A PROOFS

A.1 ASSUMPTIONS AND NOTATION

Assumption 1. *For the XOR-GMM data model, the means of the Gaussian mixture are such that* $\langle \boldsymbol{\mu}, \boldsymbol{\nu} \rangle = 0$ *and* $\|\boldsymbol{\mu}\|_2 = \|\boldsymbol{\nu}\|_2$.

We denote $[x]_+ = \mathrm{ReLU}(x)$ and $\varphi(x) = \mathrm{sigmoid}(x) = 1/1+e^{-x}$, applied element-wise on the inputs. For any vector $\mathbf{v}$, $\hat{\mathbf{v}} = \frac{\mathbf{v}}{\|\mathbf{v}\|_2}$ denotes the normalized $\mathbf{v}$. We use $\gamma = \|\boldsymbol{\mu} - \boldsymbol{\nu}\|_2$ to denote the distance between the means of the inter-class components of the mixture model, and γ' to denote the norm of the means, $\gamma' = \gamma/\sqrt{2} = \|\boldsymbol{\mu}\|_2 = \|\boldsymbol{\nu}\|_2$.

Given intra-class and inter-class edge probabilities p and q, we define $\Gamma(p, q) = \frac{|p-q|}{p+q}$. We denote the probability density function of a standard Gaussian by $\phi(x)$, and the cumulative distribution function by $\Phi(x)$. The complementary distribution function is denoted by $\Phi_{\mathrm{c}}(x) = 1 - \Phi(x)$.

A.2 ELEMENTARY RESULTS

In this section, we state preliminary results about the concentration of the degrees of all nodes and the number of common neighbours for all pairs of nodes, along with the effects of a graph convolution on the mean and the variance of some data. Our results regarding the merits of graph convolutions rely heavily on these arguments.

Proposition A.1 (Concentration of degrees)**.** *Assume that the graph density is* $p, q = \Omega(\frac{\log^2 n}{n})$. *Then for any constant* $c > 0$, *with probability at least* $1 - 2n^{-c}$, *we have for all* $i \in [n]$ *that*

$$\mathbf{deg}(i) = \frac{n}{2}(p+q)(1 \pm o_n(1)), \qquad \frac{1}{\mathbf{deg}(i)} = \frac{2}{n(p+q)}(1 \pm o_n(1)),$$

$$\frac{1}{\mathbf{deg}(i)} \left(\sum_{j \in C_1} a_{ij} - \sum_{j \in C_0} a_{ij} \right) = (2\varepsilon_i - 1)\frac{p-q}{p+q}(1 + o_n(1)),$$

where the error term $o_n(1) = O\left(\sqrt{\frac{c}{\log n}}\right)$.

Proof. Note that $\mathbf{deg}(i)$ is a sum of n Bernoulli random variables, hence, we have by the Chernoff bound (Vershynin, 2018, Section 2) that

$$\mathbf{Pr}\left[\mathbf{deg}(i) \in \left[\frac{n}{2}(p+q)(1-\delta), \frac{n}{2}(p+q)(1+\delta)\right]^{\mathsf{c}}\right] \leq 2\exp(-Cn(p+q)\delta^2),$$

for some $C > 0$. We now choose $\delta = \sqrt{\frac{(c+1)\log n}{Cn(p+q)}}$ for a large constant $c > 0$. Note that since $p, q = \Omega(\log^2 n/n)$, we have that $\delta = O(\sqrt{\frac{c}{\log n}}) = o_n(1)$. Then following a union bound over $i \in [n]$, we obtain that with probability at least $1 - 2n^{-c}$,

$$\mathbf{deg}(i) = \frac{n}{2}(p+q)\left(1 \pm O\Big(\sqrt{\frac{c}{\log n}}\Big)\right) \text{ for all } i \in [n],$$
$$\frac{1}{\mathbf{deg}(i)} = \frac{2}{n(p+q)}\left(1 \pm O\Big(\sqrt{\frac{c}{\log n}}\Big)\right) \text{ for all } i \in [n].$$

Note that $\frac{1}{\mathbf{deg}(i)} \sum_{j \in C_b} a_{ij}$ for any $b \in \{0, 1\}$ is a sum of independent Bernoulli random variables. Hence, by a similar argument, we have that with probability at least $1 - 2n^{-c}$,

$$\frac{1}{\mathbf{deg}(i)} \left(\sum_{j \in C_1} a_{ij} - \sum_{j \in C_0} a_{ij} \right) = (2\varepsilon_i - 1)\frac{p-q}{p+q}(1 + o_n(1)) \text{ for all } i \in [n]. \qquad \square$$

Proposition A.2 (Concentration of the number of common neighbours)**.** *Assume that the graph density is $p, q = \Omega(\frac{\log n}{\sqrt{n}})$. Then for any constant $c > 0$, with probability at least $1 - 2n^{-c}$,*

$$|N_i \cap N_j| = \frac{n}{2}(p^2 + q^2)(1 \pm o_n(1)) \qquad \text{for all } i \sim j,$$
$$|N_i \cap N_j| = npq(1 \pm o_n(1)) \qquad \text{for all } i \nsim j,$$

where the error term $o_n(1) = O\left(\sqrt{\frac{c}{\log n}}\right)$.

Proof. For any two distinct nodes $i, j \in [n]$ we have that the number of common neighbours of i and j is $|N_i \cap N_j| = \sum_{k\in[n]} a_{ik}a_{jk}$. This is a sum of independent Bernoulli random variables, with mean $\mathbb{E}|N_i \cap N_j| = \frac{n}{2}(p^2 + q^2)$ for $i \sim j$ and $\mathbb{E}|N_i \cap N_j| = npq$ for $i \nsim j$. Denote $\mu_{ij} = \mathbb{E}|N_i \cap N_j|$. Therefore, by the Chernoff bound (Vershynin, 2018, Section 2), we have for a fixed pair of nodes (i, j) that

$$\mathbf{Pr}\left[|N_i \cap N_j| \in [\mu_{ij}(1 - \delta_{ij}), \mu_{ij}(1 + \delta_{ij})]^{\mathsf{c}}\right] \leq 2\exp(-C\mu_{ij}\delta_{ij}^2)$$

for some constant $C > 0$. We now choose $\delta_{ij} = \sqrt{\frac{(c+2)\log n}{C\mu_{ij}}}$ for any large $c > 0$. Note that since $p, q = \Omega(\log n/\sqrt{n})$, we have that $\delta_{ij} = O(\sqrt{\frac{c}{\log n}}) = o_n(1)$. Then following a union bound over all pairs $(i, j) \in [n] \times [n]$, we obtain that with probability at least $1 - 2n^{-c}$, for all pairs of nodes (i, j) we have

$$|N_i \cap N_j| = \frac{n}{2}(p^2 + q^2)(1 \pm o_n(1)) \qquad \text{for all } i \sim j,$$
$$|N_i \cap N_j| = npq(1 \pm o_n(1)) \qquad \text{for all } i \nsim j. \qquad \square$$

Lemma A.3 (Variance reduction)**.** *Denote the event from Proposition A.1 to be B. Let $\{\mathbf{X}_i\}_{i\in[n]} \in \mathbb{R}^{n\times d}$ be an iid sample of data. For a graph with adjacency matrix $\mathbf{A}$ (including self-loops) and a fixed integer $K > 0$, define a K-convolution to be $\tilde{\mathbf{X}} = (\mathbf{D}^{-1}\mathbf{A})^K\mathbf{X}$. Then we have*

$$\mathbf{Cov}(\tilde{\mathbf{X}}_i \mid B) = \rho(K)\mathbf{Cov}(\mathbf{X}_i), \text{ where } \rho(K) = \left(\frac{1 + o_n(1)}{\Delta}\right)^{2K} \sum_{j\in[n]} \mathbf{A}^K(i, j)^2.$$

Here, $\mathbf{A}^K(i, j)$ is the entry in the ith row and jth column of the exponentiated matrix $\mathbf{A}^K$ and $\Delta = \mathbb{E}\,\mathbf{deg} = \frac{n}{2}(p + q)$.

Proof. For a matrix $\mathbf{M}$, the ith convolved data point is $\tilde{\mathbf{X}}_i = \mathbf{M}_i^\top\mathbf{X}$, where $\mathbf{M}_i^\top$ denotes the ith row of $\mathbf{M}$. Since $\mathbf{X}_i$ are iid, we have

$$\mathbf{Cov}(\tilde{\mathbf{X}}_i) = \sum_{j\in[n]} (\mathbf{M}_{ij})^2\mathbf{Cov}(\mathbf{X}_j).$$

It remains to compute the entries of the matrix $\mathbf{M} = (\mathbf{D}^{-1}\mathbf{A})^K$. Note that we have $\mathbf{D}^{-1}\mathbf{A}(i, j) = a_{ij}/\mathbf{deg}(i)$, so we obtain that

$$\mathbf{M}_{ij} = (\mathbf{D}^{-1}\mathbf{A})^K(i, j) = \sum_{j_1=1}^{n}\sum_{j_2=1}^{n}\cdots\sum_{j_{K-1}=1}^{n} \frac{a_{ij_1}a_{j_1j_2}\cdots a_{j_{K-2}j_{K-1}}a_{j_{K-1}j}}{\mathbf{deg}(i)\mathbf{deg}(j_1)\cdots\mathbf{deg}(j_{K-1})}.$$

Recall that on the event B, the degrees of all nodes are $\Delta(1 \pm o_n(1))$, and hence, we have that

$$\mathbf{M}_{ij} = \frac{(1 \pm o_n(1))^K}{\Delta^K}\sum_{j_1=1}^{n}\sum_{j_2=1}^{n}\cdots\sum_{j_{K-1}=1}^{n} a_{ij_1}\cdots a_{j_{K-2}j_{K-1}}a_{j_{K-1}j},$$

where the error $o_n(1) = O(\frac{1}{\sqrt{\log n}})$. The sum of these products of the entries of $\mathbf{A}$ is simply the number of length-K paths from node i to j, i.e., $\mathbf{A}^K(i, j)$. Thus, we have

$$\mathbf{Cov}(\tilde{\mathbf{X}}_i \mid B) = \sum_{j\in[n]} (\mathbf{M}_{ij})^2\mathbf{Cov}(\mathbf{X}_j) = \left(\frac{1 + o_n(1)}{\Delta}\right)^{2K}\sum_{j\in[n]} \mathbf{A}^K(i, j)^2\mathbf{Cov}(\mathbf{X}_j).$$

Since $\mathbf{X}_j$ are iid, we obtain that $\rho(K) = \left(\frac{1+o_n(1)}{\Delta}\right)^{2K}\sum_{j\in[n]} \mathbf{A}^K(i, j)^2$. $\square$

Let us briefly discuss the implications of Lemma A.3. Consider a sample $(\mathbf{A}, \mathbf{X})$ drawn from XOR-CSBM$(n, d, \boldsymbol{\mu}, \boldsymbol{\nu}, \sigma^2, p, q)$ for the symmetric case where exactly $n/2$ nodes are in each of the two classes. We have that

$$\mathbb{E}\mathbf{A} = \begin{pmatrix} p\mathbf{I}_{n/2} & q\mathbf{I}_{n/2} \\ q\mathbf{I}_{n/2} & p\mathbf{I}_{n/2} \end{pmatrix}.$$

This gives us $\mathbb{E}\rho(K) \approx \frac{1}{n}(1 + \Gamma(p,q)^{2K})$ for any $K \geq 2$. Recall that a single graph convolution reduces the distance between the means by a factor of $\Gamma(p,q)$. Hence, to comment on the performance of an arbitrary number of convolutions, K, we might hope to compare the reduction in this distance, $\Gamma(p,q)^K$ with the reduction in the variance ($\rho(K)$) to obtain a condition on K in terms of n, p, and q. The challenge, however, lies in the fact that in deeper layers, computing $\rho(K)$ is non-trivial due to node features being highly correlated. Moreover, an argument to claim that $\rho(K) \approx \mathbb{E}\rho(K)$ is needed for this approach, which seems to require strong density assumptions on the graph.

We now state a result about the output of the (Bayes) optimal classifier for the XOR-GMM data model that is used in several of our proofs.

