Information Theoretic Sample Complexity Lower Bound for
Feed-Forward Fully-Connected Deep Networks

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Abstract

In this paper, we study the sample complexity lower bound of a \(d\)-layer feed-forward, fully-connected neural network for binary classification, using information-theoretic tools. Specifically, we propose a backward data generating process, where the input is generated based on the binary output, and the network is parametrized by weight parameters for the hidden layers. The sample complexity lower bound is of order \(\Omega(\log(r) + p/(rd))\), where \(p\) is the dimension of the input, \(r\) is the rank of the weight matrices, and \(d\) is the number of hidden layers. To the best of our knowledge, our result is the first information theoretic sample complexity lower bound.

1 Introduction

Motivation. There has been an abundance of studies on the generalization upper bound on fully-connected, feed-forward neural networks. Various methods have been applied to obtain generalization and error probability upper bounds, including shattering coefficients [1], margin-based bounds [2], PAC-Bayes methods [3] and Rademacher complexity [4], among others. With further assumptions, there have also been less size-dependent upper bounds [5]. Regardless, one factor common in these upper bounds is the product of norms of parameter matrices, \(\prod_{j=1}^{d} \|W_j\|\) where \(\| \cdot \|\) is some matrix norm (e.g. Frobenius norm, spectral norm, (2,1)-norm) and \(W_j\)'s are the parameter matrices of for each layer in the network.

One interesting behavior of deep learning is that over-parametrized networks seem to generalize well, yet it is not well understood which sample size makes an over-parametrized network perform well and which does not. To the best of our knowledge, there is no sample complexity lower bound yet, and in this paper we provide such a bound with information-theoretic tools.

Contribution. In this paper, we consider a backward data generating process, where the output, binary labels, are first generated, and then the input is generated conditioned on the output and intermediate hidden layers. Moreover, we consider a setup where the parameter matrices are permutation matrices of low rank, and we show that \(\Omega(\log(r) + p/(r \cdot d))\) samples are necessary, where \(p\) is the dimension of input, \(r\) is the rank of the parameter matrices, and \(d\) is the number of hidden layers in the deep network.

The paper is organized as follows: we introduce our neural network setup and the backward data generating process in Section 2, provide the proof of our sample complexity lower bound in Section 3 and compare existing upper bounds with our lower bound in Section 4.
2 Model

In this section we describe our $d$-layer deep network and the backward data generating process, on which our analysis of sample complexity is based.

2.1 Preliminaries

Consider a fully-connected feed-forward neural network with $d$ hidden layers. A common representation is

$$x \mapsto w_{d+1} \sigma(W_d \sigma(W_{d-1} \cdots \sigma(W_1 x)))$$

where $x \in \mathbb{R}^p$, $\sigma$ is some activation function possibly applied elementwise, $W_1, W_2, \cdots W_d$ are matrices parametrizing the hidden layers, and $w_{d+1}$ is a parameter vector.

We focus on the binary classification setting, where each input $x_i$ is associated with a label, $y_i \in \{-1, +1\}$, and the data set $S = \{(x_i, y_i)\}_{i=1}^n$ contains $n$ i.i.d. samples. For the common representation introduced above, there is a Markov chain from input $x$ to output $y$, formally described as:

$$x \mapsto \sigma(W_1 x) \mapsto \cdots \mapsto W_d \sigma(W_{d-1} \cdots \sigma(W_1 x)) \mapsto w_{d+1} \sigma(W_d \sigma(W_{d-1} \cdots \sigma(W_1 x))) \mapsto y$$

Our argument will build on this Markov chain, but we will consider the reverse of this Markov chain, and utilize the symmetry of the mutual information between $x$ and $y$ when the parameter $W$ is given.

2.2 Backward data generation

Next we propose a backward data generating process, where the input $x$ is generated based on the label $y$ and some other parameters $\tilde{W}$ different from the parameters $W$ above. Our information-theoretic result relies on the construction of a restricted class of functions. The use of restricted ensembles is customary for information-theoretic lower bounds ([10, 13, 11]). Specifically,

$$y \sim \text{Unif}\{-1, +1\}$$
$$z_0 | y \sim N(y w_0, \text{covar} = \sigma^2 I_{n_0}), \tilde{w}_0 \in \mathbb{R}^{n_0}$$
$$z_1 | z_0 \sim N(\tilde{W}_1 z_0, \text{covar} = \sigma^2 I_{n_1}), \tilde{W}_1 \in \mathbb{R}^{n_1 \times n_0}$$
$$z_2 | z_1 \sim N(\tilde{W}_2 z_1, \text{covar} = \sigma^2 I_{n_2}), \tilde{W}_2 \in \mathbb{R}^{n_2 \times n_1}$$
$$\cdots$$
$$x := z_d | z_{d-1} \sim N(\tilde{W}_d z_{d-1}, \text{covar} = \sigma^2 I_{n_d} = \sigma^2 I_p), \tilde{W}_d \in \mathbb{R}^{n_d \times n_{d-1}} = \mathbb{R}^{p \times n_{d-1}}$$

The above defines a Markov chain from label $y$ to output $x$, formally described as:

$$y \mapsto z_0 \mapsto z_1 \mapsto \cdots \mapsto z_{d-1} \mapsto z_d =: x$$

The parameters characterizing this data generating process are a collection of weight matrices and vector $\tilde{W} := (\tilde{w}_0, \tilde{W}_1, \cdots, \tilde{W}_d)$. The above describes a deep network with identity activation function. We will show that the sample complexity lower bound of this network holds for a larger
class of deep networks with the same parameter space and any activation function. That is, if learning with the identity activation function is difficult, then learning with any activation is harder.

One thing to note is that the dimension of $\tilde{W}_i$ is different from that of $W_i$ for $i \in \{1, 2, \cdots, d\}$. In fact, there is also no guarantee that $\tilde{W}_i$ will be the (pseudo-)inverse of $W_i$. The hypothesis class of the network defined in (3) is different from that in (1). However, we will show that learning the network in (3) is as hard as learning the network in (1) using information theoretic tools.

## 3 Results

In this section we present our sample complexity lower bound. In order to achieve this, we first prove claims about the joint distribution of $(z_0, z_1, z_2, \cdots, z_d)|y; \tilde{W}$, the marginal distribution of $z_d|y; \tilde{W}$, and some KL divergence upper bounds which we will use for our sample complexity lower bound. We discuss three cases: the 1-layer network, the 2-layer network, and the general $d$-layer network. Each case depends on the previous case, and we will employ a recursive argument for the general $d$-layer network.

### 3.1 One hidden layer

We first consider a 1-layer model, which is described below:

$$y \sim \text{Unif}\{-1, +1\}$$

$$z_0|y \sim N(y\tilde{w}_0, \text{covar} = \sigma^2 I_{n_0}), \tilde{w}_0 \in \mathbb{R}^{n_0}$$

$$x := z_1|z_0 \sim N(\tilde{W}_1 z_0, \text{covar} = \sigma^2 I_{n_1} = \sigma^2 I_p), \tilde{W}_1 \in \mathbb{R}^{n_1 \times n_0} = \mathbb{R}^{p \times n_0}$$

(5)

Here we first find the joint distribution of $(z_0, z_1)|y$ and then show an upper bound on the KL divergence of interest. These results for the 1-layer network will be a building block for our analysis of the 2-hidden layer network. We use $x$ and $z_1$ interchangeably in this subsection.

We first find the joint distribution of $(z_0, z_1)|y; \tilde{W}$.

**Lemma 3.1.** The random variable $(z_0, z_1)|y; \tilde{W}$ is normally distributed with mean $(y\tilde{w}_0, y\tilde{W}_1\tilde{w}_0)$ and covariance matrix

$$
\begin{bmatrix}
\tilde{\Sigma}_0 + \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1 & -(\tilde{\Sigma}_1 \tilde{W}_1)^\top \\
-(\tilde{\Sigma}_1 \tilde{W}_1) & \tilde{\Sigma}_1
\end{bmatrix}^{-1}
$$

where $\tilde{\Sigma}_i = (\sigma^2 I_{n_i})^{-1}$ is the precision matrix of $z_i$ as defined in (3). (Detailed proofs can be found in Appendix A)

Now based on Lemma 3.1, we give an upper bound on the KL divergence between the distribution of $(z_1, y); \tilde{W}$ and a prior distribution, where $\tilde{W} = (\tilde{w}_0, \tilde{W}_1, \tilde{W}_2)$. This upper bound of the KL divergence sheds light on the analysis for networks with more layers.

**Lemma 3.2.** Let $\mathbb{P}_{(z_1, y)|\tilde{W}}$ be the joint distribution of $(z_1, y)$ parametrized by $\tilde{W}$, then we have

$$\text{KL}(\mathbb{P}_{(z_1, y)|\tilde{W}}||Q) \leq \frac{1}{2} \left[ \frac{\sigma^2}{\tau} \sum_i (1 + d_{i, i}) + \frac{1}{\tau} \|	ilde{W}_1 \tilde{w}_0\|^2 + n_1 \ln \left( \frac{\tau^2}{\sigma^2} \right) - n_1 \right]$$

where $Q = N(0, \tau^2 I_{n_1}) \times \text{Unif}\{-1, +1\}$ is a prior distribution, $\tau$ is a fixed constant, and $\text{diag}(d_{i, i})$ is the diagonal matrix of singular values in the decomposition of $\tilde{W}_1$.  


3.2 Two hidden layers

Now we consider a neural network with the same backward data generating process with 2 hidden layers:

\[
y \sim \text{Unif}\{-1, +1\}
\]

\[
z_0 | y \sim N(y\tilde{w}_0, \text{covar} = \sigma^2 I_{n_0}), \tilde{w}_0 \in \mathbb{R}^{n_0}
\]

\[
z_1 | z_0 \sim N(\tilde{W}_1 z_0, \text{covar} = \sigma^2 I_{n_1}), \tilde{W}_1 \in \mathbb{R}^{n_1 \times n_0}
\]

\[
x := z_2 | z_1 \sim N(\tilde{W}_2 z_2, \text{covar} = \sigma^2 I_{n_2} = \sigma^2 I_p), \tilde{W}_2 \in \mathbb{R}^{n_2 \times n_1} = \mathbb{R}^{p \times n_1}
\]

where \(\sigma\) is a constant. We will use \(z_2\) and \(x\) interchangeably, and such definition of \(x\) helps us present the arguments. We will also use \(n_2\) and \(p\) interchangeably.

In this section we have similar analysis for the entire network. We first generalize the technique in Lemma 3.1 to \((z_0, z_1, x)|y\).

