 15.38 ± 0.12 & 15.13 ± 0.13 & 14.86 ± 0.25 & 14.69 ± 0.24 & 15.23 ± 0.12 & 15.35 ± 0.10 \\
\hline
l = 4 & & & & & \\
Rademacher & 27.92 ± 0.02 & 29.57 ± 0.12 & 30.64 ± 0.18 & 31.34 ± 0.20 & 29.35 ± 0.14 & 28.87 ± 0.07 \\
PAC-Bayes & 27.00 ± 0.04 & 28.32 ± 0.07 & 29.18 ± 0.12 & 29.70 ± 0.14 & 28.14 ± 0.05 & 27.74 ± 0.04 \\
\hline
l = 6 & & & & & \\
Rademacher & 37.10 ± 0.29 & 40.22 ± 0.19 & 42.00 ± 0.26 & 43.08 ± 0.39 & 40.04 ± 0.25 & 39.02 ± 0.19 \\
PAC-Bayes & 36.85 ± 0.25 & 39.65 ± 0.14 & 41.30 ± 0.22 & 42.24 ± 0.34 & 39.50 ± 0.17 & 38.63 ± 0.17 \\
\hline
l = 8 & & & & & \\
Rademacher & 46.72 ± 0.51 & 51.16 ± 0.21 & 53.44 ± 0.39 & 55.06 ± 0.38 & 56.60 ± 0.17 & 49.29 ± 0.34 \\
PAC-Bayes & 46.70 ± 0.48 & 51.02 ± 0.21 & 53.10 ± 0.36 & 54.87 ± 0.38 & 50.44 ± 0.16 & 49.22 ± 0.36 \\
\hline
\end{array}
\]

Table 7: Bound (log value) comparisons on synthetic datasets.