Lemma A.4. *Let* $h(\boldsymbol{x}) = |\langle \boldsymbol{x}, \hat{\boldsymbol{\nu}} \rangle| - |\langle \boldsymbol{x}, \hat{\boldsymbol{\mu}} \rangle|$ *for all* $\boldsymbol{x} \in \mathbb{R}^d$ *and define*

$$\zeta(t) = t\,\mathrm{erf}(t) - \frac{1}{\sqrt{\pi}}\left(1 - e^{-t^2}\right)$$

for $x, y \in \mathbb{R}$. *Then we have*

1. *The expectation* $\mathbb{E}h(\mathbf{X}_i) = \begin{cases} -\sqrt{2}\sigma\zeta(\gamma/2\sigma) & i \in C_0 \\ \sqrt{2}\sigma\zeta(\gamma/2\sigma) & i \in C_1 \end{cases}$.
2. *For any* $\gamma, \sigma > 0$ *such that* $\gamma = \Omega_n(\sigma)$, *we have that* $\zeta(\frac{\gamma}{\sigma}) = \Omega(\frac{\gamma}{\sigma})$.
3. *For any* $\gamma, \sigma > 0$ *such that* $\gamma = o_n(\sigma)$, *we have that* $\zeta(\frac{\gamma}{\sigma}) = \Omega(\frac{\gamma^2}{\sigma^2})$.

Proof. For part one, observe that $\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}} \rangle$ and $\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}} \rangle$ are Gaussian random variables with variance σ^2 and means $\gamma/\sqrt{2}, 0$ if $\varepsilon_i = 0$ and $0, \gamma/\sqrt{2}$ if $\varepsilon_i = 1$, respectively. Thus, $|\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}} \rangle|$ and $|\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}} \rangle|$ are folded-Gaussian random variables and we have $\mathbb{E}h(\mathbf{X}_i) = -\sqrt{2}\zeta(\gamma/\sqrt{2}\sigma)$ if $i \in C_0$ and $\mathbb{E}h(\mathbf{X}_i) = \sqrt{2}\zeta(\gamma/\sqrt{2}\sigma)$ otherwise.

We now write

$$\zeta(t) = t\left(\mathrm{erf}(t) - \frac{1}{t\sqrt{\pi}}(1 - e^{-t^2})\right) = tH(t),$$

where $H(t) = \mathrm{erf}(t) - 1/t\sqrt{\pi}(1 - e^{-t^2})$.

For part two, note that $H(t)$ is an increasing function in the range $[-1, 1]$ and $H(t) > 0$ for $t > 0$. Hence, for $t \geq C$ for some positive constant C, $H(t) \geq H(C) = C'$, therefore, $\zeta(t) = tH(t) \geq C't$.

For part three when $t = o_n(1)$, we use the series expansion of $h(t)$ about $t = 0$ to obtain that

$$h(t) = \frac{t}{\sqrt{\pi}} - \frac{t^3}{6\sqrt{\pi}} + O(t^5) \geq \frac{t}{\sqrt{\pi}} - \frac{t^3}{6\sqrt{\pi}} = \Omega(t).$$

Hence, $\zeta(t) = th(t) = \Omega(t^2)$. Putting $t = \gamma/\sigma$ completes the proof. □

Fact A.5. *For any* $x \in [0, 1]$, $\frac{x}{2} \leq \log(1 + x) \leq x$.

A.3 Proof of Theorem 1 part one

In this section we prove our first result about the fraction of misclassified points in the absence of graphical information. We begin by computing the Bayes optimal classifier for the data model XOR-GMM (see Section 2.1). A Bayes classifier, denoted by $h^*(\boldsymbol{x})$, maximizes the posterior probability of observing a label given the input data $\boldsymbol{x}$. More precisely, $h^*(\boldsymbol{x}) = \mathrm{argmax}_{b \in \{0,1\}} \mathbf{Pr}[y = b \mid \mathbf{x} = \boldsymbol{x}]$, where $\boldsymbol{x} \in \mathbb{R}^d$ represents a single data point.

Lemma A.6. *For some fixed $\boldsymbol{\mu}, \boldsymbol{\nu} \in \mathbb{R}^d$ and $\sigma^2 > 0$, the Bayes optimal classifier, $h^*(\boldsymbol{x}) : \mathbb{R}^d \to \{0, 1\}$ for the data model XOR-GMM$(n, d, \boldsymbol{\mu}, \boldsymbol{\nu}, \sigma^2)$ is given by*

$$h^*(\boldsymbol{x}) = \mathbb{1}(|\langle \boldsymbol{x}, \boldsymbol{\mu} \rangle| < |\langle \boldsymbol{x}, \boldsymbol{\nu} \rangle|) = \begin{cases} 0 & |\langle \boldsymbol{x}, \boldsymbol{\mu} \rangle| \geq |\langle \boldsymbol{x}, \boldsymbol{\nu} \rangle| \\ 1 & |\langle \boldsymbol{x}, \boldsymbol{\mu} \rangle| < |\langle \boldsymbol{x}, \boldsymbol{\nu} \rangle| \end{cases},$$

where $\mathbb{1}$ is the indicator function.

Proof. Note that $\mathbf{Pr}[y = 0] = \mathbf{Pr}[y = 1] = \frac{1}{2}$. Let $f_{\mathbf{x}}(\boldsymbol{x})$ denote the density function of a continuous random vector $\mathbf{x}$. Therefore, for any $b \in \{0, 1\}$,

$$\mathbf{Pr}[y = b \mid \mathbf{x} = \boldsymbol{x}] = \frac{\mathbf{Pr}[y = b] f_{\mathbf{x}|y}(\boldsymbol{x} \mid y = b)}{\sum_{c \in \{0,1\}} \mathbf{Pr}[y = c] f_{\mathbf{x}|y}(\boldsymbol{x} \mid y = c)} = \frac{1}{1 + \frac{f_{\mathbf{x}|y}(\boldsymbol{x}|y=1-b)}{f_{\mathbf{x}|y}(\boldsymbol{x}|y=b)}}.$$

Let's compute this for $b = 0$. We have

$$\frac{f_{\mathbf{x}|y}(\boldsymbol{x} \mid y = 1)}{f_{\mathbf{x}|y}(\boldsymbol{x} \mid y = 0)} = \frac{\cosh(\langle \boldsymbol{x}, \boldsymbol{\nu} \rangle / \sigma^2)}{\cosh(\langle \boldsymbol{x}, \boldsymbol{\mu} \rangle / \sigma^2)} \exp\left(\frac{\|\boldsymbol{\mu}\|^2 - \|\boldsymbol{\nu}^2\|}{2\sigma^2}\right) = \frac{\cosh(\langle \boldsymbol{x}, \boldsymbol{\nu} \rangle / \sigma^2)}{\cosh(\langle \boldsymbol{x}, \boldsymbol{\mu} \rangle / \sigma^2)},$$

where in the last equation we used the assumption that $\|\boldsymbol{\mu}\| = \|\boldsymbol{\nu}\|$. The decision regions are then identified by: $\mathbf{Pr}[y = 0 \mid \mathbf{x}] \geq 1/2$ for label 0 and $\mathbf{Pr}[y = 0 \mid \mathbf{x}] < 1/2$ for label 1.

Thus, for label 0, we need $\frac{f_{\mathbf{x}|y}(\boldsymbol{x}|y=1)}{f_{\mathbf{x}|y}(\boldsymbol{x}|y=0)} < 1$, which implies that $\frac{\cosh(\langle \boldsymbol{x}, \boldsymbol{\nu} \rangle / \sigma^2)}{\cosh(\langle \boldsymbol{x}, \boldsymbol{\mu} \rangle / \sigma^2)} \leq 1$. Now we note that $\cosh(x) \leq \cosh(y) \implies |x| \leq |y|$ for all $x, y \in \mathbb{R}$, hence, we have $|\langle \boldsymbol{x}, \boldsymbol{\mu} \rangle| \geq |\langle \boldsymbol{x}, \boldsymbol{\nu} \rangle|$. Similarly, we have the complementary condition for label 1. □

Next, we design a two-layer and a three-layer network and show that for a particular choice of parameters $\theta = (\mathbf{W}^{(l)}, \mathbf{b}^{(l)})$ for $l \in \{1, 2\}$ for the two-layer case and $l \in \{1, 2, 3\}$ for the three-layer case, the networks realize the optimal classifier described in Lemma A.6.

Proposition A.7. *Consider two-layer and three-layer networks of the form described in Section 2.2 without biases (i.e., $\mathbf{b}^{(l)} = \mathbf{0}$ for all layers l), for parameters $\mathbf{W}^{(l)}$ and some $R \in \mathbb{R}^+$ as follows.*

1. *For the two-layer network,*

$$\mathbf{W}^{(1)} = R\begin{pmatrix} \hat{\boldsymbol{\mu}} & -\hat{\boldsymbol{\mu}} & \hat{\boldsymbol{\nu}} & -\hat{\boldsymbol{\nu}} \end{pmatrix}, \qquad \mathbf{W}^{(2)} = \begin{pmatrix} -1 & -1 & 1 & 1 \end{pmatrix}^\top.$$

2. *For the three-layer network,*

$$\mathbf{W}^{(1)} = R\begin{pmatrix} \hat{\boldsymbol{\mu}} & -\hat{\boldsymbol{\mu}} & \hat{\boldsymbol{\nu}} & -\hat{\boldsymbol{\nu}} \end{pmatrix}, \quad \mathbf{W}^{(2)} = \begin{pmatrix} -1 & 1 \\ -1 & 1 \\ 1 & -1 \\ 1 & -1 \end{pmatrix}, \quad \mathbf{W}^{(3)} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

Then for any $\sigma > 0$, the defined networks realize the Bayes optimal classifier for the data model XOR-GMM$(n, d, \boldsymbol{\mu}, \boldsymbol{\nu}, \sigma^2)$.

Proof. Note that the output of the two-layer network is $\varphi([\mathbf{X}\mathbf{W}^{(1)}]_+ \mathbf{W}^{(2)})$, which is interpreted as the probability with which the network believes that the input is in the class with label 1. The final prediction for the class label is thus assigned to be 1 if the output is ≥ 0.5, and 0 otherwise. For each $i \in [n]$, we have that the output of the network on data point i is

$$\begin{aligned} \hat{y}_i &= \varphi(R(-[\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}} \rangle]_+ - [-\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}} \rangle]_+ + [\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}} \rangle]_+ + [-\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}} \rangle]_+)) \\ &= \varphi((R(|\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}} \rangle| - |\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}} \rangle|)), \end{aligned}$$

where we used the fact that $[t]_+ + [-t]_+ = |t|$ for all $t \in \mathbb{R}$. Similarly, for the three-layer network, the output is $\varphi([[\mathbf{X}\mathbf{W}^{(1)}]_+\mathbf{W}^{(2)}]_+\mathbf{W}^{(3)})$. So we have for each $i \in [n]$ that

$$\begin{aligned}\hat{y}_i = \varphi\Bigg(R\Big([-[\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle]_+ - [-\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle]_+ + [\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle]_+ + [-\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle]_+]_+ \\ - [[\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle]_+ + [-\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle]_+ - [\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle]_+ - [-\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle]_+]_+\Big)\Bigg) \\ = \varphi\left(R([|\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle| - |\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle|]_+ - [|\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle| - |\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle|]_+)\right) \\ = \varphi\left(R(|\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle| - |\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle|)\right),\end{aligned}$$

where in the last equation we used the fact that $[t]_+ - [-t]_+ = t$ for all $t \in \mathbb{R}$.

The final prediction is then obtained by considering the maximum posterior probability among the class labels 0 and 1, and thus,

$$\text{pred}(\mathbf{X}_i) = \mathbb{1}(R\,|\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle| < R\,|\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle|) = \mathbb{1}(|\langle \mathbf{X}_i, \boldsymbol{\mu}\rangle| < |\langle \mathbf{X}_i, \boldsymbol{\nu}\rangle|),$$

which matches the Bayes classifier in Lemma A.6. □

We now restate the relevant theorem below for convenience.