**Lemma 3.3** (Joint distribution of \((z_0, z_1, x)|y; (\tilde{w}_0, \tilde{W}_1, \tilde{W}_2))
. The random variable \((z_0, z_1, x)|y; (\tilde{w}_0, \tilde{W}_1, \tilde{W}_2)\) is normally distributed with mean \((y\tilde{w}_0, y\tilde{W}_1\tilde{w}_0, y\tilde{W}_2\tilde{w}_0)\) and covariance matrix

\[
\begin{bmatrix}
\Sigma_0 + \tilde{W}_1^\top \Sigma_1 \tilde{W}_1 & - (\Sigma_1 \tilde{W}_1)^\top & 0 \\
-(\Sigma_1 \tilde{W}_1) & \tilde{\Sigma}_1 + \tilde{W}_2^\top \tilde{\Sigma}_2 \tilde{W}_2 & -(\tilde{\Sigma}_2 \tilde{W}_2)^\top \\
0 & -(\tilde{\Sigma}_2 \tilde{W}_2) & \tilde{\Sigma}_2
\end{bmatrix}^{-1}
\]

where \(\tilde{\Sigma}_i := (\sigma^2 I_{n_i})^{-1}\).

Next we find the marginal distribution of \(z_2|y; \tilde{W}\).

**Lemma 3.4** (Marginal Distribution of \(z_2|y; (\tilde{w}_0, \tilde{W}_1, \tilde{W}_2))
. The random variable \(x|y; (\tilde{w}_0, \tilde{W}_1, \tilde{W}_2)\) is normally distributed with mean \(y\tilde{W}_2\tilde{w}_0\) and covariance matrix

\[
\sigma^2 \left[ I_p - \tilde{W}_2 \left( I_{n_1} + \tilde{W}_1^\top \tilde{W}_2 \right) - \tilde{W}_1 (I_{n_0} + \tilde{W}_1^\top \tilde{W}_1)^{-1} \tilde{W}_1^\top \right]^{-1} \tilde{W}_2^\top
\]

Now that we have the marginal distribution of \((x|y; \tilde{W}) = (z_2|y; \tilde{W})\), we can again find an upper bound on the KL divergence.

**Lemma 3.5** (Upper bound on KL divergence between \((x, y); W\) and a prior distribution \(Q\)). We have that

\[
\text{KL}(P_{(x,y)}; \tilde{W})||Q) \leq \frac{1}{2} \left[ \frac{\sigma^2}{\tau^2} \left( p + \sum_{i=1}^{r} d_{2,i}^2 (1 + d_{1,i}^2) \right) + \frac{1}{\tau^2} \| \tilde{W}_2 \tilde{W}_1 \tilde{w}_0 \|^2 + p \ln \left( \frac{\tau^2}{\sigma^2} \right) - p \right]
\]

where \(Q \sim N(0, \tau^2 I_p) \times \text{Unif}\{-1, +1\}\) with \(\tau\) being a fixed constant, \(P_{(x,y)}; \tilde{W}\) is the joint distribution of \((x, y)\) when \(\tilde{W}\) is viewed as a parameter, \(\text{diag}(d_{1,i})\) is the diagonal matrix of the singular values in the decomposition of \(\tilde{W}_1\) with diagonal entries in decreasing order, \(d_{2,1}\) is the largest singular value of \(\tilde{W}_2\), and \(r = \text{rank}(\tilde{W}_1) = \text{rank}(\tilde{W}_2)\).

Below we list two lemmas regarding properties of a matrix key to the analysis of the KL divergence in Lemma 3.3. Moreover, Lemma 3.7 will be generalized later in the discussion of the general \(d\)-layer network.
Lemma 3.6. Let

\[
M_1 := \tilde{W}_1 \left( I_{n_0} + \tilde{W}_1^T \tilde{W}_1 \right)^{-1} \tilde{W}_1^T
\]
\[
M_2 := \tilde{W}_2 \left( I_{n_1} + \tilde{W}_2^T \tilde{W}_2 - M_1 \right)^{-1} \tilde{W}_2^T
\]

then \(M_2\) is positive semi-definite and has all eigenvalues strictly less than 1.

Lemma 3.7. For \(M_2\) defined in Lemma 3.6, let \(\lambda(M_2) = \{\lambda_i^\top(M_2) : i = 1, 2, \cdots, p\}\) be the set of eigenvalues of \(M_2\) in decreasing order, and \(\lambda(M_2)\) may contain zero. Then

\[
\text{Tr} \left( (I_p - M_2)^{-1} \right) = \sum_{i=1}^{p} \frac{1}{1 - \lambda_i^\top(M_2)} \leq p + \sum_{i=1}^{r} d_{2,i}^2 (1 + d_{1,1}^2)
\]

where \(r = \text{rank}(M_2)\), \(D_1 = \text{diag}(d_{1,i})\) is the diagonal matrix of singular values of the decomposition of \(\tilde{W}_1\), \(D_2 = \text{diag}(d_{2,i})\) is the diagonal matrix of singular values of the decomposition of \(\tilde{W}_2\), and the diagonal entries in both matrices are in decreasing order.

3.3 General \(d\) hidden layers

Now consider a general setting where the neural network has \(d\) hidden layers.

\[
y \sim \text{Unif}\{-1, +1\} \\
z_0 | y \sim N(y\tilde{w}_0, \text{covar} = \sigma^2 I_{n_0}), \tilde{w}_0 \in \mathbb{R}^{n_0} \\
z_1 | z_0 \sim N(\tilde{W}_1 z_0, \text{covar} = \sigma^2 I_{n_1}), \tilde{W}_1 \in \mathbb{R}^{n_1 \times n_0} \\
z_2 | z_1 \sim N(\tilde{W}_2 z_1, \text{covar} = \sigma^2 I_{n_2}), \tilde{W}_2 \in \mathbb{R}^{n_2 \times n_1} \\
\vdots \\
x := z_d | z_{d-1} \sim N(\tilde{W}_d z_{d-1}, \text{covar} = \sigma^2 I_{n_d} = \sigma^2 I_p), \tilde{W}_d \in \mathbb{R}^{n_d \times n_{d-1}} = \mathbb{R}^{p \times n_{d-1}}
\]

As shown above, the dimension of the "input" \(x\) is \(n_d\), and later we will use \(p\) and \(n_d\) interchangeably, as most readers are familiar with \(p\) being the dimension of the feature. We will also sometimes use \(\tilde{W}\) as a shorthand for \((\tilde{w}_0, \tilde{W}_1, \tilde{W}_2, \cdots, \tilde{W}_{d-1}, \tilde{W}_d)\). We will also use \(x\) and \(z_d\) interchangeably.

For the sake of simplicity, we consider the case where all \(\tilde{W}_i(i = 1, \cdots, d)\) have the same rank \(r\), i.e., \(\text{rank}(\tilde{W}_1) = \text{rank}(\tilde{W}_2) = \cdots = \text{rank}(\tilde{W}_d) = r\).

As done before, we first identify the joint distribution of \((z_0, z_1, z_2, \cdots, z_d) | y; \tilde{W}\), and then find the marginal distribution of \((z_d | y; \tilde{W}) = (x | y; \tilde{W})\).

Lemma 3.8. The joint distribution of \((z_0, z_1, z_2, \cdots, z_d) | y; (\tilde{w}_0, \tilde{W}_1, \tilde{W}_2, \cdots, \tilde{W}_{d-1}, \tilde{W}_d)\) is multivariate normal with mean \((y\tilde{w}_0, y\tilde{W}_1 \tilde{w}_0, \cdots, y\tilde{W}_{d-1} \tilde{w}_0, y\tilde{W}_d \tilde{w}_{d-1} \cdots \tilde{w}_1 \tilde{w}_0)\) and precision matrix \(\kappa^{(d)}\) of dimension \((\sum_{i=0}^{d} n_i) \times (\sum_{i=0}^{d} n_i)\) being a block matrix with \((d + 1) \times (d + 1)\) blocks. Let \(\kappa_{i,j}^{(d)}\) represent the \((i, j)\)-th block of \(\kappa^{(d)}\) \((0 \leq i, j \leq d)\), and let \(\Sigma_i := (\sigma^2 I_{n_i})^{-1}\) be the
precision matrix of $z_i$ as in \cite{10}, then $\kappa^{(d)}$ has tri-diagonal blocks and

\begin{align}
For 0 \leq i \leq d - 1: & \kappa_{i,i}^{(d)} = \tilde{\Sigma}_i + \tilde{W}_{i+1}^\top \tilde{\Sigma}_{i+1} \tilde{W}_{i+1}, \\
& \kappa_{i,i+1}^{(d)} = - (\tilde{\Sigma}_{i+1} \tilde{W}_{i+1})^\top \\
& \kappa_{i+1,i}^{(d)} = - (\tilde{\Sigma}_{i+1} \tilde{W}_{i+1}) \\
\end{align}

(11)

For $i = d : \kappa_{dd}^{(d)} = \tilde{\Sigma}_d$

For all other $i, j : \kappa_{i,j}^{(d)} = [0]_{n_i \times n_j}$

Then we find the marginal distribution of $(z_d | y; \tilde{W}) = (x | y; \tilde{W})$ with a recursively defined covariance matrix.

**Lemma 3.9** (Marginal distribution of $x | y; \tilde{W}$). $x | y; \tilde{W}$ is multivariate normal with mean $y \tilde{W}_d \tilde{W}_{d-1} \cdots \tilde{W}_2 \tilde{W}_1$ and covariance matrix $\sigma^2 (\mathbf{I}_p - M_d)^{-1}$, which has the following recursive definition:

\begin{align}
M_1 &= \tilde{W}_1 \left( \mathbf{I}_{n_0} + \tilde{W}_1^\top \tilde{W}_1 \right)^{-1} \tilde{W}_1^\top \\
M_2 &= \tilde{W}_2 \left( \mathbf{I}_{n_1} + \tilde{W}_2^\top \tilde{W}_2 - M_1 \right)^{-1} \tilde{W}_2^\top \\
\vdots \\
M_d &= \tilde{W}_d \left( \mathbf{I}_{n_{d-1}} + \tilde{W}_d^\top \tilde{W}_d - M_{d-1} \right)^{-1} \tilde{W}_d^\top \\
\end{align}

(12)

With the marginal distribution of $x | y; \tilde{W}$, and using the fact that the label $y \sim \text{Unif}\{-1, +1\}$ is first generated, we can find the distribution of $(x, y); \tilde{W}$ and then obtain an upper bound of the KL divergence between itself and a prior distribution $Q$. This upper bound will be used in our sample complexity lower bound.

**Lemma 3.10** (Upper bound on KL divergence between $(x, y); \tilde{W}$ and a prior distribution $Q$). We have that

\[
\text{KL}(p_{(x,y);\tilde{W}} || Q) \leq \frac{1}{2} \left[ \frac{\sigma^2}{\tau^2} \left( p + \sum_{i=1}^r m_{d,i} \right) + \frac{1}{\tau^2} \| \tilde{W}_d \tilde{W}_{d-1} \cdots \tilde{W}_1 \tilde{W}_0 \|^2_2 + p \ln \left( \frac{\tau^2}{\sigma^2} \right) - p \right]
\]

where $Q \sim N(0, \tau^2 \mathbf{I}_p) \times \text{Unif}\{-1, +1\}$ with $\tau$ being a fixed constant is a prior distribution, $p_{(x,y);\tilde{W}}$ is the joint distribution of $(x, y)$ when $\tilde{W} = (\tilde{W}_0, \tilde{W}_1, \tilde{W}_2, \cdots, \tilde{W}_{d-1}, \tilde{W}_d)$ is viewed as a parameter, $r = \text{rank}(\tilde{W}_1) = \cdots = \text{rank}(\tilde{W}_d)$, and $m_{d,i}$ is defined recursively as:

\begin{align}
m_{1,i} &= d_{1,i}^2 \\
m_{2,i} &= d_{2,i}^2 (m_{1,1} + 1) = d_{2,i}^2 (d_{1,1}^2 + 1) \\
m_{3,i} &= d_{3,i}^2 (m_{2,1} + 1) = d_{3,i}^2 (d_{2,1}^2 (d_{1,1}^2 + 1) + 1) \\
\vdots \\
m_{d,i} &= d_{d,i}^2 (m_{d-1,1} + 1)
\end{align}

(13)

where $d_{\ell,i}$ is the $i$-th largest singular value of $\tilde{W}_\ell$, $\ell \in \{1, 2, \cdots, d\}$. 