Theorem (Restatement of part one of Theorem 1)**.** *Let $\mathbf{X} \in \mathbb{R}^{n\times d} \sim$ XOR-GMM$(n, d, \boldsymbol{\mu}, \boldsymbol{\nu}, \sigma^2)$. Assume that $\|\boldsymbol{\mu} - \boldsymbol{\nu}\|_2 \le K\sigma$ and let $h(\mathbf{x}) : \mathbb{R}^d \to \{0, 1\}$ be any binary classifier. Then for any $K > 0$ and any $\epsilon \in (0, 1)$, at least a fraction $2\Phi_{\text{c}}\left(K/2\right)^2 - O(n^{-\epsilon/2})$ of all data points are misclassified by h with probability at least $1 - \exp(-2n^{1-\epsilon})$.*

Proof. Recall from Lemma A.6 that for successful classification, we require for every $i \in [n]$,

$$\begin{aligned}|\langle \mathbf{X}_i, \boldsymbol{\mu}\rangle| \ge |\langle \mathbf{X}_i, \boldsymbol{\nu}\rangle| \qquad i \in C_0, \\ |\langle \mathbf{X}_i, \boldsymbol{\mu}\rangle| < |\langle \mathbf{X}_i, \boldsymbol{\nu}\rangle| \qquad i \in C_1.\end{aligned}$$

Let's try to upper bound the probability of the above event, i.e., the probability that the data is classifiable. We consider only class C_0, since the analysis for C_1 is symmetric and similar. For $i \in C_0$, we can write $\mathbf{X}_i = \boldsymbol{\mu} + \sigma\mathbf{g}_i$, where $\mathbf{g}_i \sim \mathcal{N}(\mathbf{0}, I)$. Recall that $\gamma = \|\boldsymbol{\mu} - \boldsymbol{\nu}\|_2$ and $\gamma' = \gamma/\sqrt{2} = \|\boldsymbol{\mu}\|_2 = \|\boldsymbol{\nu}\|_2$. Then we have for any fixed $i \in C_0$ that

$$\begin{aligned}\mathbf{Pr}\left[|\langle \mathbf{X}_i, \boldsymbol{\mu}\rangle| \ge |\langle \mathbf{X}_i, \boldsymbol{\nu}\rangle|\right] &= \mathbf{Pr}\left[|\gamma' + \sigma\langle \mathbf{g}_i, \hat{\boldsymbol{\mu}}\rangle| \ge |\sigma\langle \mathbf{g}_i, \hat{\boldsymbol{\nu}}\rangle|\right] \\ &\le \mathbf{Pr}\left[\gamma' + \sigma|\langle \mathbf{g}_i, \hat{\boldsymbol{\mu}}\rangle| \ge \sigma|\langle \mathbf{g}_i, \hat{\boldsymbol{\nu}}\rangle|\right] \qquad \text{(by triangle inequality)} \\ &\le \mathbf{Pr}\left[|\langle \mathbf{g}_i, \hat{\boldsymbol{\nu}}\rangle| - |\langle \mathbf{g}_i, \hat{\boldsymbol{\mu}}\rangle| \le K/\sqrt{2}\right] \qquad \text{(using } \gamma \le K\sigma\text{)}.\end{aligned}$$

We now define random variables $Z_1 = \langle \mathbf{g}_i, \hat{\boldsymbol{\nu}}\rangle$ and $Z_2 = \langle \mathbf{g}_i, \hat{\boldsymbol{\mu}}\rangle$ and note that $Z_1, Z_2 \sim \mathcal{N}(0, 1)$ and $\mathbb{E}[Z_1 Z_2] = 0$. Let $K' = K/\sqrt{2}$. We now have

$$\begin{aligned}\mathbf{Pr}\left[|Z_1| - |Z_2| \le K'\right] &= 4\mathbf{Pr}\left[Z_1 - Z_2 \le K',\, Z_1, Z_2 \ge 0\right] \\ &= 4\int_0^\infty \mathbf{Pr}\left[0 \le Z_1 \le z + K'\right]\phi(z)dz \\ &= 4\int_0^\infty \left(\Phi(z + K') - \frac{1}{2}\right)\phi(z)dz = 4\int_0^\infty \Phi(z + K')\,\phi(z)dz - 1 \\ &= 2\Phi(K/2) + 2\Phi(K/2)\Phi_{\text{c}}(K/2) - 1 = 1 - 2\Phi_{\text{c}}(K/2)^2.\end{aligned}$$

To evaluate the integral above, we used (Owen, 1980, Table 1:10,010.6 and Table 2:2.3). Thus, the probability that a point $i \in C_0$ is misclassified is lower bounded as follows

$$\mathbf{Pr}\left[\mathbf{X}_i \text{ is misclassified}\right] \ge 2\Phi_{\text{c}}\left(K/2\right)^2 = \tau_K.$$

Note that this is a decreasing function of K, implying that the probability of misclassification decreases as we increase the distance between the means, and is maximum for $K = 0$.

Define $M(n)$ for a fixed K to be the fraction of misclassified nodes in C_0. Define x_i to be the indicator random variable $\mathbb{1}(\mathbf{X}_i \text{ is misclassified})$. Then x_i are Bernoulli random variables with mean

at least τ_K, and $\mathbb{E}M(n) = \frac{2}{n}\sum_{i\in C_0}\mathbb{E}x_i \geq \tau_K$. Using Hoeffding's inequality (Vershynin, 2018, Theorem 2.2.6), we have that for any $t > 0$,

$$\mathbf{Pr}\left[M(n) \geq \tau_K - t\right] \geq \mathbf{Pr}\left[M(n) \geq \mathbb{E}M(n) - t\right] \geq 1 - \exp(-nt^2).$$

Choosing $t = n^{-\epsilon/2}$ for any $\epsilon \in (0,1)$ yields

$$\mathbf{Pr}\left[M(n) \geq \tau_K - n^{-\epsilon/2}\right] \geq 1 - \exp(-n^{1-\epsilon}). \qquad \square$$

A.4 Proof of Theorem 1 part two

In this section, we show that in the positive regime (sufficiently large distance between the means), there exists a two-layer MLP that obtains an arbitrarily small loss, and hence, successfully classifies a sample drawn from the XOR-GMM model with overwhelming probability.

Theorem (Restatement of part two of Theorem 1)**.** *Let $\mathbf{X} \in \mathbb{R}^{n\times d} \sim$ XOR-GMM$(n, d, \boldsymbol{\mu}, \boldsymbol{\nu}, \sigma^2)$. For any $\epsilon > 0$, if the distance between the means is $\|\boldsymbol{\mu} - \boldsymbol{\nu}\|_2 = \Omega(\sigma(\log n)^{\frac{1}{2}+\epsilon})$, then for any $c > 0$, with probability at least $1 - O(n^{-c})$, the two-layer and three-layer networks described in Proposition A.7 classify all data points, and obtain a cross-entropy loss given by*

$$\ell_\theta(\mathbf{X}) = C\exp\left(-\frac{R}{\sqrt{2}}\|\boldsymbol{\mu} - \boldsymbol{\nu}\|_2\left(1 \pm \sqrt{c}/(\log n)^{\epsilon}\right)\right),$$

where $C \in [1/2, 1]$ is an absolute constant.

Proof. Consider the two-layer and three-layer MLPs described in Proposition A.7, for which we have $\hat{y}_i = \varphi\left(R(|\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle| - |\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle|)\right)$. We now look at the loss for a single data point $\mathbf{X}_i$,

$$\begin{aligned}\ell_i(\mathbf{X}, \theta) &= -y_i\log(\hat{y}_i) - (1-y_i)\log(1-\hat{y}_i)\\ &= \log\left(1 + \exp\left((1-2y_i)R(|\langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle| - |\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle|)\right)\right).\end{aligned}$$

Note that $\langle \mathbf{X}_i - \mathbb{E}\mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle$ and $\langle \mathbf{X}_i - \mathbb{E}\mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle$ are mean 0 Gaussian random variables with variance σ^2. So for any fixed $i \in [n]$ and $\mathbf{m}_c \in \{\boldsymbol{\mu}, \boldsymbol{\nu}\}$, we use (Vershynin, 2018, Proposition 2.1.2) to obtain

$$\mathbf{Pr}\left[|\,\langle \mathbf{X}_i - \mathbb{E}\mathbf{X}_i, \hat{\mathbf{m}}_c\rangle\,| > t\right] \leq \frac{\sigma}{t\sqrt{2\pi}}\exp\left(-\frac{t^2}{2\sigma^2}\right).$$

Then by a union bound over all $i \in [n]$ and $\mathbf{m}_c \in \{\boldsymbol{\mu}, \boldsymbol{\nu}\}$, we have that

$$\mathbf{Pr}\left[|\,\langle \mathbf{X}_i - \mathbb{E}\mathbf{X}_i, \hat{\mathbf{m}}_c\rangle\,| \leq t\ \forall i \in [n],\ \mathbf{m}_c \in \{\boldsymbol{\mu}, \boldsymbol{\nu}\}\right] \geq 1 - \frac{n\sigma}{t}\sqrt{\frac{2}{\pi}}\exp\left(-\frac{t^2}{2\sigma^2}\right).$$

We now set $t = \sigma\sqrt{2(c+1)\log n}$ for any large constant $c > 0$. We now have with probability at least $1 - \frac{n^{-c}}{\sqrt{\pi(c+1)\log n}}$ that

$$\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle = \langle \mathbb{E}\mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle \pm O(\sigma\sqrt{c\log n}), \quad \langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle = \langle \mathbb{E}\mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle \pm O(\sigma\sqrt{c\log n})\ \forall i \in [n].$$

Thus, we can write

$$\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle = \gamma'\left(1 \pm O\left(\sqrt{\frac{c}{\log n}}\right)\right), \qquad \langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle = \gamma' \cdot O\left(\sqrt{\frac{c}{\log n}}\right) \qquad \forall i \in C_0, \quad (2)$$

$$\langle \mathbf{X}_i, \hat{\boldsymbol{\mu}}\rangle = \gamma' \cdot O\left(\sqrt{\frac{c}{\log n}}\right), \qquad \langle \mathbf{X}_i, \hat{\boldsymbol{\nu}}\rangle = \gamma'\left(1 \pm O\left(\sqrt{\frac{c}{\log n}}\right)\right) \qquad \forall i \in C_1. \quad (3)$$

Using Eqs. (2) and (3) in the expression for the loss, we obtain for all $i \in [n]$,

$$\ell_i(\mathbf{X}, \theta) = \log(1 + \exp(-R\gamma'(1 \pm o_n(1)))),$$

where the error term $o_n(1) = \sqrt{c/\log n}$. The total loss is then given by

$$\ell_\theta(\mathbf{X}) = \frac{1}{n}\sum \ell_i(\mathbf{X}, \theta) = \log(1 + \exp(-R\gamma'(1 + o_n(1)))).$$

Next, Fact A.5 implies that for $t < 0$, $e^t/2 \leq \log(1 + e^t) \leq e^t$, hence, we have that there exists a constant $C \in [1/2, 1]$ such that

$$\ell_\theta(\mathbf{X}) = C\exp\left(-R\gamma'(1 + o_n(1))\right).$$

Note that by scaling the optimality constraint R, the loss can go arbitrarily close to 0. $\square$

A.5 GRAPH CONVOLUTION IN THE FIRST LAYER

In this section, we show precisely why a graph convolution operation in the first layer is detrimental to the classification task.

Proposition A.8. *Fix a positive integer $d > 0$, $\sigma \in \mathbb{R}^+$ and $\boldsymbol{\mu}, \boldsymbol{\nu} \in \mathbb{R}^d$. Let $(\mathbf{A}, \mathbf{X}) \sim$ XOR-CSBM$(n, d, \boldsymbol{\mu}, \boldsymbol{\nu}, \sigma^2, p, q)$. Define $\tilde{\mathbf{X}}$ to be the transformed data after applying a graph convolution on $\mathbf{X}$, i.e., $\tilde{\mathbf{X}} = \mathbf{D}^{-1}\mathbf{A}\mathbf{X}$. Then in the regime where $p, q = \Omega(\frac{\log^2 n}{n})$, with probability at least $1 - 1/\mathrm{poly}(n)$ we have that*

$$\mathbb{E}\tilde{\mathbf{X}}_i = \begin{cases} \dfrac{p\boldsymbol{\mu} + q\boldsymbol{\nu}}{2(p+q)} \cdot o_n(1) & i \in C_0 \\ \dfrac{p\boldsymbol{\nu} + q\boldsymbol{\mu}}{2(p+q)} \cdot o_n(1) & i \in C_1 \end{cases}.$$

Hence, the distance between the means of the convolved data, given by $\frac{p-q}{2(p+q)} \|\boldsymbol{\mu} - \boldsymbol{\nu}\|_2 \cdot o_n(1)$ diminishes to 0 for $n \to \infty$.