6
3.4 Covering number of the hypothesis class

In what follows we state all the assumptions we need for the covering number.

Assumption A1: The hypothesis class is \( \mathcal{F} = \mathcal{F}_d \times \cdots \times \mathcal{F}_1 \times \mathcal{F}_0 \). Let \( c \in (0, 1) \) be a constant to be determined, we define

\[
\forall i \in \{1, \cdots, d\}, \mathcal{F}_i := \left\{ \begin{bmatrix} R_i \ 0 \\ 0 \ cI_{p-r} \end{bmatrix} : R_i \in \{0, 1\}^r \text{ is any rank-}r \text{ permutation matrix on } \mathbb{R}^r, c \in (0, 1) \right\},
\]

\[
\mathcal{F}_0 := \left\{ \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \in \mathbb{R}^p : v_1 \in B_r \left(0, \frac{1}{\sqrt{2}}\right) \text{ at angular distance at least } \frac{\pi}{3} \text{ with each other, } v_2 \in \left\{ \pm \sqrt{\frac{1}{2(p-r)}} \right\}^{p-r} \right\},
\]

(14)

where \( B_r \left(0, \frac{1}{\sqrt{2}}\right) \) denotes the sphere centered at \( 0 \in \mathbb{R}^r \) with radius \( 1/\sqrt{2} \).

Assumption A2: \( \tau^2 = \sigma^2 \).

We first give an explicit construction of \( \mathcal{F} \) and then we show an upper bound on \( k = |\mathcal{F}| \) based on our construction.

It is easy to see that the size of \( \mathcal{F}_i \) for \( i \in \{1, \cdots, d\} \) is the number of \( r \)-permutations, meaning that

\[
|\mathcal{F}_d| = \cdots = |\mathcal{F}_1| = r!
\]

(15)

For \( \mathcal{F}_0 \), it is easy to see that the number of choices for \( v_1 \) is the same as the number of unit-length vectors that are at least \( \pi/3 \) angular distance apart with one another in \( \mathbb{R}^r \), which equals to \( K(r) \), where \( K(r) \) is defined as the maximum number of non-overlapping unit spheres that can touch a single unit sphere in dimension \( r \). The number of choices for \( v_2 \) is \( 2^{p-r} \). Therefore, \( |\mathcal{F}_0| = K(r) \cdot 2^{p-r} \).

By Equation (1) in [6],

\[
K(r) \geq (1 + o(1)) \sqrt{\frac{3\pi r}{8} \left( \frac{2}{\sqrt{3}} \right)^r}
\]

(16)

Combine (15) and (16), we get

\[
|\mathcal{F}| = |\mathcal{F}_d| \times \cdots \times |\mathcal{F}_1| \times |\mathcal{F}_0| \geq (r!)^d \cdot (1 + o(1)) \sqrt{\frac{3\pi r}{8} \left( \frac{2}{\sqrt{3}} \right)^r} \cdot 2^{p-r}
\]

(17)

Therefore, we conclude that the hypothesis class in assumption A1 fulfills

\[
\log |\mathcal{F}| \geq d \left( \sum_{i=1}^{r} \log(i) \right) + o(1) + \frac{1}{2} \left( \log \frac{3\pi}{8} + \log(r) \right) + r \log \frac{2}{\sqrt{3}} + (p-r) \log(2)
\]

(18)

Now we impose a third assumption on the value of \( c \in (0, 1) \) to further improve our KL divergence upper bound. The reason of such choice of \( c \) is given in the proof in the appendix.

Assumption A3: \( c = \frac{1}{p-r+1} \).

3.5 Sample complexity lower bound for the exact recovery of the network parameters

In this section we provide our sample complexity lower bound for the exact recovery of the network parameters. To show the sample complexity lower bound with Fano’s inequality, we need two more information theoretic results.
Lemma 3.11 (Upper bound on mutual information between parameters and $n$-sample). We have that

$$I(\hat{\mathbf{W}}; S) \leq nI(\hat{\mathbf{W}}; (x, y))$$

where $\hat{\mathbf{W}} = (\hat{W}_d, \cdots, \hat{W}_1, \hat{W}_0)$ are the parameters in (10), $S = ((x_1, y_1), \cdots, (x_n, y_n))$, $(x_i, y_i)|\hat{\mathbf{W}}$ are i.i.d. data points generated as in (10), and $(x_i, y_i)|\hat{\mathbf{W}} = (x, y)|\hat{\mathbf{W}}$.

Lemma 3.12 (Conditional mutual information is sum of weighted "conditional" mutual information). We have that

$$I(\hat{\mathbf{W}}; (x, y)) = \frac{1}{2}(I(\hat{\mathbf{W}}; x | y = -1) + I(\hat{\mathbf{W}}; x | y = +1))$$

where $I(\hat{\mathbf{W}}; x | y = -1)$ denotes the 'conditional' mutual information when $y$ is held fixed.

Now given the upper bounds on the KL divergence and the information theoretic results, we can utilize Fano's inequality to obtain a sample complexity lower bound.

Theorem 3.13 (Sample complexity lower bound of a $d$-layer network). Under assumptions $A1$, $A2$ and $A3$, for a $d$-layer network described in (10) with truth parameter $\hat{\mathbf{W}}^*$, and $\hat{\mathbf{W}} \in \mathcal{F}$ is a hypothesis recovered by any conceivable method, if $n \leq \frac{d \sum_{i=1}^{2d} \log(i)}{r^2 + \sigma^2}$

then $P(\hat{\mathbf{W}} \neq \hat{\mathbf{W}}^*) \geq \frac{1}{2}$, where $n$ is the sample size, $p$ is the dimension of input $x$, and $r$ is the rank of the parameter matrices.

From the above theorem, we can conclude that the sample complexity lower bound for the exact recovery of the network parameters is $n \in \Omega(\frac{d^2}{r^2} + \log(r))$.

3.6 Sample complexity lower bound for the expected risk

In order to transform the above bound into a risk bound, we consider the following definition of the expected risk,

$$R(\hat{\mathbf{W}}) = P_{(x, y) \in \mathcal{W}} \left[ y \cdot (\hat{W}_d \cdots \hat{W}_1 \hat{W}_0) \top \leq 0 \right]$$

where $\hat{\mathbf{W}} = (\hat{W}_d, \cdots, \hat{W}_1, \hat{W}_0)$ is any hypothesis in $\mathcal{F}$, and the truth is $\hat{\mathbf{W}}^* = (\hat{W}_d^*, \cdots, \hat{W}_1^*, \hat{W}_0^*)$, which implies the random variable $x|y; \hat{\mathbf{W}}^*$ is multivariate normal with mean $y \hat{W}_d \cdots \hat{W}_1 \hat{W}_0$ and covariance $\sigma^2 (I_p - M_d)^{-1}$.

For a more concise proof, let $\hat{\mathbf{w}} = \hat{W}_d \cdots \hat{W}_1 \hat{W}_0$ for any $\hat{\mathbf{W}} \in \mathcal{F}$.

Lemma 3.14 (Risk lower bound of a $d$-layer network). For a $d$-layer network as described in (10) with truth $\hat{\mathbf{W}}^*$, under assumptions $A1$, $A2$ and $A3$, if $\hat{\mathbf{W}} \neq \hat{\mathbf{W}}^*$, then

$$R(\hat{\mathbf{W}}) - R(\hat{\mathbf{W}}^*) \geq 1 \{ \hat{\mathbf{w}}^\top \hat{\mathbf{w}}^* \leq 0 \} \cdot \frac{1}{2} \cdot \text{erf} \left( \frac{1 + c^{2d}}{2 \sqrt{\sigma^2 ((d + 1) + \frac{c^{2d} - 1}{1 - c^2})}} \right)$$

where $c = \frac{1}{p^2 + r^2}$.

Aimed with the above lemma, similar to Lemma 3.13, we have
Theorem 3.15 (Sample complexity lower bound for the risk). Under assumptions \( A1 \), \( A2 \) and \( A3 \), for a \( d \)-layer network described in (10) with truth parameter \( \hat{W}^* \), and \( \hat{W} \in \mathcal{F} \) is a hypothesis recovered by any conceivable method, if

\[
n \leq \frac{d \left( \sum_{i=1}^{r} \log(i) \right) + o(1) + \frac{1}{2} \left( \log \frac{3p}{8} + \log(r) \right) + r \log \frac{2}{r} + (p - r) \log(2) - \log(4)}{r \cdot d + 1 + \frac{1}{\sigma^2}}
\]

then the expected risk fulfills

\[
P \left( R(\hat{W}) - R(\hat{W}^*) \geq 1 \{ \hat{w}^\top \hat{w}^* \leq 0 \} \cdot \frac{1}{2} \cdot \text{erf} \left( \frac{1 + c^{2d}}{2 \sqrt{\sigma^2 \left[ (d + 1) + \frac{c^{2d} - c^{2(d+1)}}{1-c^2} \right]} \right) \right) \geq \frac{1}{2}
\]

where \( n \) is the sample size, \( p \) is the dimension of input \( x \), \( r \) is the rank of the parameter matrices, and \( c = \frac{1}{p - r + 1} \).

4 Comparison with Existing Upper Bounds

We mainly compare with the four existing upper bounds, either on Rademacher complexity, or on generalization error. All those existing bounds are discussed based on the assumption that the input \( x \) is bounded, while our model has unbounded \( x \). Therefore we ignore all terms involving norm of \( x \) when comparing the bounds.

Theorem 1 in [9] gives an upper bound on the Rademacher complexity of a class of \( d \)-layer network with ReLU activation. Further imposing our assumption \( A1 \), which assumes the parameter matrices are permutation matrices of rank \( r \), the upper bound in Theorem 1 [9], ignoring \( \max_{i} \| x_i \|^2 \), becomes

\[
O \left( \frac{1}{n} \left( \left( \frac{1}{2} \right)^{2(d)} \min \{ 2, 4 \log(2 \cdot 2) \} \right) \right)
\]

which implies the sample size \( n \) must be of order \( \Omega(r^d) \) to have a decaying Rademacher complexity.

Theorem 1.1 in [2] gives an upper bound on the prediction error probability for a given \( d \)-layer network with ReLU activation. The upper bound in Theorem 1.1 in [2] includes a spectral density \( R_A \), where \( A \) is equivalent to \( \hat{W} \) in our analysis. Under our assumption this upper bound becomes

\[
O \left( \frac{R_A \ln(p) + \sqrt{1/\delta}}{n} \right)
\]

where \( R_A = \left( \prod_{i=1}^{d} \lambda_{\text{max}}(\hat{W}_i) \right) \cdot \left( \sum_{i=1}^{d} \left( \frac{\| \hat{W}_i \|^2_{2,1}}{\lambda_{\text{max}}(\hat{W}_i)} \right)^{2/3} \right)^{3/2} = r q^{\beta/2} \). Thus this upper bound says at least we need \( n \in \Omega(d^2 \cdot r \cdot \ln(p)) \) to have a decreasing error probability.

Theorem 1 in [8] gives an upper bound on the generalization error for a given \( d \)-layer network with ReLU activation. The upper bound holds with probability \( 1 - \delta \):

\[
O \left( \sqrt{d^2 p \ln(dp) \prod_{i=1}^{d} \frac{1}{\gamma^2} \sum_{i=1}^{d} \frac{r}{\gamma} + \ln \frac{dp}{\delta}} \right)
\]
which says at least we need $n \in \Omega \left( r^d p \ln(dp) \right)$ to have a decreasing error probability.

There has also been a size-independent upper bound on the Rademacher complexity, i.e., the width of the network, which is $p$ in our analysis, does not appear in the bound. Theorem 5 in [3] gives such a size-independent upper bound for a given $d$-layer network with ReLU activation.

\[
O \left( \left( \prod_{j=1}^{d} r^{1/2} \right) \cdot \min \left\{ \sqrt{\log \left( \frac{1}{\sqrt{n}} \prod_{j=1}^{d} r^{1/2} \right)}, \sqrt{\frac{d}{n}} \right\} \right) \tag{24}
\]

If the minimum evaluates to the first term, we need $n \in \Omega \left( r^{2d} \cdot d^2 (\log r)^2 \right)$ to have a decreasing Rademacher complexity. If the minimum evaluates to the second term, we need $n \in \Omega \left( r^d \cdot d \right)$.

Meanwhile, our sample complexity lower bound suggests that we need $n \in \Omega \left( \log(r) + p/(r \cdot d) \right)$. This is compatible with observation in practice, as the network tends to fit better with more layers ($d$) and higher rank ($r$), and if the network is deep enough, then the number of samples needed does not necessarily grow with dimension of input, $p$.

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Most of the supplementary material contains proofs of the lemmas and theorems in the main text.

A Detailed proofs

A.1 One hidden layer

A.1.1 Proof of Lemma 3.1

Proof. We just need to show that the exponent of the proposed distribution in the claim above matches the exponent in \( p(z_0|y; \tilde{W})p(z_1|z_0; \tilde{W}) \) and then check the positive-definiteness of the precision matrix.

\[
p(z_0, z_1|y) = p(z_0|y)p(z_1|z_0)
\]

\[
\propto \exp \left( -\frac{1}{2}(z_0 - y\tilde{w}_0)^\top \tilde{\Sigma}_0(z_0 - y\tilde{w}_0) \right) \exp \left( -\frac{1}{2}(z_1 - \tilde{W}_1 z_0)^\top \tilde{\Sigma}_1(z_1 - \tilde{W}_1 z_0) \right)
\]

(25)

and the exponent, ignoring the \(-1/2\) factor, becomes

\[
z_0^\top \tilde{\Sigma}_0 z_0 - 2z_0^\top \tilde{\Sigma}_0(y\tilde{w}_0) + (y\tilde{w}_0)^\top \tilde{\Sigma}_0(y\tilde{w}_0) + z_1^\top \tilde{\Sigma}_1 z_1 - 2z_1^\top \tilde{\Sigma}_1(\tilde{W}_1 z_0) + (\tilde{W}_1 z_0)^\top \tilde{\Sigma}_1(\tilde{W}_1 z_0)
\]

\[
= z_0^\top (\tilde{\Sigma}_0 + \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1) z_0 - 2y z_0^\top \tilde{\Sigma}_0 \tilde{w}_0 - 2y \tilde{w}_0^\top \tilde{\Sigma}_0 z_0 + \tilde{w}_0^\top \tilde{\Sigma}_0 \tilde{w}_0
\]

(26)

while the density of proposed distribution is proportional to the exponential of

\[
-\frac{1}{2} \begin{bmatrix} z_0 - y\tilde{w}_0 \\ z_1 - y\tilde{W}_1 \tilde{w}_0 \end{bmatrix}^\top \begin{bmatrix} \tilde{\Sigma}_0 + \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1 & -(\tilde{\Sigma}_1 \tilde{W}_1) \\ -(\tilde{\Sigma}_1 \tilde{W}_1) & \tilde{\Sigma}_1 \end{bmatrix} \begin{bmatrix} z_0 - y\tilde{w}_0 \\ z_1 - y\tilde{W}_1 \tilde{w}_0 \end{bmatrix}
\]

(27)

ignoring the factor of \(-1/2\). (27) evaluates to

\[
\begin{align*}
&\begin{bmatrix} z_0 - y\tilde{w}_0 \\ z_1 - y\tilde{W}_1 \tilde{w}_0 \end{bmatrix}^\top \begin{bmatrix} \tilde{\Sigma}_0 + \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1 & -(\tilde{\Sigma}_1 \tilde{W}_1) \\ -(\tilde{\Sigma}_1 \tilde{W}_1) & \tilde{\Sigma}_1 \end{bmatrix} \begin{bmatrix} z_0 - y\tilde{w}_0 \\ z_1 - y\tilde{W}_1 \tilde{w}_0 \end{bmatrix} \\
= & (z_0 - y\tilde{w}_0)^\top (\tilde{\Sigma}_0 + \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1)(z_0 - y\tilde{w}_0) - (z_0 - y\tilde{w}_0)^\top (\tilde{\Sigma}_1 \tilde{W}_1)(z_1 - y\tilde{W}_1 \tilde{w}_0) - (z_1 - y\tilde{W}_1 \tilde{w}_0)^\top (\tilde{\Sigma}_1 \tilde{W}_1)(z_0 - y\tilde{w}_0) - (z_1 - y\tilde{W}_1 \tilde{w}_0)^\top \tilde{\Sigma}_1(z_1 - y\tilde{W}_1 \tilde{w}_0) \\
= & [z_0^\top \tilde{\Sigma}_0 z_0 - 2z_0^\top \tilde{\Sigma}_0(y\tilde{w}_0) + (y\tilde{w}_0)^\top \tilde{\Sigma}_0(y\tilde{w}_0) + z_0^\top \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1 z_0 - 2z_0^\top \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1 y\tilde{w}_0 + 2y \tilde{w}_0^\top \tilde{\Sigma}_0 \tilde{w}_0 - 2y \tilde{w}_0^\top \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1 \tilde{w}_0 + 2y \tilde{w}_0^\top \tilde{\Sigma}_0 \tilde{w}_0] \\
+ & \tilde{w}_0^\top \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1 \tilde{w}_0 + [z_0^\top \tilde{\Sigma}_1 z_1 - 2yz_0^\top \tilde{\Sigma}_1 \tilde{W}_1 \tilde{w}_0 + \tilde{w}_0^\top \tilde{\Sigma}_0 \tilde{w}_0] \\
= & [z_0^\top (\tilde{\Sigma}_0 + \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1) z_0 + z_0^\top [-2y \tilde{\Sigma}_0 \tilde{w}_0 - 2y \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1 \tilde{w}_0 + 2y \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1 \tilde{w}_0] \\
+ & z_0^\top [-2 \tilde{W}_1^\top \tilde{\Sigma}_1] z_1 + z_0^\top [2y \tilde{\Sigma}_1 \tilde{W}_1 \tilde{w}_0 - 2y \tilde{\Sigma}_1 \tilde{W}_1 \tilde{w}_0] \\
+ & [\tilde{w}_0^\top \tilde{\Sigma}_0 \tilde{w}_0 + \tilde{w}_0^\top \tilde{\Sigma}_0 \tilde{w}_0 + \tilde{w}_0^\top \tilde{\Sigma}_0 \tilde{w}_0] \\
= & z_0^\top (\tilde{\Sigma}_0 + \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1) z_0 + z_0^\top [-2y \tilde{\Sigma}_0 \tilde{w}_0 + z_0^\top [-2 \tilde{W}_1^\top \tilde{\Sigma}_1] z_1 + \tilde{w}_0^\top \tilde{\Sigma}_0 \tilde{w}_0]
\end{align*}
\]

which is exactly same as in (26). Now we check the positive-definiteness of the precision matrix

\[
\begin{bmatrix} \tilde{\Sigma}_0 + \tilde{W}_1^\top \tilde{\Sigma}_1 \tilde{W}_1 & -(\tilde{\Sigma}_1 \tilde{W}_1) \\ -(\tilde{\Sigma}_1 \tilde{W}_1) & \tilde{\Sigma}_1 \end{bmatrix}
\]

in the claim. Note \( \tilde{\Sigma}_0 \) and \( \tilde{\Sigma}_1 \) are both positive-definite, as they
are precision matrices of normal distribution. Consider any vector $x \neq 0$ and write $x = (x_0, x_1)$ where $x_0 \in \mathbb{R}^{n_0}$ and $x_1 \in \mathbb{R}^{n_1}$, then

$$
\begin{bmatrix}
  x_0^T \\
  x_1^T
\end{bmatrix}
\begin{bmatrix}
  \Sigma_0 + \tilde{W}_1^T \tilde{\Sigma}_1 \tilde{W}_1 & - (\tilde{\Sigma}_1 \tilde{W}_1)^T \\
  -(\tilde{\Sigma}_1 \tilde{W}_1) & \Sigma_1
\end{bmatrix}
\begin{bmatrix}
  x_0 \\
  x_1
\end{bmatrix}
= x_0^T \Sigma_0 x_0 + x_1^T \tilde{W}_1^T \tilde{\Sigma}_1 \tilde{W}_1 x_0 - 2x_0^T \tilde{\Sigma}_1 \tilde{W}_1 x_1 + x_1^T \tilde{\Sigma}_1 x_1 
$$

$$
= \|\Sigma_0^{1/2} x_0\|^2 + \|\tilde{\Sigma}_1^{1/2} \tilde{W}_1 x_0\|^2 + \|\tilde{\Sigma}_1^{1/2} x_1\|^2 - 2 \tilde{\Sigma}_1 \tilde{W}_1 x_0 x_1 
$$

$$
\geq \|\Sigma_0^{1/2} x_0\|^2 + \|\tilde{\Sigma}_1^{1/2} \tilde{W}_1 x_0\|^2 + \|\tilde{\Sigma}_1^{1/2} x_1\|^2 - 2 \tilde{\Sigma}_1 \tilde{W}_1 x_0 \tilde{\Sigma}_1 \tilde{W}_1 x_1 
$$

$$
= \|\Sigma_0^{1/2} x_0\|^2 + \|\tilde{\Sigma}_1^{1/2} \tilde{W}_1 \tilde{\Sigma}_1 x_1\|^2
$$

by the Cauchy-Schwarz inequality. It is easy to see that there are two cases: either $x_0 = 0$ or not. If $x_0 \neq 0$, then the RHS of (29) is positive. Otherwise, if $x_0 = 0$, then from (29) before the Cauchy-Schwarz inequality is applied, we can see

$$
\begin{bmatrix}
  0 \\
  x_1^T
\end{bmatrix}
\begin{bmatrix}
  \Sigma_0 + \tilde{W}_1^T \tilde{\Sigma}_1 \tilde{W}_1 & - (\tilde{\Sigma}_1 \tilde{W}_1)^T \\
  -(\tilde{\Sigma}_1 \tilde{W}_1) & \Sigma_1
\end{bmatrix}
\begin{bmatrix}
  0 \\
  x_1
\end{bmatrix}
= x_1^T \tilde{\Sigma}_1 x_1 
$$

which is zero iff $x_1 = 0$ as well. Therefore we conclude the precision matrix is indeed positive definite.