Proof. Fix $\boldsymbol{\mu}, \boldsymbol{\nu} \in \mathbb{R}^d$ and define the following sets:

$$C_{-\boldsymbol{\mu}} = \{i \mid \varepsilon_i = 0, \eta_i = 0\}, \qquad C_{\boldsymbol{\mu}} = \{i \mid \varepsilon_i = 0, \eta_i = 1\},$$
$$C_{-\boldsymbol{\nu}} = \{i \mid \varepsilon_i = 1, \eta_i = 0\}, \qquad C_{\boldsymbol{\nu}} = \{i \mid \varepsilon_i = 1, \eta_i = 1\}.$$

Denote $\tilde{\mathbf{X}} = \mathbf{D}^{-1}\mathbf{A}\mathbf{X}$ and note that for any $i \in [n]$, the row vector

$$\begin{aligned} \tilde{\mathbf{X}}_i &= \frac{1}{\mathbf{deg}(i)} \sum_{j \in [n]} a_{ij} \mathbf{X}_j = \frac{1}{\mathbf{deg}(i)} \sum_{j \in [n]} a_{ij} (\mathbb{E}\mathbf{X}_j + \sigma \mathbf{g}_j) \\ &= \frac{1}{\mathbf{deg}(i)} \left[\boldsymbol{\mu} \left(\sum_{j \in C_{\boldsymbol{\mu}}} a_{ij} - \sum_{j \in C_{-\boldsymbol{\mu}}} a_{ij} \right) + \boldsymbol{\nu} \left(\sum_{j \in C_{\boldsymbol{\nu}}} a_{ij} - \sum_{j \in C_{-\boldsymbol{\nu}}} a_{ij} \right) + \sigma \sum_{j \in [n]} a_{ij} \mathbf{g}_j \right], \end{aligned}$$

where we used the fact that $\mathbf{X}_j = (2\eta_j - 1)((1-\varepsilon_j)\boldsymbol{\mu} + \varepsilon_j \boldsymbol{\nu} + \sigma \mathbf{g}_j)$ for a set of iid Gaussian random vectors $\mathbf{g}_j \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$.

Note that since ϵ_i, η_i are Bernoulli random variables, using the Chernoff bound (Vershynin, 2018, Section 2), we have that with probability at least $1 - 1/\mathrm{poly}(n)$,

$$|C_{-\boldsymbol{\mu}}| = |C_{\boldsymbol{\mu}}| = |C_{-\boldsymbol{\nu}}| = |C_{\boldsymbol{\nu}}| = \frac{n}{4}(1 \pm o_n(1)).$$

We now use an argument similar to Proposition A.1 to obtain that for any $c > 0$, with probability at least $1 - O(n^{-c})$, the following holds for all $i \in [n]$:

$$\frac{1}{\mathbf{deg}(i)} \left(\sum_{j \in C_{\boldsymbol{\mu}}} a_{ij} - \sum_{j \in C_{-\boldsymbol{\mu}}} a_{ij} \right) = O\left(\frac{(1-\varepsilon_i)p + \varepsilon_i q}{2(p+q)} \sqrt{\frac{c}{\log n}} \right),$$
$$\frac{1}{\mathbf{deg}(i)} \left(\sum_{j \in C_{\boldsymbol{\nu}}} a_{ij} - \sum_{j \in C_{-\boldsymbol{\nu}}} a_{ij} \right) = O\left(\frac{\varepsilon_i p + (1-\varepsilon_i) q}{2(p+q)} \sqrt{\frac{c}{\log n}} \right).$$

Hence, we have that for all $i \in [n]$,

$$\begin{aligned} \mathbb{E}\tilde{\mathbf{X}}_i &= \left[\left(\frac{(1-\varepsilon_i)p + \varepsilon_i q}{2(p+q)} \right) \boldsymbol{\mu} + \left(\frac{\varepsilon_i p + (1-\varepsilon_i) q}{2(p+q)} \right) \boldsymbol{\nu} \right] \cdot O\left(\sqrt{\frac{c}{\log n}} \right) \\ &= \begin{cases} \dfrac{p\boldsymbol{\mu} + q\boldsymbol{\nu}}{2(p+q)} \cdot o_n(1) & i \in C_0 \\ \dfrac{p\boldsymbol{\nu} + q\boldsymbol{\mu}}{2(p+q)} \cdot o_n(1) & i \in C_1 \end{cases} \end{aligned}$$

Using the above result, we obtain the distance between the means, which is of the order $o_n(\gamma)$ and thus, diminishes to 0 as $n \to \infty$. □

A.6 PROOF OF THEOREM 2 PART ONE

We begin by computing the output of the network when one graph convolution is applied at any layer other than the first.

Lemma A.9. *Let $h(\boldsymbol{x}) = |\langle \boldsymbol{x}, \hat{\boldsymbol{\nu}} \rangle| - |\langle \boldsymbol{x}, \hat{\boldsymbol{\mu}} \rangle|$ for any $\boldsymbol{x} \in \mathbb{R}^d$. Consider the two-layer and three-layer networks in Proposition A.7 where the weight parameter of the last layer, $W^{(L)}$, is scaled by a factor of $\xi = \operatorname{sgn}(p-q)$. If a graph convolution is added to these networks in either the second or the third layer then for a sample $(\mathbf{A}, \mathbf{X}) \sim$ XOR-CSBM$(n, d, \boldsymbol{\mu}, \boldsymbol{\nu}, \sigma^2, p, q)$, the output of the networks for a point $i \in [n]$ is*

$$\hat{y}_i = \varphi(f_i^{(L)}(\mathbf{X})) = \varphi\left(\frac{R \operatorname{sgn}(p-q)}{\mathbf{deg}(i)} \sum_{j \in [n]} a_{ij} h(\mathbf{X}_j)\right).$$

Proof. The networks with scaled parameters are given as follows.

1. For the two-layer network,

$$\mathbf{W}^{(1)} = R\begin{pmatrix}\hat{\boldsymbol{\mu}} & -\hat{\boldsymbol{\mu}} & \hat{\boldsymbol{\nu}} & -\hat{\boldsymbol{\nu}}\end{pmatrix}, \qquad \mathbf{W}^{(2)} = \xi\begin{pmatrix}-1 & -1 & 1 & 1\end{pmatrix}^\top.$$

2. For the three-layer network,

$$\mathbf{W}^{(1)} = R\xi\begin{pmatrix}\hat{\boldsymbol{\mu}} & -\hat{\boldsymbol{\mu}} & \hat{\boldsymbol{\nu}} & -\hat{\boldsymbol{\nu}}\end{pmatrix}, \quad \mathbf{W}^{(2)} = \begin{pmatrix}-1 & 1\\ -1 & 1\\ 1 & -1\\ 1 & -1\end{pmatrix}, \quad \mathbf{W}^{(3)} = \xi\begin{pmatrix}1\\ -1\end{pmatrix}.$$

When a graph convolution is applied at the second layer of this two-layer MLP, the output of the last layer for data $(\mathbf{A}, \mathbf{X})$ is $f_i^{(2)}(\mathbf{X}) = \mathbf{D}^{-1}\mathbf{A}[\mathbf{X}\mathbf{W}^{(1)}]_+\mathbf{W}^{(2)}$. Then we have

$$f_i^{(2)}(\mathbf{X}) = \frac{R\xi}{\mathbf{deg}(i)} \sum_{j \in [n]} a_{ij}(|\langle \mathbf{X}_j, \hat{\boldsymbol{\nu}} \rangle| - |\langle \mathbf{X}_j, \hat{\boldsymbol{\mu}} \rangle|) = \frac{R\xi}{\mathbf{deg}(i)} \sum_{j \in [n]} a_{ij} h(\mathbf{X}_j).$$

Similarly, when the graph convolution is applied at the second layer of the three-layer MLP, the output is $f_i^{(3)}(\mathbf{X}) = [\mathbf{D}^{-1}\mathbf{A}[\mathbf{X}\mathbf{W}^{(1)}]_+\mathbf{W}^{(2)}]_+\mathbf{W}^{(3)}$, and we have

$$f_i^{(3)}(\mathbf{X}) = \frac{R\xi}{\mathbf{deg}(i)}\left(\left[\sum_{j \in [n]} a_{ij} h(\mathbf{X}_j)\right]_+ - \left[-\sum_{j \in [n]} a_{ij} h(\mathbf{X}_j)\right]_+\right) = \frac{R\xi}{\mathbf{deg}(i)} \sum_{j \in [n]} a_{ij} h(\mathbf{X}_j).$$

Finally, when the graph convolution is applied at the third layer of the three-layer MLP, the output is $f_i^{(3)}(\mathbf{X}) = \mathbf{D}^{-1}\mathbf{A}[[\mathbf{X}\mathbf{W}^{(1)}]_+\mathbf{W}^{(2)}]_+\mathbf{W}^{(3)}$, and we have

$$\begin{aligned} f_i^{(3)}(\mathbf{X}) &= \frac{R\xi}{\mathbf{deg}(i)} \sum_{j \in [n]} a_{ij}\left([|\langle \mathbf{X}_j, \hat{\boldsymbol{\nu}} \rangle| - |\langle \mathbf{X}_j, \hat{\boldsymbol{\mu}} \rangle|]_+ - [|\langle \mathbf{X}_j, \hat{\boldsymbol{\mu}} \rangle| - |\langle \mathbf{X}_j, \hat{\boldsymbol{\nu}} \rangle|]_+\right)\\ &= \frac{R}{\mathbf{deg}(i)} \sum_{j \in [n]} a_{ij}(|\langle \mathbf{X}_j, \hat{\boldsymbol{\nu}} \rangle| - |\langle \mathbf{X}_j, \hat{\boldsymbol{\mu}} \rangle|) = \frac{R\xi}{\mathbf{deg}(i)} \sum_{j \in [n]} a_{ij} h(\mathbf{X}_j). \end{aligned}$$

Therefore, in all cases where we have a single graph convolution, the output of the last layer is

$$f_i^{(L)}(\mathbf{X}) = \frac{R \operatorname{sgn}(p-q)}{\mathbf{deg}(i)} \sum_{j \in [n]} a_{ij} h(\mathbf{X}_j),$$

where $L \in \{2, 3\}$ is the number of layers. □

Theorem (Restatement of part one of Theorem 2)**.** *Let $(\mathbf{A}, \mathbf{X}) \sim$ XOR-CSBM$(n, d, \boldsymbol{\mu}, \boldsymbol{\nu}, \sigma^2, p, q)$. Assume that $p, q = \Omega(\frac{\log^2 n}{n})$, and it holds that $\Gamma(p,q)\zeta(\gamma/2\sigma) = \omega\left(\sqrt{\frac{\log n}{n(p+q)}}\right)$, then for any $c > 0$,*

with probability at least $1 - O(n^{-c})$, the networks equipped with a graph convolution in the second or the third layer perfectly classify the data, and obtain the following loss:

$$\ell_\theta(\mathbf{A}, \mathbf{X}) = C' \exp\left(-C\sigma R\Gamma(p,q)\zeta(\gamma/2\sigma)(1 \pm \sqrt{c/\log n})\right),$$

where $C > 0$ and $C' \in [1/2, 1]$ are constants and R is the constraint from Eq. (1).