A.1.2 Proof of Lemma 3.2

Proof. By Lemma 3.1 taking the inverse of the precision matrix, we know

$$
Cov(z_0, z_1 | y) = \left[ \begin{array}{cc}
\tilde{\Sigma}_0 + \tilde{W}_1^T \tilde{\Sigma}_1 \tilde{W}_1 & - (\tilde{\Sigma}_1 \tilde{W}_1)^T \\
-(\tilde{\Sigma}_1 \tilde{W}_1) & \Sigma_1
\end{array} \right]^{-1}
$$

where $\tilde{\Sigma}_0 = (\sigma^2 I_{n_0})^{-1}$ and $\tilde{\Sigma}_1 = (\sigma^2 I_{n_1})^{-1}$. By the block matrix inversion formula,

$$
Cov(z_1 | y) = (\Sigma_1 - (\Sigma_1 \tilde{W}_1) (\tilde{\Sigma}_0 + \tilde{W}_1^T \tilde{\Sigma}_1 \tilde{W}_1)^{-1} (\tilde{\Sigma}_1 \tilde{W}_1)^T - 1 (\tilde{\Sigma}_1 \tilde{W}_1)^T)^{-1}
$$

Denote the density of $Q$ by $q(z, y)$, and denote the density of $P(z_1, y) \| W$ by $p(z, y)$. Also denote the marginal distribution of $z$ under $Q$ and $P(z_1, y) \| W$ by $q(\cdot)$ and $p(\cdot)$, respectively. Note $q(z)$ is density of $N(0, \tau^2 I_{n_1})$, and $q(y)$ and $p(y)$ are both $1/2$ for $y \in \{-1, +1\}$. The KL divergence between $P(z_1, y) \| W$ and $Q$ is

$$
KL(P(z_1, y) \| W || Q) = \sum_{y \in \{-1, +1\}} \int p(z, y) \log \frac{p(z, y)}{q(z, y)} dz
$$

$$
= \sum_{y \in \{-1, +1\}} \int p(z | y) p(y) \log \frac{p(z | y) p(y)}{q(z | y) q(y)} dz
$$

$$
= \frac{1}{2} \int p(z | y = -1) \log \frac{p(z | y = -1)}{q(z)} dz + \frac{1}{2} \int p(z | y = +1) \log \frac{p(z | y = +1)}{q(z)} dz
$$

$$
= \frac{1}{2} KL(P(z_1 | y = -1) \| W || N(0, \tau^2 I_{n_1})) + \frac{1}{2} KL(P(z_1 | y = +1) \| W || N(0, \tau^2 I_{n_1}))
$$

(33)
Note $P(z_1|y=-1; \tilde{w})$ is a normal distribution with mean $-\tilde{W}_1\tilde{w}_0$ and covariance $\left(\Sigma_1 - (\Sigma_1 \tilde{w}_1)(\Sigma_0 + \tilde{w}_1^T \Sigma_1 \tilde{w}_1)^{-1}(\Sigma_1 \tilde{w}_1)^T\right)$. Thus

$$
\mathbb{KL}(P(z_1|y=-1; \tilde{w})|N(0, \tau^2 I_{n_1})) = \frac{1}{2} \text{Tr} \left[ (\tau^2 I_{n_1})^{-1} (\Sigma_1 - (\Sigma_1 \tilde{w}_1)(\Sigma_0 + \tilde{w}_1^T \Sigma_1 \tilde{w}_1)^{-1}(\Sigma_1 \tilde{w}_1)^T)^{-1} \right]
+ \frac{1}{2} \left( -\tilde{W}_1\tilde{w}_0 - 0 \right)^T (\tau^2 I_{n_1})^{-1} (-\tilde{W}_1\tilde{w}_0 - 0)
+ \frac{1}{2} \ln \left( \frac{\det(\tau^2 I_{n_1})}{\det((\Sigma_1 - (\Sigma_1 \tilde{w}_1)(\Sigma_0 \tilde{w}_1^T \Sigma_1 \tilde{w}_1)^{-1}(\Sigma_1 \tilde{w}_1)^T)^{-1})} \right) - \frac{n_1}{2}
$$

(34)

Recall $\tilde{\Sigma}_0 = (\sigma^2 I_{n_0})^{-1}$ and $\tilde{\Sigma}_1 = (\sigma^2 I_{n_1})^{-1}$. Thus

$$
I = \frac{1}{\tau^2} \text{Tr} \left[ (\tilde{\Sigma}_1 - (\tilde{\Sigma}_1 \tilde{w}_1)(\tilde{\Sigma}_0 + \tilde{w}_1^T \tilde{\Sigma}_1 \tilde{w}_1)^{-1}(\tilde{\Sigma}_1 \tilde{w}_1)^T)^{-1} \right]
= \frac{\sigma^2}{\tau^2} \text{Tr} \left[ (I_{n_1} - \tilde{W}_1(I_{n_0} + \tilde{w}_1^T \tilde{w}_1)^{-1}\tilde{w}_1^T)^{-1} \right]
= \frac{\sigma^2}{\tau^2} \sum_{i=1}^{n_1} \lambda_i \left( (I_{n_1} - \tilde{W}_1(I_{n_0} + \tilde{w}_1^T \tilde{w}_1)^{-1}\tilde{w}_1^T)^{-1} \right)^{-1}
$$

(35)

where $\lambda_i(\cdot)$ denotes the $i$-th largest eigenvalue of a matrix.

It is known that the eigenvalues of $(I - A)^{-1}$ are $\{\frac{1}{1-\lambda_i(A)}\}$ for positive semi-definite matrix $A$ with eigenvalues less than 1. Thus we need to show that $\tilde{W}_1(I_{n_0} + \tilde{w}_1^T \tilde{w}_1)^{-1}\tilde{w}_1^T$ is positive semi-definite and has all eigenvalues less than 1. It is easy to see that $\tilde{W}_1(I_{n_0} + \tilde{w}_1^T \tilde{w}_1)^{-1}\tilde{w}_1^T$ is symmetric, thus it remains to show the eigenvalues are in $[0, 1)$.

It is also known that $\tilde{W}_1(I_{n_0} + \tilde{w}_1^T \tilde{w}_1)^{-1}\tilde{w}_1^T$ and $(I_{n_0} + \tilde{w}_1^T \tilde{w}_1)^{-1}\tilde{w}_1^T \tilde{w}_1^T$ have same eigenvalues. Suppose $\mu$ is an eigenvalue of $(I_{n_0} + \tilde{w}_1^T \tilde{w}_1)^{-1}\tilde{w}_1^T \tilde{w}_1$ with corresponding eigenvector $x \in \mathbb{R}^{n_0} \setminus \{0\}$. Thus

$$
(I_{n_0} + \tilde{w}_1^T \tilde{w}_1)^{-1}\tilde{w}_1^T \tilde{w}_1 x = \mu x
\tilde{w}_1^T \tilde{w}_1 x = \mu (I_{n_0} + \tilde{w}_1^T \tilde{w}_1) x
\tilde{w}_1^T \tilde{w}_1 x = \mu x^T (I_{n_0} + \tilde{w}_1^T \tilde{w}_1) x
\mu = \frac{\|\tilde{w}_1 x\|^2}{\|x\|^2 + \|\tilde{w}_1 x\|^2} \in [0, 1)
$$

(36)

Consider the singular value decomposition of $\tilde{W}_1 = U_1 D_1 V_1^T$, where $U_1 \in \mathbb{R}^{n_1 \times n_1}$ is orthonor-
mal, $D_1 = \text{diag}(d_{1,i}) \in \mathbb{R}^{n_1 \times n_0}$ and $V_1 \in \mathbb{R}^{n_0 \times n_0}$ is orthonormal. Then

$$\lambda \left( \tilde{W}_1 (I_{n_0} + \tilde{W}_1^T \tilde{W}_1)^{-1} \tilde{W}_1^T \right) = \lambda \left( U_1 D_1 V_1^T (V_1 V_1^T + V_1 D_1^T U_1^T U_1 D_1 V_1^T)^{-1} V_1 D_1^T U_1^T \right)$$

$$= \lambda \left( U_1 D_1 (I_{n_0} + D_1^T D_1)^{-1} D_1^T U_1^T \right)$$

$$= \lambda \left( D_1 (I_{n_0} + D_1^T D_1)^{-1} D_1^T \right)$$

$$= \left\{ \frac{d_{1,i}^2}{1 + d_{1,i}^2} \right\}$$

Therefore

$$I = \frac{\sigma^2}{\tau^2} \sum_{i=1}^{n_1} \lambda_i \left( \{I_{n_1} - \tilde{W}_1 (I_{n_0} + \tilde{W}_1^T \tilde{W}_1)^{-1} \tilde{W}_1^T \} \right)^{-1} = \frac{\sigma^2}{\tau^2} \sum_{i=1}^{n_1} \frac{1}{1 - \frac{d_{1,i}^2}{1 + d_{1,i}^2}} = \frac{\sigma^2}{\tau^2} \sum_{i=1}^{n_1} (1 + d_{1,i}^2) \quad (37)$$

It is easy to see that $II = \frac{1}{\tau^2} \| \tilde{W}_1 \tilde{w}_0 \|_2^2$. Furthermore, we have

$$III = \ln \left( \frac{\det(\tau^2 I_{n_1})}{\det \left( (\Sigma_1 - (\Sigma_1 \tilde{W}_1)(\Sigma_0 \tilde{W}_1^T \Sigma_1 \tilde{W}_1)^{-1} (\Sigma_1 \tilde{W}_1^T)^{-1} \right) \right)$$

$$= \ln \left( \frac{\tau^{2n_1}}{\det \left( \sigma^2 \{I_{n_1} - \tilde{W}_1 (I_{n_0} + \tilde{W}_1^T \tilde{W}_1)^{-1} \tilde{W}_1^T \} \right)^{-1} \right) \right)$$

$$= \ln \left( \frac{\tau^{2n_1}}{\det \left( \sigma^2 \prod_{i=1}^{n_1} \lambda_i \left( \{I_{n_1} - \tilde{W}_1 (I_{n_0} + \tilde{W}_1^T \tilde{W}_1)^{-1} \tilde{W}_1^T \} \right)^{-1} \right) \right)$$

$$= \ln \left( \frac{\tau^{2n_1}}{\sigma^{2n_1} \prod_{i=1}^{n_1} \lambda_i \left( \{I_{n_1} - \tilde{W}_1 (I_{n_0} + \tilde{W}_1^T \tilde{W}_1)^{-1} \tilde{W}_1^T \} \right)^{-1} \right) \right)$$

$$= \ln \left( \frac{\tau^{2n_1}}{\sigma^{2n_1} \prod_{i=1}^{n_1} (1 + d_{1,i}^2)} \right) \leq \ln \left( \frac{\tau^{2n_1}}{\sigma^{2n_1}} \right) = n_1 \ln \left( \frac{\tau^2}{\sigma^2} \right)$$

Thus $\mathbb{KL}(P_{(z_1|y=1)}; \tilde{W}|N(0, \tau^2 I_{n_1})) \leq \frac{1}{2} \left[ \frac{\sigma^2}{\tau^2} \sum_i 1 + d_{1,i}^2 + \frac{1}{\tau^2} \| \tilde{W}_1 \tilde{w}_0 \|_2^2 + n_1 \ln \left( \frac{\tau^2}{\sigma^2} \right) \right]$. Similar reasoning gives the same upper bound on $\mathbb{KL}(P_{(z_1|y=-1)}; \tilde{W}|N(0, \tau^2 I_{n_1}))$. □

### A.2 Two hidden layers

#### A.2.1 Proof of Lemma 3.3

**Proof.** Similarly, we want to check the exponent in $p(z_0, z_1, x|y) = p(z_0|y)p(z_1|z_0)p(x|z_1)$ matches that of the distribution stated in the claim.