Proof. First, we analyze the output conditioned on the adjacency matrix $\mathbf{A}$. Note that $\frac{1}{R} f_i^{(L)}(\mathbf{X})$ in Lemma A.9 is Lipschitz with constant $\sqrt{\frac{2}{\mathbf{deg}(i)}}$, and $h(\mathbf{X}_j)$ are mutually independent for $j \in [n]$. Therefore, by Gaussian concentration (Vershynin, 2018, Theorem 5.2.2) we have that for a fixed $i \in [n]$,

$$\mathbf{Pr}\left[\frac{1}{R}|f_i^{(L)}(\mathbf{X}) - \mathbb{E}[f_i^{(L)}(\mathbf{X})]| > \delta \mid \mathbf{A}\right] \leq 2\exp\left(-\frac{\delta^2 \mathbf{deg}(i)}{4\sigma^2}\right).$$

We refer to the event from Proposition A.1 as B and define $Q(t)$ to be the event that

$$|f_i^{(L)}(\mathbf{X}) - \mathbb{E}[f_i^{(L)}(\mathbf{X})]| \leq t \text{ for all } i \in [n].$$

Then we can write

$$\begin{aligned}
\mathbf{Pr}\left[Q(t)^{\mathsf{c}}\right] &= \mathbf{Pr}\left[Q(t)^{\mathsf{c}} \cap B\right] + \mathbf{Pr}\left[Q(t)^{\mathsf{c}} \cap B^{\mathsf{c}}\right] \\
&\leq 2n\exp\left(-\frac{t^2 n(p+q)}{8\sigma^2}\right) + \mathbf{Pr}\left[B^{\mathsf{c}}\right] \\
&\leq 2n\exp\left(-\frac{t^2 n(p+q)}{8\sigma^2}\right) + 2n^{-c}.
\end{aligned}$$

Let $\xi = \operatorname{sgn}(p-q)$ and note that $\frac{\xi(p-q)}{p+q} = \frac{|p-q|}{p+q} = \Gamma(p,q)$. We now choose $t = 2\sigma\sqrt{\frac{2(c+1)\log n}{n(p+q)}}$ to obtain that with probability at least $1 - 4n^{-c}$, the following holds for all $i \in [n]$:

$$\begin{aligned}
\frac{1}{\sigma} f_i^{(L)}(\mathbf{X}) &= \mathbb{E}[f_i^{(L)}(\mathbf{X})]/\sigma \pm O\left(R\sqrt{\frac{c\log n}{n(p+q)}}\right) \\
&= \frac{R\xi}{\sigma\,\mathbf{deg}(i)} \sum_{j\in[n]} a_{ij}\mathbb{E}h(\mathbf{X}_j) \pm O\left(R\sqrt{\frac{c\log n}{n(p+q)}}\right) \\
&= \frac{\sqrt{2}R\xi\zeta(\gamma/2\sigma)}{\sigma\,\mathbf{deg}(i)}\left(\sum_{j\in C_1} a_{ij} - \sum_{j\in C_0} a_{ij}\right) \pm O\left(R\sqrt{\frac{c\log n}{n(p+q)}}\right) \qquad \text{(Lemma A.4)} \\
&= \sqrt{2}(2\varepsilon_i - 1)R\Gamma(p,q)\zeta(\gamma/2\sigma)(1 \pm o_n(1)) \pm O\left(R\sqrt{\frac{c\log n}{n(p+q)}}\right) \qquad \text{(Proposition A.1)} \\
&= \sqrt{2}(2\varepsilon_i - 1)R\Gamma(p,q)\zeta(\gamma/2\sigma)(1 \pm o_n(1)),
\end{aligned}$$

where in the last equation we used the assumption that $\Gamma(p,q)\zeta(\gamma/2\sigma) = \omega\left(\sqrt{\frac{\log n}{n(p+q)}}\right)$. Overall, we obtain that with probability at least $1 - 4n^{-c}$,

$$f_i^{(L)}(\mathbf{X}) = (2\varepsilon_i - 1)C\sigma R\Gamma(p,q)\zeta(\gamma/2\sigma)(1 \pm o_n(1)), \text{ for all } i \in [n].$$

Recall that the loss for node i is given by

$$\ell_\theta^{(i)}(\mathbf{A}, \mathbf{X}) = \log(1 + e^{(1-2\varepsilon_i)f_i^{(L)}(\mathbf{X})}) = \log\left(1 + \exp\left(-C\sigma R\Gamma(p,q)\zeta(\gamma/2\sigma)(1 \pm o_n(1))\right)\right).$$

The total loss is given by $\frac{1}{n}\sum_{i\in[n]} \ell_\theta^{(i)}(\mathbf{A}, \mathbf{X})$. Next, Fact A.5 implies that for any $t < 0$, $e^t/2 \leq \log(1 + e^t) \leq e^t$, hence, we have for some $C' \in [1/2, 1]$ that

$$\ell_\theta(\mathbf{A}, \mathbf{X}) = C' \exp\left(-C\sigma R\Gamma(p,q)\zeta(\gamma/2\sigma)(1 \pm o_n(1))\right). \qquad \square$$

A.7 PROOF OF THEOREM 2 PART TWO

We begin by computing the output of the networks constructed in Proposition A.7 when two graph convolutions are placed among any layer in the networks other than the first.

Lemma A.10. *Let $h(\boldsymbol{x}) : \mathbb{R}^d \to \mathbb{R} = |\langle \boldsymbol{x}, \hat{\boldsymbol{\nu}} \rangle| - |\langle \boldsymbol{x}, \hat{\boldsymbol{\mu}} \rangle|$. Consider the networks constructed in Proposition A.7 equipped with two graph convolutions in the following combinations:*

1. *Both convolutions in the second layer of the two-layer network.*
2. *Both convolutions in the second layer of the three-layer network.*
3. *One convolution in the second layer and one in the third layer of the three-layer network.*
4. *Both convolutions in the third layer of the three-layer network.*

Then for a sample $(\mathbf{A}, \mathbf{X}) \sim$ XOR-CSBM$(n, d, \boldsymbol{\mu}, \boldsymbol{\nu}, \sigma^2, p, q)$, the output of the networks in all the above described combinations for a point $i \in [n]$ is

$$\hat{y}_i = \varphi(f_i^{(L)}(\mathbf{X})) = \varphi\left(\frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \tau_{ij} h(\mathbf{X}_j)\right), \text{ where } \tau_{ij} = \sum_{k\in[n]} \frac{a_{ik}a_{jk}}{\mathbf{deg}(k)}.$$

Proof. For the two-layer network, the output of the last layer when both convolutions are at the second layer is given by $f_i^{(2)}(\mathbf{X}) = (\mathbf{D}^{-1}\mathbf{A})^2[\mathbf{X}\mathbf{W}^{(1)}]_+\mathbf{W}^{(2)}$. Then we have

$$f_i^{(2)}(\mathbf{X}) = \frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \sum_{k\in[n]} \frac{a_{ij}a_{jk}}{\mathbf{deg}(j)} h(\mathbf{X}_k) = \frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \tau_{ij} h(\mathbf{X}_j).$$

Next, for the three-layer network, the output of the last layer when both convolutions are at the second layer is given by $f_i^{(3)}(\mathbf{X}) = [(\mathbf{D}^{-1}\mathbf{A})^2[\mathbf{X}\mathbf{W}^{(1)}]_+\mathbf{W}^{(2)}]_+\mathbf{W}^{(3)}$, hence, we have

$$\begin{aligned}
f_i^{(3)}(\mathbf{X}) &= \frac{R}{\mathbf{deg}(i)} \left(\left[\sum_{j\in[n]} \frac{a_{ij}}{\mathbf{deg}(j)} \sum_{k\in[n]} a_{jk} h(\mathbf{X}_k) \right]_+ - \left[- \sum_{j\in[n]} \frac{a_{ij}}{\mathbf{deg}(j)} \sum_{k\in[n]} a_{jk} h(\mathbf{X}_k) \right]_+ \right) \\
&= \frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \frac{a_{ij}}{\mathbf{deg}(j)} \sum_{k\in[n]} a_{jk} h(\mathbf{X}_k) \qquad \text{(using } [t]_+ - [-t]_+ = t \text{ for any } t \in \mathbb{R}) \\
&= \frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \tau_{ij} h(\mathbf{X}_j).
\end{aligned}$$

Similarly, the output of the last layer when one convolution is at the second layer and the other one is at the third layer is given by $f_i^{(3)}(\mathbf{X}) = \mathbf{D}^{-1}\mathbf{A}[\mathbf{D}^{-1}\mathbf{A}[\mathbf{X}\mathbf{W}^{(1)}]_+\mathbf{W}^{(2)}]_+\mathbf{W}^{(3)}$, hence, we have

$$\begin{aligned}
f_i^{(3)}(\mathbf{X}) &= \frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \frac{a_{ij}}{\mathbf{deg}(j)} \left(\left[\sum_{k\in[n]} a_{jk} h(\mathbf{X}_k) \right]_+ - \left[- \sum_{k\in[n]} a_{jk} h(\mathbf{X}_k) \right]_+ \right) \\
&= \frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \frac{a_{ij}}{\mathbf{deg}(j)} \sum_{k\in[n]} a_{jk} h(\mathbf{X}_k) \qquad \text{(using } [t]_+ - [-t]_+ = t \text{ for any } t \in \mathbb{R}) \\
&= \frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \tau_{ij} h(\mathbf{X}_j).
\end{aligned}$$

Finally, the output of the last layer when both convolutions are at the third layer is given by $f_i^{(3)}(\mathbf{X}) = (\mathbf{D}^{-1}\mathbf{A})^2[[\mathbf{X}\mathbf{W}^{(1)}]_+\mathbf{W}^{(2)}]_+\mathbf{W}^{(3)}$, hence, we have

$$\begin{aligned} f_i^{(3)}(\mathbf{X}) &= \frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \frac{a_{ij}}{\mathbf{deg}(j)} \left(\sum_{k\in[n]} a_{jk} \left([h(\mathbf{X}_k)]_+ - [-h(\mathbf{X}_k)]_+ \right) \right) \\ &= \frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \frac{a_{ij}}{\mathbf{deg}(j)} \sum_{k\in[n]} a_{jk} h(\mathbf{X}_k) = \frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \tau_{ij} h(\mathbf{X}_j). \end{aligned}$$

Hence, the output for two graph convolutions is the same for any combination of the placement of convolutions, as long as no convolution is placed at the first layer. □

We are now ready to prove the positive result for two convolutions.

Theorem (Restatement of part two of Theorem 2)**.** *Let* $(\mathbf{A}, \mathbf{X}) \sim$ *XOR-CSBM*$(n, d, \boldsymbol{\mu}, \boldsymbol{\nu}, \sigma^2, p, q)$. *Assume that* $p, q = \Omega(\frac{\log n}{\sqrt{n}})$ *and* $\Gamma(p,q)^2\zeta(\gamma/2\sigma) = \omega\left(\sqrt{\frac{\log n}{n}}\right)$. *Then for any* $c > 0$, *with probability at least* $1 - O(n^{-c})$, *the networks with any combination of two graph convolutions in the second and/or the third layers perfectly classify the data, and obtain the following loss:*

$$\ell_\theta(\mathbf{A}, \mathbf{X}) = C' \exp\left(-C\sigma R \Gamma(p,q)^2 \zeta(\gamma/\sigma)(1 \pm \sqrt{c/\log n}) \right),$$

where $C > 0$ *and* $C' \in [1/2, 1]$ *are constants and* R *is the constraint from Eq. (1).*

Proof. The proof strategy is similar to that of part one of the theorem. Note that $\frac{1}{R} f_i^{(L)}(\mathbf{X})$ in Lemma A.10 is Lipschitz with constant

$$\left\| \frac{1}{R} f_i^{(L)}(\mathbf{X}) \right\|_{\text{Lip}} \leq \sqrt{\frac{2}{\mathbf{deg}(i)^2} \sum_{j\in[n]} \tau_{ij}^2}.$$

Since $h(\mathbf{X}_j)$ are mutually independent for $j \in [n]$, by Gaussian concentration (Vershynin, 2018, Theorem 5.2.2) we have that for a fixed $i \in [n]$,

$$\mathbf{Pr}\left[\frac{1}{R} |f_i^{(L)}(\mathbf{X}) - \mathbb{E}[f_i^{(L)}(\mathbf{X})]| > \delta \mid \mathbf{A} \right] \leq 2\exp\left(-\frac{\delta^2 \mathbf{deg}(i)^2}{4\sigma^2 \sum_{j\in[n]} \tau_{ij}^2} \right).$$