The exponent of the density of the multivariate normal proposed in the lemma, ignoring the $-\frac{1}{2}$...
factor, is

\[
\begin{bmatrix}
    z_0 - y\hat{w}_0 \\
    z_1 - y\hat{W}_1\hat{w}_0 \\
    x - y\hat{W}_2\hat{W}_1\hat{w}_0
\end{bmatrix}^\top \begin{bmatrix}
    \hat{\Sigma}_0 + \hat{W}_1^\top \hat{\Sigma}_1 \hat{W}_1 & - (\hat{\Sigma}_1 \hat{W}_1)^\top & \mathbf{0} \\
    - (\hat{\Sigma}_1 \hat{W}_1) & \hat{\Sigma}_1 + \hat{W}_2^\top \hat{\Sigma}_2 \hat{W}_2 & - (\hat{\Sigma}_2 \hat{W}_2)^\top \\
    \mathbf{0} & - (\hat{\Sigma}_2 \hat{W}_2) & \hat{\Sigma}_2
\end{bmatrix} \begin{bmatrix}
    z_0 - y\hat{w}_0 \\
    z_1 - y\hat{W}_1\hat{w}_0 \\
    x - y\hat{W}_2\hat{W}_1\hat{w}_0
\end{bmatrix}
\]

\[
= \left\{ (z_0 - y\hat{w}_0)^\top \hat{\Sigma}_0 (z_0 - y\hat{w}_0) + (z_0 - y\hat{w}_0)^\top \hat{W}_1^\top \hat{\Sigma}_1 \hat{W}_1 (z_0 - y\hat{w}_0) \\
- (z_0 - y\hat{w}_0)^\top (\hat{\Sigma}_1 \hat{W}_1)^\top (z_1 - y\hat{W}_1\hat{w}_0) - (z_1 - y\hat{W}_1\hat{w}_0)^\top (\hat{\Sigma}_1 \hat{W}_1) (z_0 - y\hat{w}_0) \\
+ (z_1 - y\hat{W}_1\hat{w}_0)^\top \hat{\Sigma}_1 (z_1 - y\hat{W}_1\hat{w}_0) \right\}
- \left\{ (z_1 - y\hat{W}_1\hat{w}_0)^\top \hat{W}_2^\top \hat{\Sigma}_2 \hat{W}_2 (z_1 - y\hat{W}_1\hat{w}_0) - (z_1 - y\hat{W}_1\hat{w}_0)^\top (\hat{\Sigma}_2 \hat{W}_2)^\top (z_2 - y\hat{W}_2\hat{W}_1\hat{w}_0) \\
- (z_2 - y\hat{W}_2\hat{W}_1\hat{w}_0)^\top (\hat{\Sigma}_2 \hat{W}_2)^\top (z_1 - y\hat{W}_1\hat{w}_0) + (x - y\hat{W}_2\hat{W}_1\hat{w}_0)^\top \hat{\Sigma}_2 (z_2 - y\hat{W}_2\hat{W}_1\hat{w}_0) \right\}
\]

Note that the terms in the first pair of curly braces in (40) are identical to the part in the exponent of \( p(z_1, z_0|y) \) from Lemma 3.1.

This means when we compare the exponent of \( p(z_2, z_1, z_0|y) = p(z_1, z_0|y)p(z_2|z_1) \) with that of the proposed density, the terms in the first pair of curly braces will cancel out. Thus we only need to show the terms in the second pair of curly braces evaluate to \( p(z_2|z_1) \) in (47):

\[
(z_1 - y\hat{W}_1\hat{w}_0)^\top \hat{W}_2^\top \hat{\Sigma}_2 \hat{W}_2 (z_1 - y\hat{W}_1\hat{w}_0) - (z_1 - y\hat{W}_1\hat{w}_0)^\top (\hat{\Sigma}_2 \hat{W}_2)^\top (z_2 - y\hat{W}_2\hat{W}_1\hat{w}_0)
- (z_2 - y\hat{W}_2\hat{W}_1\hat{w}_0)^\top (\hat{\Sigma}_2 \hat{W}_2)(z_1 - y\hat{W}_1\hat{w}_0) + (x - y\hat{W}_2\hat{W}_1\hat{w}_0)^\top \hat{\Sigma}_2 (z_2 - y\hat{W}_2\hat{W}_1\hat{w}_0)
= \left( z_1^\top \hat{W}_2^\top \hat{\Sigma}_2 \hat{W}_2 z_1 - 2z_1^\top (y\hat{W}_2^\top \hat{\Sigma}_2 \hat{W}_2 \hat{W}_1\hat{w}_0) + \hat{w}_0^\top \hat{W}_1^\top \hat{W}_2^\top \hat{\Sigma}_2 \hat{W}_2 \hat{W}_1\hat{w}_0 \right)
+ \left( -z_1^\top \hat{W}_2^\top \hat{\Sigma}_2 z_2 + z_1^\top [y\hat{W}_2^\top \hat{\Sigma}_2 \hat{W}_2 \hat{W}_1\hat{w}_0] + y\hat{w}_0^\top \hat{W}_1^\top \hat{W}_2^\top \hat{\Sigma}_2 z_2 - \hat{w}_0^\top \hat{W}_1^\top \hat{W}_2^\top \hat{\Sigma}_2 \hat{W}_2 \hat{W}_1\hat{w}_0 \right)
+ \left( -z_2^\top \hat{\Sigma}_2 z_2 + z_2^\top [y\hat{\Sigma}_2 \hat{W}_2 \hat{W}_1\hat{w}_0] + y\hat{w}_0^\top \hat{W}_1^\top \hat{W}_2^\top \hat{\Sigma}_2 \hat{W}_2 z_1 - \hat{w}_0^\top \hat{W}_1^\top \hat{W}_2^\top \hat{\Sigma}_2 \hat{W}_2 \hat{W}_1\hat{w}_0 \right)
+ \left( z_2^\top \hat{\Sigma}_2 z_2 - 2yz_2^\top \hat{\Sigma}_2 \hat{W}_2 \hat{W}_1\hat{w}_0 + \hat{w}_0^\top \hat{W}_1^\top \hat{W}_2^\top \hat{\Sigma}_2 \hat{W}_2 \hat{W}_1\hat{w}_0 \right)
\]

which cancels out to \( (z_2 - \hat{W}_2 z_1)^\top \hat{\Sigma}_2 (z_2 - \hat{W}_2 z_1) \) and is indeed the exponent of the kernel density of \( z_2|z_1 \).

Now it remains to show the proposed covariance matrix is positive definite, which is equivalent to show that the inverse is positive definite. Consider any vector \( x \neq 0 \) and write \( x = (x_0, x_1, x_2) \)
where $x_0 \in \mathbb{R}^{n_0}$, $x_1 \in \mathbb{R}^{n_1}$ and $x_2 \in \mathbb{R}^{n_2}$, then,

$$
\begin{bmatrix}
  x_0 \\
  x_1 \\
  x_2 
\end{bmatrix}^T
\begin{bmatrix}
  \Sigma_0 + \tilde{W}_1^T \Sigma_1 \tilde{W}_1 & - (\tilde{\Sigma}_1 \tilde{W}_1)^T & 0 \\
  - (\tilde{\Sigma}_1 \tilde{W}_1) & \tilde{\Sigma}_1 + \tilde{W}_2^T \Sigma_2 \tilde{W}_2 & - (\tilde{\Sigma}_2 \tilde{W}_2)^T \\
  0 & - (\tilde{\Sigma}_2 \tilde{W}_2) & \tilde{\Sigma}_2 
\end{bmatrix}
\begin{bmatrix}
  x_0 \\
  x_1 \\
  x_2 
\end{bmatrix}
$$

$$= x_0^T (\Sigma_0 + \tilde{W}_1^T \Sigma_1 \tilde{W}_1) x_0 - x_0^T (\Sigma_1 \tilde{W}_1)^T x_1 - x_1^T (\Sigma_1 \tilde{W}_1) x_0 + x_1^T (\Sigma_1 + \tilde{W}_2^T \Sigma_2 \tilde{W}_2) x_1 \\
- x_1^T (\Sigma_2 \tilde{W}_2)^T x_2 - x_2^T (\tilde{\Sigma}_2 \tilde{W}_2) x_1 + x_2^T \tilde{\Sigma}_2 x_2
$$

$$= ||\Sigma_0^{1/2} x_0||^2_2 + ||\Sigma_1^{1/2} \tilde{W}_1 x_0||^2_2 - 2x_0^T \tilde{W}_1^T \Sigma_1 x_1 + ||\Sigma_1^{1/2} x_1||^2_2 + ||\Sigma_2^{1/2} \tilde{W}_2 x_1||^2_2 - 2x_1^T \tilde{W}_2^T \Sigma_2 x_2 + ||\Sigma_2^{1/2} x_2||^2_2
$$

$$\geq ||\Sigma_0^{1/2} x_0||^2_2 + \left(||\Sigma_1^{1/2} \tilde{W}_1 x_0||^2_2 - 2||\Sigma_1^{1/2} \tilde{W}_1 x_0||^2_2 ||\Sigma_1^{1/2} x_1||^2_2 + ||\Sigma_1^{1/2} x_1||^2_2\right) \\
+ \left(||\Sigma_2^{1/2} \tilde{W}_2 x_1||^2_2 - 2||\Sigma_2^{1/2} \tilde{W}_2 x_1||^2_2 ||\Sigma_2^{1/2} x_2||^2_2 + ||\Sigma_2^{1/2} x_2||^2_2\right)
$$

$$= ||\Sigma_1^{1/2} x_0||^2_2$$

(42)