We refer to the event from Proposition A.2 as B. Note that since the graph density assumption is stronger than $\Omega(\frac{\log^2 n}{n})$, Proposition A.1 trivially holds in this regime, hence, the degrees also concentrate strongly around $\Delta = \frac{n}{2}(p+q)$. On event B, we have that

$$\begin{aligned} \sum_{j\in[n]} \tau_{ij}^2 &= \sum_{j\in[n]} \left(\sum_{k\in[n]} \frac{a_{ik}a_{jk}}{\mathbf{deg}(k)} \right)^2 = \frac{1}{\Delta^2} \sum_{j\in[n]} \left(\sum_{k\in[n]} a_{ik}a_{jk} \right)^2 (1 \pm o_n(1)) \\ &= \frac{1}{\Delta^2} \left(\sum_{j\sim i} |N_i \cap N_j|^2 + \sum_{j\nsim i} |N_i \cap N_j|^2 \right) (1 \pm o_n(1)) \\ &= \frac{1}{\Delta^2} \left(\sum_{j\sim i} \left(\frac{n}{2}(p^2+q^2) \right)^2 + \sum_{j\nsim i} (npq)^2 \right) (1 \pm o_n(1)) \qquad \text{(using Proposition A.2)} \\ &= \frac{n}{2\Delta^2} \left(\frac{n^2}{4}(p^2+q^2)^2 + n^2p^2q^2 \right) (1 \pm o_n(1)) = \frac{n^3}{8\Delta^2} \left(p^4 + q^4 + 6p^2q^2 \right) (1 \pm o_n(1)). \end{aligned}$$

Therefore, under this event we have that

$$\left\| \frac{1}{R} f_i^{(L)}(\mathbf{X}) \right\|_{\text{Lip}} \leq \sqrt{\frac{2}{\mathbf{deg}(i)^2} \sum_{j\in[n]} \tau_{ij}^2} = \sqrt{\frac{4(p^4+q^4+6p^2q^2)}{n(p+q)^4}} (1 \pm o_n(1)).$$

Note that $K = K(p,q) = \frac{4(p^4+q^4+6p^2q^2)}{(p+q)^4} \leq 4$. We now define $Q(t)$ to be the event that $|f_i^{(L)}(\mathbf{X}) - \mathbb{E}[f_i^{(L)}(\mathbf{X})]| \leq t$ for all $i \in [n]$. Then we have

$$\mathbf{Pr}\left[Q(t)^{\mathsf{c}}\right] = \mathbf{Pr}\left[Q(t)^{\mathsf{c}} \cap B\right] + \mathbf{Pr}\left[Q(t)^{\mathsf{c}} \cap B^{\mathsf{c}}\right] \leq 2n \exp\left(-\frac{nt^2}{2K^2\sigma^2}\right) + 2n^{-c}.$$

We now choose $t = \sigma\sqrt{\frac{2K(c+1)\log n}{n}}$ to obtain that with probability at least $1 - 4n^{-c}$, the following holds for all $i \in [n]$:

$$f_i^{(L)}(\mathbf{X}) = \mathbb{E}[f_i^{(L)}(\mathbf{X})] \pm O\left(R\sigma\sqrt{\frac{\log n}{n}}\right) = \frac{R}{\mathbf{deg}(i)} \sum_{j\in[n]} \tau_{ij}\mathbb{E}h(\mathbf{X}_j) \pm O\left(R\sigma\sqrt{\frac{\log n}{n}}\right).$$

Note that we have

$$\begin{aligned}
\frac{1}{\mathbf{deg}(i)} \sum_{j\in[n]} \tau_{ij}\mathbb{E}h(\mathbf{X}_j) &= \frac{\sqrt{2}\zeta(\gamma/2\sigma)}{\mathbf{deg}(i)} \left(\sum_{j\in C_1} \tau_{ij} - \sum_{j\in C_0} \tau_{ij}\right) \qquad \text{(using Lemma A.4)} \\
&= \frac{\sqrt{2}\zeta(\gamma/2\sigma)}{\mathbf{deg}(i)} \left(\sum_{j\in C_1}\sum_{k\in[n]} \frac{a_{ik}a_{jk}}{\mathbf{deg}(k)} - \sum_{j\in C_0}\sum_{k\in[n]} \frac{a_{ik}a_{jk}}{\mathbf{deg}(k)}\right) \\
&= \frac{\sqrt{2}\zeta(\gamma/2\sigma)}{\mathbf{deg}(i)} \left(\sum_{k\in[n]} \frac{a_{ik}}{\mathbf{deg}(k)} \left(\sum_{j\in C_1} a_{jk} - \sum_{j\in C_0} a_{jk}\right)\right) \\
&= \frac{\sqrt{2}\zeta(\gamma/2\sigma)\Gamma(p,q)}{\mathbf{deg}(i)} \left(\sum_{k\in C_1} a_{ik} - \sum_{k\in C_0} a_{ik}\right)(1 + o_n(1)) \\
&= \sqrt{2}\zeta(\gamma/2\sigma)\Gamma(p,q)^2(1 + o_n(1)).
\end{aligned}$$

In the last two equations above, we used Proposition A.1 to replace, respectively,

$$\begin{aligned}
\frac{1}{\mathbf{deg}(k)} \left(\sum_{j\in C_1} a_{kj} - \sum_{j\in C_0} a_{kj}\right) &= (2\varepsilon_k - 1)\Gamma(p,q)(1 + o_n(1)), \\
\frac{1}{\mathbf{deg}(i)} \left(\sum_{j\in C_1} a_{ik} - \sum_{j\in C_0} a_{ik}\right) &= (2\varepsilon_k - 1)\Gamma(p,q)(1 + o_n(1)).
\end{aligned}$$

Therefore, we obtain that

$$\begin{aligned}
f_i^{(L)}(\mathbf{X}) &= C\sigma R\zeta(\gamma/2\sigma)\Gamma(p,q)^2(1 + o_n(1)) \pm O\left(R\sigma\sqrt{\frac{\log n}{n}}\right) \\
&= C\sigma R\zeta(\gamma/2\sigma)\Gamma(p,q)^2(1 + o_n(1)),
\end{aligned}$$

where in the last equation we used $\Gamma(p,q)^2\zeta(\gamma/2\sigma) = \omega\left(\sqrt{\frac{\log n}{n}}\right)$.

Recall that the loss for node i is given by

$$\begin{aligned}
\ell_\theta^{(i)}(\mathbf{A}, \mathbf{X}) &= \log(1 + \exp((1 - 2\varepsilon_i)f_i^{(L)}(\mathbf{X}))) \\
&= \log\left(1 + \exp\left(-C\sigma R\zeta(\gamma/2\sigma)\Gamma(p,q)^2(1 \pm o_n(1))\right)\right).
\end{aligned}$$

The total loss is $\frac{1}{n}\sum_{i\in[n]} \ell_\theta^{(i)}(\mathbf{A}, \mathbf{X})$. Now, using Fact A.5 we have for some $C' \in [1/2, 1]$ that

$$\ell_\theta(\mathbf{A}, \mathbf{X}) = C' \exp\left(-C\sigma R\zeta(\gamma/2\sigma)\Gamma(p,q)^2(1 \pm o_n(1))\right). \qquad \square$$

A.8 ANALYSIS FOR A SIMPLER CASE

Although Theorem 2 encapsulates the general condition for networks with up to two graph convolutions to achieve perfect classification, let us discuss the meaning of the theorem in a simplified setting where $\Gamma(p,q) = \Omega(1)$. In this regime, one can analyze two cases for both parts of the theorem:

1. Case $\gamma = \Omega(\sigma)$: Using part two of Lemma A.4 implies that $\zeta(\gamma/\sigma) = \Omega(\frac{\gamma}{\sigma})$. Hence, for one graph convolution, the condition $\Gamma(p,q)\zeta(\gamma/2\sigma) = \omega\left(\sqrt{\frac{\log n}{n(p+q)}}\right)$ is satisfied when $\frac{\gamma}{\sigma} = \omega\left(\sqrt{\frac{\log n}{n(p+q)}}\right)$, implying that $\gamma = \omega\left(\sigma\sqrt{\frac{\log n}{n(p+q)}}\right)$. Similarly, for two graph convolutions, the condition $\Gamma(p,q)^2\zeta(\gamma/2\sigma) = \omega\left(\sqrt{\frac{\log n}{n}}\right)$ is satisfied when $\gamma = \omega\left(\sigma\sqrt{\frac{\log n}{n}}\right)$.

2. Case $\gamma = o(\sigma)$: Using part three of Lemma A.4 implies that $\zeta(\gamma/\sigma) = \Omega(\frac{\gamma^2}{\sigma^2})$. Hence, for one graph convolution, the condition $\Gamma(p,q)\zeta(\gamma/2\sigma) = \omega\left(\sqrt{\frac{\log n}{n(p+q)}}\right)$ is satisfied when $\left(\frac{\gamma}{\sigma}\right)^2 = \omega\left(\sqrt{\frac{\log n}{n(p+q)}}\right)$, implying that $\gamma = \omega\left(\sigma\sqrt[4]{\frac{\log n}{n(p+q)}}\right)$. Similarly, for two graph convolutions, the condition $\Gamma(p,q)^2\zeta(\gamma/2\sigma) = \omega\left(\sqrt{\frac{\log n}{n}}\right)$ is satisfied when $\gamma = \omega\left(\sigma\sqrt[4]{\frac{\log n}{n}}\right)$.

Combining both cases, we find that the theorems imply perfect classification if the following holds:

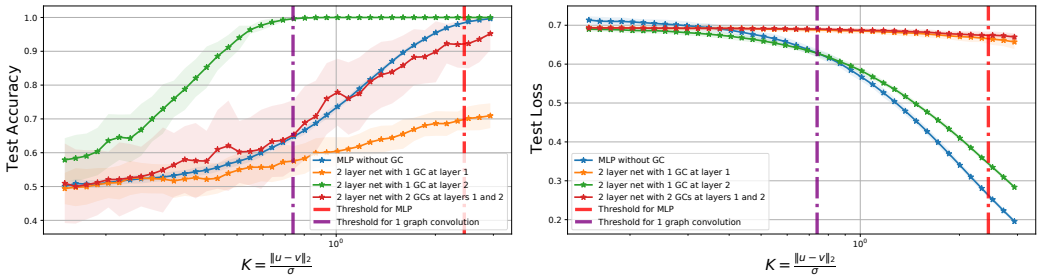
$$\gamma = \|\boldsymbol{\mu} - \boldsymbol{\nu}\|_2 = \begin{cases} \Omega\left(\frac{\sigma\sqrt{\log n}}{\sqrt[4]{n(p+q)}}\right) & \text{for networks wth one graph convolution,} \\ \Omega\left(\frac{\sigma\sqrt{\log n}}{\sqrt[4]{n}}\right) & \text{for networks with two graph convolutions.} \end{cases}$$

B ADDITIONAL EXPERIMENTS

For all synthetic and real-data experiments, we used PyTorch Geometric (Fey & Lenssen, 2019), using public splits for the real datasets. The models were trained on an Nvidia Titan Xp GPU, using the Adam optimizer with learning rate 10^{-3}, weight decay 10^{-5}, and 50 to 500 epochs varying among the datasets.

B.1 SYNTHETIC DATA

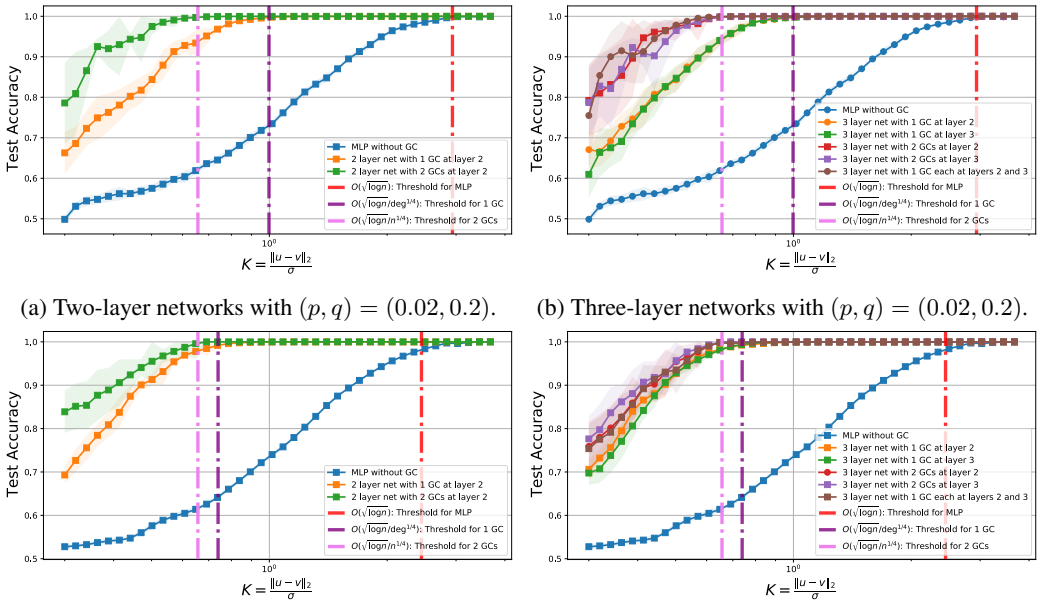
In this section we show additional results on the synthetic data. First, we show that placing a graph convolution in the first layer makes the classification task difficult since the means of the convolved data collapse towards 0. This is shown in Fig. 4.



(a) Test accuracy. (b) Test loss.

Figure 4: Comparing the accuracy and loss for various networks with and without graph convolutions, averaged over 50 trials. Networks with a graph convolution in the first layer (red and orange) fail to generalize even for a large distance between the means of the data. For this experiment, we set $n = 400$ and $d = 4$, with $\sigma^2 = 1/d$.

Next, we show experiments for two sets of values of $p < q$ to demonstrate that graph convolutions also work in this setting. In Figs. 5a and 5b we have $\Gamma(p, q) \approx 0.82$, while in Figs. 5c and 5d we have a lower signal in the graph, $\Gamma(p, q) \approx 0.66$. We observe that in the latter case that there is less gap in the performance of networks with one graph convolution and those with two graph convolutions. In comparison to Fig. 2, we observe similar trends about the performance of all the networks in different regimes of interest. In particular, networks with one graph convolution perform mutually similarly, and networks with two graph convolutions perform mutually similarly, as claimed in Theorem 2.



(a) Two-layer networks with $(p, q) = (0.02, 0.2)$.

(b) Three-layer networks with $(p, q) = (0.02, 0.2)$.

(c) Two-layer networks with $(p, q) = (0.1, 0.5)$.

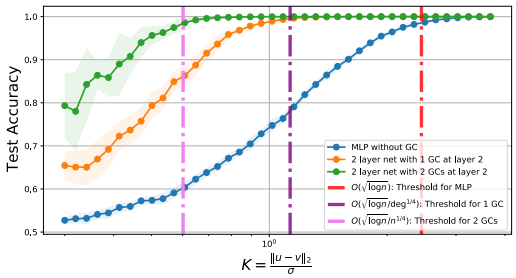
(d) Three-layer networks with $(p, q) = (0.1, 0.5)$.

Figure 5: Averaged accuracy (over 50 trials) for various networks with and without graph convolutions on the XOR-CSBM data model with $n = 400, d = 4$ and $\sigma^2 = 1/d$ for $p < q$. The x-axis denotes the ratio $K = \|\boldsymbol{\mu} - \boldsymbol{\nu}\|_2 / \sigma$ on a logarithmic scale. The vertical lines indicate the classification thresholds mentioned in part two of Theorem 1 (red), and in Theorem 2 (violet and pink).

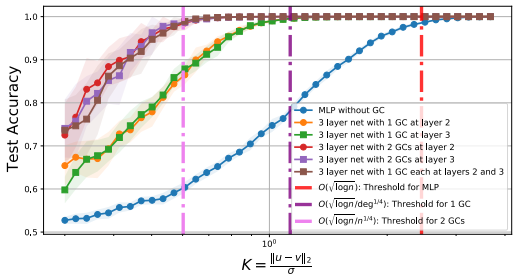
Finally, in Fig. 6, we show the trends for the accuracy of various networks with and without graph convolutions, for different values of $\Gamma(p, q)$. For cases where $\Gamma(p, q)$ is relatively larger, networks with graph convolutions perform much better than a standard MLP (see Figs. 6a to 6d), while for the cases where $\Gamma(p, q)$ is much smaller, the networks with graph convolutions degrade in performance (see Figs. 6e to 6h). The intuition behind this behaviour is that a smaller value of $\Gamma(p, q)$ represents more noise in the data, thus, networks with graph convolutions gather roughly an equivalent amount of information from nodes in both the classes, making the feature representations noisy.

B.2 Real-world data

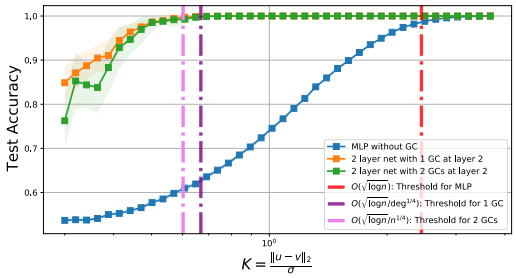
This section contains additional experiments on real-world data. In Fig. 7, we plot the accuracy of the networks measured on the three benchmark datasets, averaged across 50 different trials (random initialization of the network parameters). This corresponds to the plots in Fig. 3 that show the maximum accuracy across all trials. Next, we evaluate the performance of the original GCN normalization (Kipf & Welling, 2017), $\mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}$ instead of $\mathbf{D}^{-1}\mathbf{A}$, and show that we observe the same trends about the number of convolutions and their placement. These results are shown in Figs. 8 and 9. Note the two general trends that are consistent: first, networks with two graph convolutions perform better than those with one graph convolution, and second, placing all graph convolutions in the first layer yields worse accuracy as compared to networks where the convolutions are placed in deeper layers.



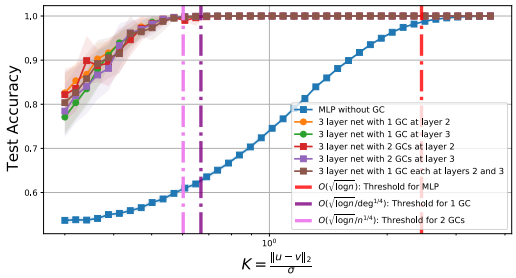
(a) Two layers, $(p, q) = (0.1, 0.01)$, $\Gamma(p, q) \approx 0.82$.



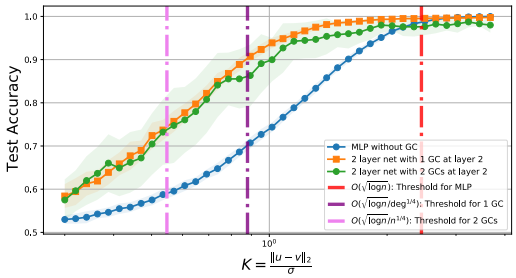
(b) Three layers, $\Gamma(p, q) \approx 0.82$.



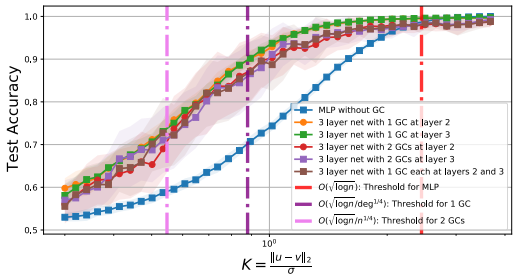
(c) Two layers, $(p, q) = (0.8, 0.1)$, $\Gamma(p, q) \approx 0.78$.



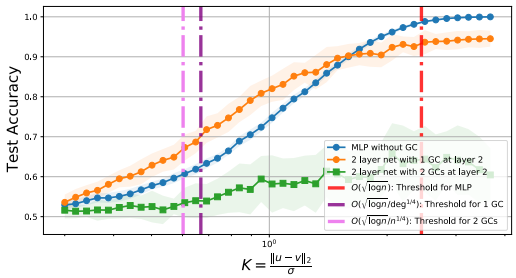
(d) Three layers, $\Gamma(p, q) \approx 0.78$.



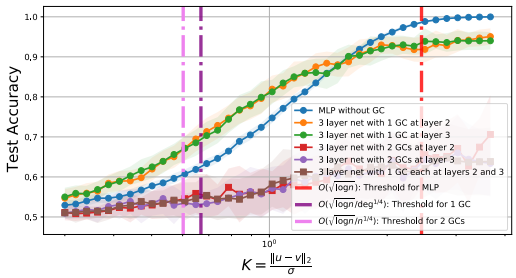
(e) Two layers, $(p, q) = (0.2, 0.1)$, $\Gamma(p, q) \approx 0.33$.



(f) Three layers, $\Gamma(p, q) \approx 0.33$.



(g) Two layers, $(p, q) = (0.5, 0.4)$, $\Gamma(p, q) \approx 0.11$.

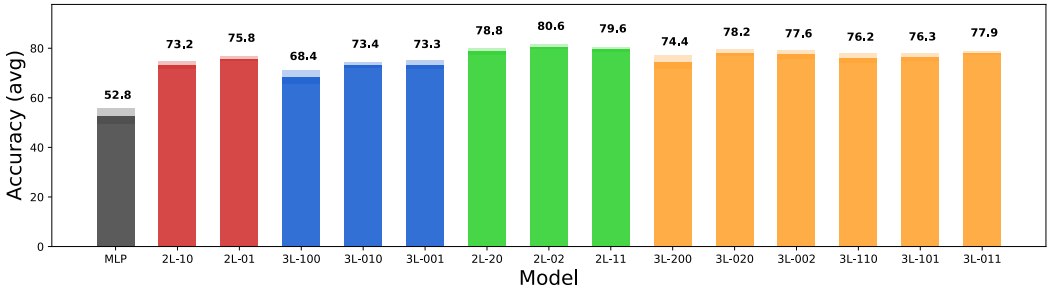


(h) Three layers, $\Gamma(p, q) \approx 0.11$.

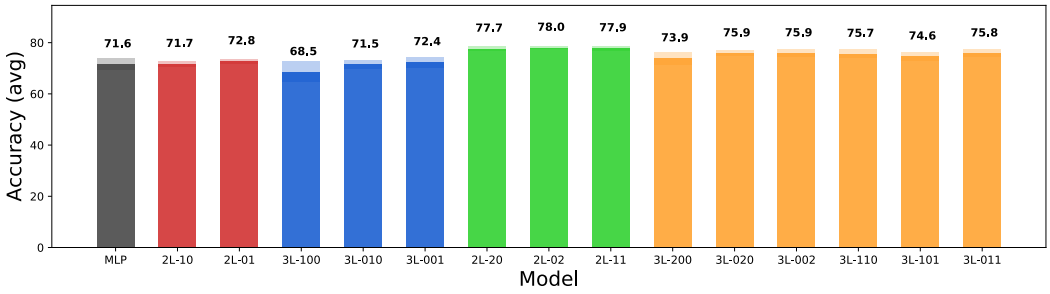
Figure 6: Test accuracy of various networks with with and without graph convolutions (GCs) for various values of p and q, on the XOR-CSBM data model. Note that networks with graph convolutions degrade in performance as $\Gamma(p, q)$ (attributed to the signal in the graph) decreases.

Similar to the results in the main paper, we observe that there are differences within the group of networks with the same number of convolutions, however, these differences are smaller in magnitude as compared to the difference between the two groups of networks, one with one graph convolution and the other two graph convolutions. We also note that in some cases, three-layer networks obtain a worse accuracy, which we attribute to the fact that three layers have a lot more parameters, and thus may either be overfitting, or may not be converging for the number of epochs used.

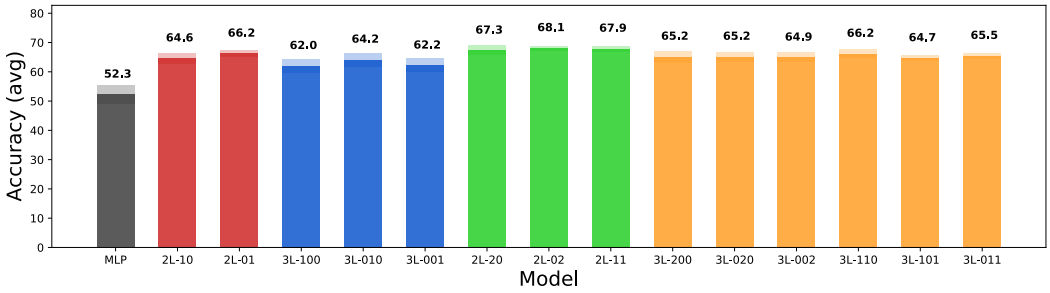
Furthermore, we perform the same experiments on relatively larger datasets, OGBN-arXiv and OGBN-products (Hu et al., 2020). We observe similar trends in these experiments. First, we observe



(a) CORA.