which is positive if $x_0 \neq 0$. Otherwise, if $x_0 = 0$, then (42) evaluates to

$$
\begin{bmatrix}
  0 \\
  x_1 \\
  x_2
\end{bmatrix}^T
\begin{bmatrix}
  \Sigma_0 + \tilde{W}_1^T \Sigma_1 \tilde{W}_1 & - (\tilde{\Sigma}_1 \tilde{W}_1)^T & 0 \\
  - (\tilde{\Sigma}_1 \tilde{W}_1) & \tilde{\Sigma}_1 + \tilde{W}_2^T \Sigma_2 \tilde{W}_2 & - (\tilde{\Sigma}_2 \tilde{W}_2)^T \\
  0 & - (\tilde{\Sigma}_2 \tilde{W}_2) & \tilde{\Sigma}_2 
\end{bmatrix}
\begin{bmatrix}
  0 \\
  x_1 \\
  x_2
\end{bmatrix}
$$

$$= ||\Sigma_1^{1/2} x_1||^2_2 + ||\Sigma_2^{1/2} \tilde{W}_2 x_1||^2_2 - 2x_1^T \tilde{W}_2^T \Sigma_2 x_2 + ||\Sigma_2^{1/2} x_2||^2_2
$$

$$\geq ||\Sigma_1^{1/2} x_1||^2_2 + \left(||\Sigma_2^{1/2} \tilde{W}_2 x_1||^2_2 - 2||\Sigma_2^{1/2} \tilde{W}_2 x_1||^2_2 ||\Sigma_2^{1/2} x_2||^2_2 + ||\Sigma_2^{1/2} x_2||^2_2\right)
$$

which is positive if $x_1 \neq 0$. Otherwise, meaning that both $x_0$ and $x_1$ are 0, (42) would evaluate to

$$
\begin{bmatrix}
  0 \\
  0 \\
  x_2
\end{bmatrix}^T
\begin{bmatrix}
  \Sigma_0 + \tilde{W}_1^T \Sigma_1 \tilde{W}_1 & - (\tilde{\Sigma}_1 \tilde{W}_1)^T & 0 \\
  - (\tilde{\Sigma}_1 \tilde{W}_1) & \tilde{\Sigma}_1 + \tilde{W}_2^T \Sigma_2 \tilde{W}_2 & - (\tilde{\Sigma}_2 \tilde{W}_2)^T \\
  0 & - (\tilde{\Sigma}_2 \tilde{W}_2) & \tilde{\Sigma}_2 
\end{bmatrix}
\begin{bmatrix}
  0 \\
  0 \\
  x_2
\end{bmatrix} = ||\Sigma_2^{1/2} x_2||^2_2
$$

(44)

which is positive if $x_2 \neq 0$. Thus we showed that the quadratic form of the precision matrix is zero iff $x = (x_0, x_1, x_2) = 0$. Thus the proposed distribution of $(z_0, z_1, z_2)|y$ is a valid multivariate normal distribution.

\textbf{A.2.2 Proof of Lemma 3.4}

\textbf{Proof.} This follows from repeated application of block matrix inversion formula, which gives the covariance matrix of $x|y$. First recall the precision matrix of $(z_0, z_1, x)|y$ is a tri-diagonal matrix, and take the inverse of the precision matrix of $(z_0, z_1, x)|y$,

$$\text{Cov} \left( \begin{bmatrix} z_0 \\ z_1 \\ x \end{bmatrix} \mid y \right) = \left[ \begin{bmatrix} \tilde{\Sigma}_0 + \bar{W}_1^T \tilde{\Sigma}_1 \bar{W}_1 \\ - \tilde{\Sigma}_1 \bar{W}_1 \\ 0 \end{bmatrix} \begin{bmatrix} - \bar{W}_1 \tilde{\Sigma}_1 \bar{W}_1 \\ \tilde{\Sigma}_1 + \bar{W}_2^T \tilde{\Sigma}_2 \bar{W}_2 \\ - \bar{W}_2 \tilde{\Sigma}_2 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ - \bar{W}_2 \tilde{\Sigma}_2 \end{bmatrix} \right]^{-1}$$

$$= \begin{bmatrix} T & Z^T & Z \end{bmatrix}^{-1} \begin{bmatrix} S_1 & S_2 \\ S_2 & S_3 \end{bmatrix}$$

(45)

17
where \( T = \begin{bmatrix} \tilde{\Sigma} + \tilde{W}_1^\top \tilde{\Sigma} \tilde{W}_1 & - (\tilde{\Sigma}_1 \tilde{W}_1)^	op \\ - (\tilde{\Sigma}_1 \tilde{W}_1) & \Sigma + \tilde{W}_2^\top \Sigma \tilde{W}_2 \end{bmatrix} \), \( Z = [0 \quad -(\tilde{\Sigma}_2 \tilde{W}_2)] \), \( Z^\top = \begin{bmatrix} 0 \\ -(\tilde{\Sigma}_2 \tilde{W}_2)^	op \end{bmatrix} \), and \( D = [\tilde{\Sigma}_2] \). We are interested in \( S_3 \), which is precisely \( \text{Cov}(x|y) \). Then by the block matrix inversion formula, we know
\[
S_3^{-1} = (D - ZT^{-1}Z^\top)
= \hat{\Sigma}_2 - \begin{bmatrix} 0 \\ -(\hat{\Sigma}_2 \tilde{W}_2)^	op \end{bmatrix}^\top \begin{bmatrix} \hat{\Sigma}_2 + \tilde{W}_1^\top \hat{\Sigma} \tilde{W}_1 & - (\hat{\Sigma}_1 \tilde{W}_1)^	op \\ - (\hat{\Sigma}_1 \tilde{W}_1) & \Sigma + \tilde{W}_2^\top \Sigma \tilde{W}_2 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ -(\hat{\Sigma}_2 \tilde{W}_2)^	op \end{bmatrix}
= \hat{\Sigma}_2 - (\hat{\Sigma}_2 \tilde{W}_2) \left( (\hat{\Sigma}_1 + \tilde{W}_2^\top \Sigma \tilde{W}_2) - (\hat{\Sigma}_1 \tilde{W}_1)(\Sigma + \tilde{W}_2^\top \Sigma \tilde{W}_2)^{-1}(\hat{\Sigma}_1 \tilde{W}_1) \right)^{-1} (\Sigma_0 \tilde{W}_1)^	op
\]
\[
= \frac{1}{\sigma^2} \left[ (I_n + (I_n)^\top + 1) \right] \left[ (I_n + \tilde{W}_2^\top \tilde{W}_2) - \tilde{W}_1 (I_n + \tilde{W}_1^\top \tilde{W}_1)^{-1} \tilde{W}_1^\top \right]^{-1} \tilde{W}_2
\]
(46)

\[\square\]

### A.2.3 Proof of Lemma 3.5

**Proof.** First we let \( M_2 \) denote \( \hat{W} \left( (I_n + \tilde{W}_2^\top \tilde{W}_2) - \tilde{W}_1 (I_n + \tilde{W}_1^\top \tilde{W}_1)^{-1} \tilde{W}_1^\top \right)^{-1} \tilde{W}_2 \). By a similar reasoning as in Lemma 3.2 we know the KL divergence has
\[
\text{KL}(P_{(x,y)}, \tilde{W}) = \sum_{y \in \{-1,1\}} \int p(x,y) \log \frac{p(x,y)}{q(x,y)} \, dx
\]
(47)

\[
= \frac{1}{2} \text{KL}(P_{(x|y=-1)}, \tilde{W}) \| N(0, \tau^2 I_p) \| + \frac{1}{2} \text{KL}(P_{(x|y=+1)}, \tilde{W}) \| N(0, \tau^2 I_p) \|
\]

where \( q(x,y) \) is the density of \( Q \) and \( p(x,y) \) is the density of \( P_{(x,y)} \).

We focus on one of the two KL-divergences. Recall the formula of KL divergence between two multivariate normal distributions, \( P \sim N(\mu_1, \Sigma_1) \) and \( Q \sim N(\mu_2, \Sigma_2) \), \( \mu_1, \mu_2 \in \mathbb{R}^k \), \( \Sigma_1, \Sigma_2 \in \mathbb{R}^{k \times k} \),
\[
\text{KL}(P \| Q) = \frac{1}{2} \left( \text{Tr}(\Sigma_2^{-1} \Sigma_1) + (\mu_2 - \mu_1)^\top \Sigma_2^{-1} (\mu_2 - \mu_1) + \ln \frac{\det \Sigma_2}{\det \Sigma_1} + k \right)
\]
(48)

Plug in the formula,
\[
\text{KL}(P_{(x|y=-1)}, \tilde{W}) \| N(0, \tau^2 I_p)) = \frac{1}{2} \frac{\sigma^2}{2 \tau^2} \text{Tr} \left( (I_p - M_2)^{-1} \right) + \frac{1}{2} \left( (\tilde{W}_2 \tilde{W}_1 \tilde{w}_0)^\top (\tau^2 I_p)^{-1} (-\tilde{W}_2 \tilde{W}_1 \tilde{w}_0) \right)
\]
\[
+ \frac{1}{2} \ln \left( \frac{\text{det}(\tau^2 I_p)}{\text{det}(\text{Cov}(x|y))} \right) - \frac{p}{2}
\]
(49)

In next lemma we show that \( M_2 \) is positive semi-definite and has largest eigenvalue strictly less than 1.

Observe \( I = \frac{\sigma^2}{\tau^2} \text{Tr} \left( (I_p - M_2)^{-1} \right) = \frac{\sigma^2}{\tau^2} \sum_i \frac{1}{\lambda_i(M_2)} \), where \( \lambda(M_2) = \{\lambda_i(M_2)\} \) is the set of eigenvalues of \( M_2 \) and may contain zero. We claim \( I \leq \frac{\sigma^2}{\tau^2} \sum_{i=1}^p (d^2_{1,i} + d^2_{2,i} + d^2_{2,i} + 1) \), where \( D_1 = \text{diag}_i(d_{1,i}) \) is the diagonal matrix of singular values in the decomposition of \( \tilde{W}_1 \), and \( D_2 = \text{diag}_i(d_{2,i}) \)
is the diagonal matrix of singular values in the decomposition of \( \tilde{W}_2 \), and the diagonal entries in both matrices are in decreasing order. We leave the proof to Lemma 3.7.

It is easy to see that \( II = \frac{\|W_2 w_0 \|^2}{\sigma^2} \).