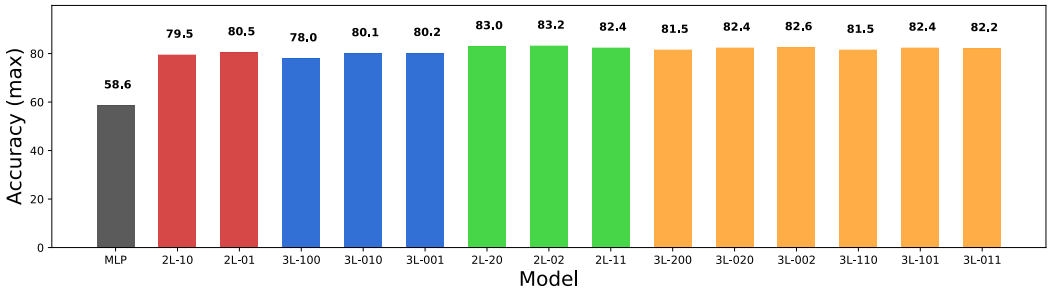
(b) Pubmed.



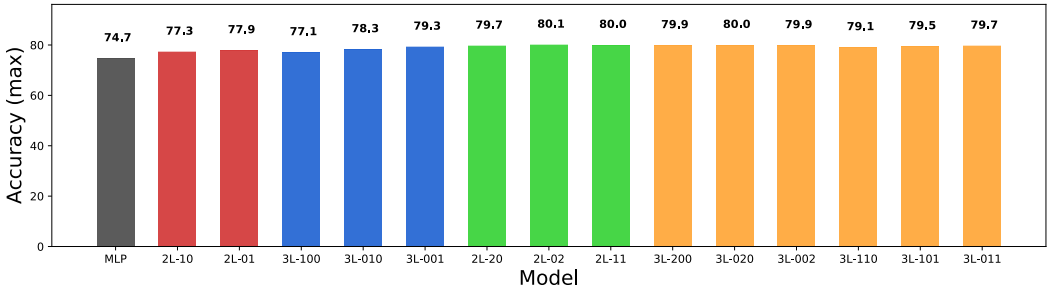
(c) CiteSeer.

Figure 7: Averaged accuracy (percentage) over 50 trials for various networks. A network with k layers and $j_1, \ldots, j_k$ convolutions in each of the layers is represented by the label kL-$j_1 \ldots j_k$.

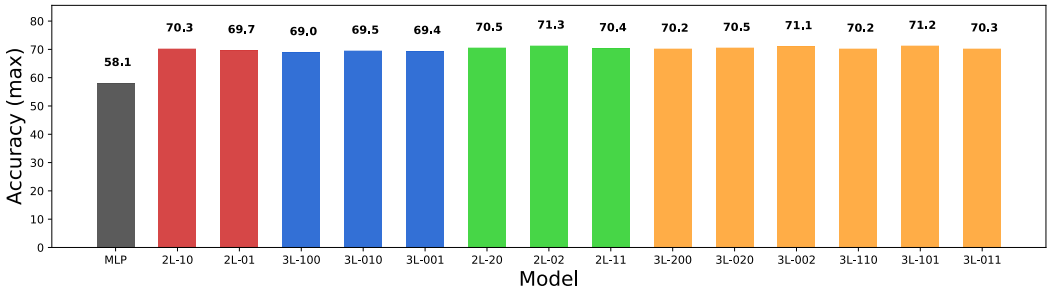
that networks with a graph convolution perform better than a simple MLP, and that two convolutions perform better than a single convolution. Furthermore, three graph convolutions do not have a significant advantage over two graph convolutions. This observation agrees with Lemma A.3, where one can compute $\rho(2)$ and $\rho(3)$ and realize that they are of the same order in n, i.e., the variance reduction offered by two graph convolutions is of the same order as three graph convolutions for sufficiently dense graphs. We present the results of these experiments in Fig. 10.



(a) CORA.

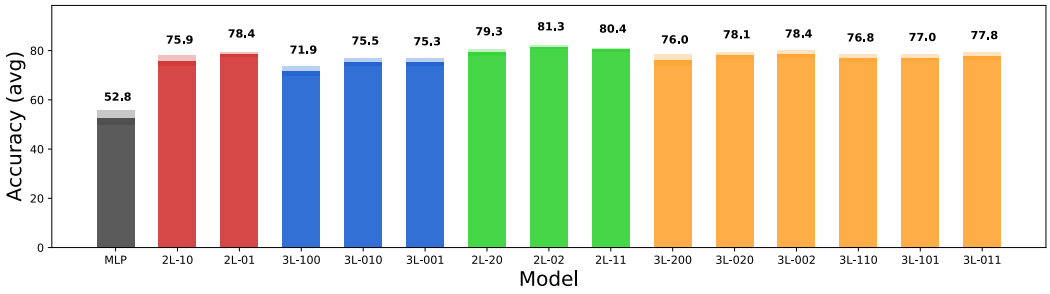


(b) Pubmed.

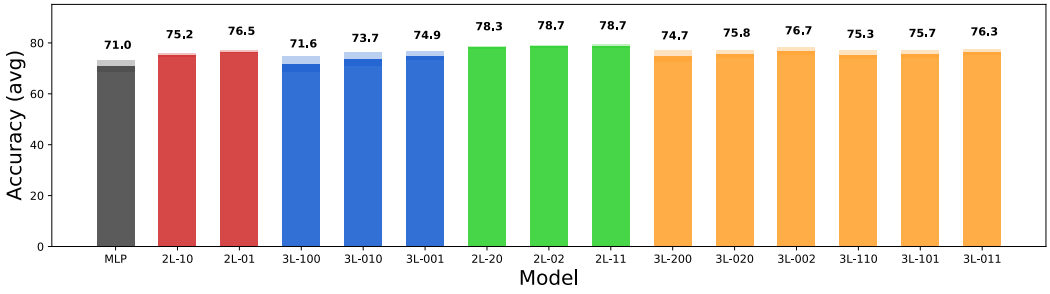


(c) CiteSeer.

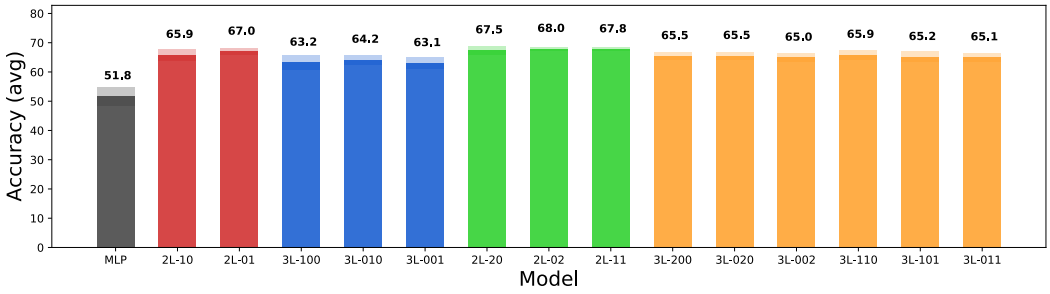
Figure 8: Maximum accuracy (percentage) over 50 trials for various networks with the original GCN normalization $\mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}$. A network with k layers and $j_1, \ldots, j_k$ convolutions in each of the layers is represented by the label kL-$j_1 \ldots j_k$.



(a) CORA.

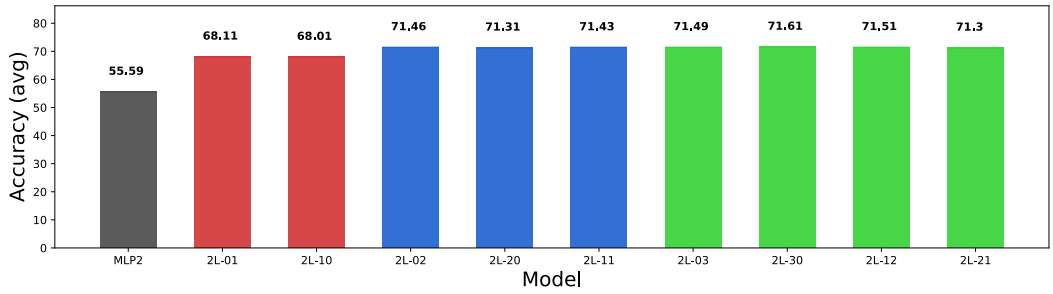


(b) Pubmed.

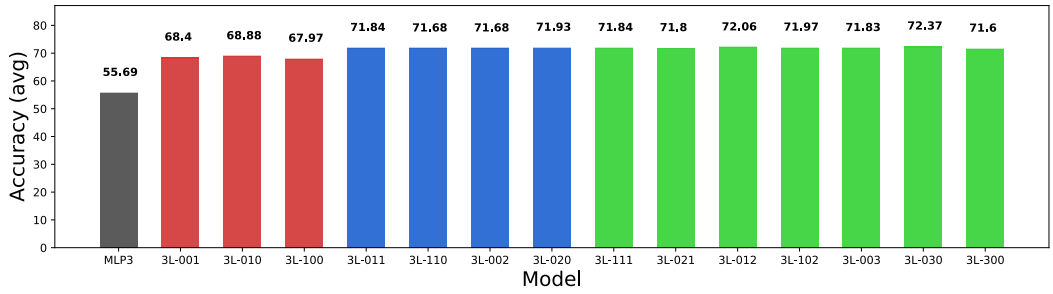


(c) CiteSeer.

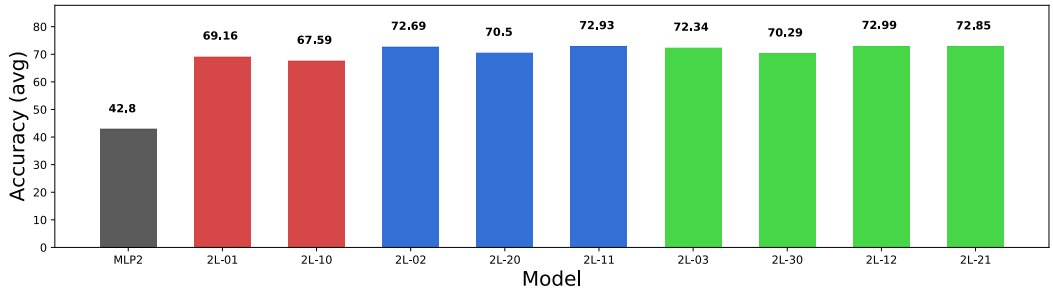
Figure 9: Averaged accuracy (percentage) over 50 trials for various networks with the original GCN normalization $\mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}$. A network with k layers and $j_1, \ldots, j_k$ convolutions in each of the layers is represented by the label kL-$j_1 \ldots j_k$.



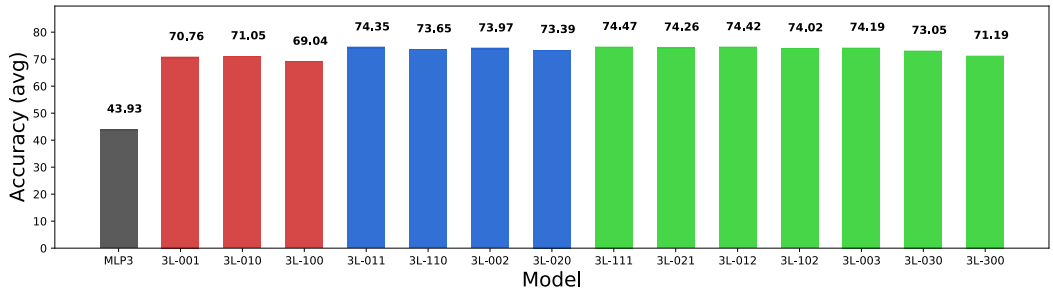
(a) OGBN-arXiv with two-layer networks.



(b) OGBN-arXiv with three-layer networks.



(c) OGBN-products with two-layer networks.



(d) OGBN-products with three-layer networks.

Figure 10: Averaged accuracy (percentage) for OGB datasets arXiv and products, over 10 trials for various networks. A network with k layers and $j_1, \ldots, j_k$ convolutions in each of the layers is represented by the label kL-$j_1 \ldots j_k$, while MLP3 denotes a three-layer MLP. Note that all models with one GC (in red) perform mutually similarly, while models with two GCs (in blue) and three GCs (in green) perform mutually similarly and better than models with one GC.