Now we provide an upper bound on term III, where the last inequality follows from Lemma 3.6.

\[
III = \ln \left( \frac{\det \left( \frac{\tau^2 I_p}{\sigma^2} \right)}{\det \left( \text{Cov}(x|y) \right)} \right) = p \ln \left( \frac{\tau^2}{\sigma^2} \right) + \ln \left( \det \left( I_p - M_2 \right) \right)
\]

\[
= p \ln \left( \frac{\tau^2}{\sigma^2} \right) + \ln \left( \prod_{i=1}^{p} (1 - \lambda_i(M_2)) \right) \leq p \ln \left( \frac{\tau^2}{\sigma^2} \right)
\]

\( \square \)

A.2.4 Proof of Lemma 3.6

Proof. First we show positive semi-definiteness. Consider any \( x \neq 0 \in \mathbb{R}^p \). Suppose \( x \not\in \text{Ker}(\tilde{W}_2) \), then \( \exists y \neq 0 \in \mathbb{R}^{n_1} \) such that \( x = \tilde{W}_2 y \), and

\[
x^T M_2 x = x^T \tilde{W}_2 \left[ (I_{n_1} + \tilde{W}_2^T \tilde{W}_2) - \tilde{W}_1(I_{n_0} + \tilde{W}_1^T \tilde{W}_1)^{-1} \tilde{W}_1^T \right]^{-1} \tilde{W}_2^T x
\]

\[
= y^T \left[ (I_{n_1} + \tilde{W}_2^T \tilde{W}_2) - \tilde{W}_1(I_{n_0} + \tilde{W}_1^T \tilde{W}_1)^{-1} \tilde{W}_1^T \right]^{-1} y
\]

Thus it suffices to show positive semi-definiteness of \( \left[ (I_{n_1} + \tilde{W}_2^T \tilde{W}_2) - \tilde{W}_1(I_{n_0} + \tilde{W}_1^T \tilde{W}_1)^{-1} \tilde{W}_1^T \right]^{-1} \), which is equivalent to show positive semi-definiteness of \( \left[ (I_{n_1} + \tilde{W}_2^T \tilde{W}_2) - \tilde{W}_1(I_{n_0} + \tilde{W}_1^T \tilde{W}_1)^{-1} \tilde{W}_1^T \right] \).

Now consider any \( v \neq 0 \in \mathbb{R}^{n_1} \), and consider the singular value decomposition of \( \tilde{W}_1 = U_1 D_1 V_1^T \), where \( U_1 \in \mathbb{R}^{n_1 \times n_1} \) is orthonormal, \( D_1 = \text{diag}(d_{1,i}) \in \mathbb{R}^{n_1 \times n_0} \) has singular values of \( \tilde{W}_1 \) along the diagonal, and \( V_1 \in \mathbb{R}^{n_0 \times n_0} \) is orthonormal.

\[
v^T \left[ (I_{n_1} + \tilde{W}_2^T \tilde{W}_2) - \tilde{W}_1(I_{n_0} + \tilde{W}_1^T \tilde{W}_1)^{-1} \tilde{W}_1^T \right] v
\]

\[
= \|v\|^2 + \|\tilde{W}_2 v\|^2 - v^T \tilde{W}_1(I_{n_0} + \tilde{W}_1^T \tilde{W}_1)^{-1} \tilde{W}_1^T v
\]

\[
= \|v\|^2 + \|\tilde{W}_2 v\|^2 - v^T U_1 D_1 (I_{n_0} + D_1^T D_1)^{-1} D_1^T U_1^T v
\]

\[
= \|v\|^2 + \|\tilde{W}_2 v\|^2 - \|\text{diag}_i \left( \sqrt{\frac{d_{1,i}^2}{1 + d_{1,i}^2}} \right) U_1^T v\|^2
\]

\[
\geq \|\tilde{W}_2 v\|^2
\]

This shows that \( M_2 \) is positive semi-definite. Now we show that the eigenvalues of \( M_2 \) are less than 1.

First, continue using the singular value decomposition \( \tilde{W}_1 = U_1 D_1 V_1^T \) and consider the singular value decomposition \( \tilde{W}_2 = U_2 D_2 V_2^T \) where \( U_2 \in \mathbb{R}^{p \times p} \) is orthonormal, \( D_2 = \text{diag}(d_{2,i}) \in \mathbb{R}^{p \times n_1} \) is the diagonal matrix of singular values of \( \tilde{W}_2 \) where the diagonal entries are in decreasing order,
and $V_2 \in \mathbb{R}^{n_1 \times n_1}$ is orthonormal, then

$$M_2 = W_2 \left[ \left( I_{n_1} + \tilde{W}_2^T \tilde{W}_2 \right) - W_1 \left( I_{n_0} + \tilde{W}_1^T \tilde{W}_1 \right)^{-1} \tilde{W}_1^T \right]^{-1} \tilde{W}_2^T$$

$$= W_2 \left[ \left( I_{n_1} + \tilde{W}_2^T \tilde{W}_2 \right) - U_1 D_1 V_1^T \left( V_1 V_1^T + V_1 D_1^T U_1^T U_1 D_1 V_1 \right)^{-1} V_1 D_1 U_1^T \right]^{-1} \tilde{W}_2^T$$

$$= W_2 \left[ \left( I_{n_1} + \tilde{W}_2^T \tilde{W}_2 \right) - U_1 D_1 V_1 \left( V_1 \text{diag}_1 \left( \frac{1}{1 + d_{1,i}^2} \right) V_1^T \right) V_1 D_1 U_1^T \right]^{-1} \tilde{W}_2^T$$

$$= \tilde{W}_2 \left[ \left( U_1 U_1^T + \tilde{W}_2^T \tilde{W}_2 \right) - U_1 \left( \text{diag}_1 \left( \frac{d_{2,i}^2}{1 + d_{1,i}^2} \right) \right) U_1^T + \tilde{W}_2^T \tilde{W}_2 \right]^{-1} \tilde{W}_2^T$$

(53)

Note the eigenvalues of $M_2$, $\lambda(M_2)$, are the same as the eigenvalues of $M'_2$, $\lambda(M'_2)$, where

$$M'_2 := \left[ U_1 \left( \text{diag}_1 \left( \frac{1}{1 + d_{1,i}^2} \right) \right) U_1^T + \tilde{W}_2^T \tilde{W}_2 \right]^{-1} \tilde{W}_2^T \tilde{W}_2$$

(54)

Now consider any eigenvalue $\mu$ of $M_2$ with corresponding eigenvector $x$, and we want to show that $\mu < 1$.

$$\left[ U_1 \left( \text{diag}_i \left( \frac{1}{1 + d_{1,i}^2} \right) \right) U_1^T + \tilde{W}_2^T \tilde{W}_2 \right]^{-1} \tilde{W}_2^T \tilde{W}_2 x = \mu x$$

$$\tilde{W}_2^T \tilde{W}_2 x = \mu \left[ U_1 \left( \text{diag}_i \left( \frac{1}{1 + d_{1,i}^2} \right) \right) U_1^T + \tilde{W}_2^T \tilde{W}_2 \right] x$$

(55)

Case 1: $\mu \neq 0$, which is equivalent to $\tilde{W}_2 x \neq 0$. Then note $x^T U_1 \left( \text{diag}_i \left( \frac{1}{1 + d_{1,i}^2} \right) \right) U_1^T x > 0$ as $U_1 \left( \text{diag}_i \left( \frac{1}{1 + d_{1,i}^2} \right) \right) U_1^T$ is positive definite. Thus $(1 - \mu) x^T \tilde{W}_2^T \tilde{W}_2 x > 0$, and therefore $\mu < 1$.

Case 2: $\mu = 0$. Then $\tilde{W}_2 x = 0$, $x \in \text{Ker}(\tilde{W}_2)$. $\square$

### A.2.5 Proof of Lemma 3.7

**Proof.** First note that matrix $M'_2$ defined below has the same spectrum as $M_2$, i.e. $\lambda(M_2) = \lambda(M'_2)$

$$M_2 := \left[ \left( I_{n_1} + \tilde{W}_2^T \tilde{W}_2 \right) - W_1 \left( I_{n_0} + \tilde{W}_1^T \tilde{W}_1 \right)^{-1} \tilde{W}_1^T \right]^{-1} \tilde{W}_2^T \tilde{W}_2$$

$$= \left[ U_1 \left( \text{diag}_i \frac{1}{1 + d_{1,i}^2} \right) U_1^T + \tilde{W}_2^T \tilde{W}_2 \right]^{-1} \tilde{W}_2^T \tilde{W}_2$$

$$= \left[ C + D \right]^{-1} D$$

(56)
with \( C := U_1 \left( \text{diag} \frac{1}{1 + d_{1,i}} \right) U_1^\top \) is positive definite and \( D := \hat{W}_2^\top \hat{W}_2 \) is positive semi-definite.

Consider diagonalization of \( D = QD'Q^\top \), where \( Q \) is an orthonormal matrix and \( D' \) is diagonal. Then there exists a matrix \( C' \) such that \( C = QCQ^\top \), and thus

\[
(C + D)^{-1}D = (QCQ^\top + QD'Q^\top)^{-1}QD'Q^\top = Q(C' + D')^{-1}QD'Q^\top \implies \lambda((C + D)^{-1}D) = \lambda((C' + D')^{-1}D')
\]

Without loss of generality we assume \( D' \) has all its diagonal entries in descending order, and \( D' \) may have zero diagonal entries. Consider below, where \( D_1 \) is a diagonal matrix as well and contains all the positive diagonal entries of \( D' \).

\[
D' = \begin{bmatrix} D_1 & 0 \\ 0 & 0 \end{bmatrix}, C' = \begin{bmatrix} X & Y^\top \\ Y & Z \end{bmatrix}
\]

\[
C' + D' = \begin{bmatrix} X + D_1 & Y^\top \\ Y & Z \end{bmatrix},
\]

\[
(C' + D')^{-1} = \begin{bmatrix} (D_1 + X - Y^\top Z^{-1}Y)^{-1} & * \\ * & * \end{bmatrix} = \begin{bmatrix} (D_1 + S)^{-1} & * \\ * & * \end{bmatrix},
\]

\[
(C' + D')^{-1}D' = \begin{bmatrix} (D_1 + S)^{-1} & * \\ * & * \end{bmatrix} \begin{bmatrix} D_1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} (I + D_1^{-1}S)^{-1} & * \\ * & * \end{bmatrix}
\]

We will use this fact below: for product of two matrices, for any two operators \( A, B \) on Hilbert space \( \mathcal{H} \) with dimension \( n \), for all \( i, j \) such that \( i + j \leq n + 1, \lambda_{i+j-1}(AB) \leq \lambda_i(A)\lambda_j(B) \), where \( \lambda_i(A) \) is the \( i \)-th largest eigenvalue of \( A \) [3].

Therefore, for any \( i \in \{1, 2, \cdots, r\} \) where \( r = \text{rank}(M_2') \), and let \( \lambda_i^j(\cdot) \) denote the \( i \)-th largest eigenvalue of a matrix, \( \alpha_i^j(\cdot) \) denote the \( i \)-th smallest eigenvalue of a matrix

\[
\lambda_i^j(M_2') = \lambda_i^j((I + D_1^{-1}S)^{-1})
\]

\[
= \frac{1}{1 + \lambda_i^j(D_1^{-1}S)} = \frac{1}{1 + \frac{1}{\lambda_i^j(S^{-1}D_1)}}
\]

\[
\leq \frac{1}{1 + \frac{1}{\lambda_i^j(S^{-1})\lambda_j^j(D_1)}}, \forall j, k \in \{1, 2, \cdots, r\} \text{ s.t. } j + k = i + 1
\]

\[
\leq \frac{1}{1 + \frac{1}{\lambda_i^j(C^{-1})\lambda_j^j(D_1)}} = \frac{1}{1 + \frac{\lambda_i^j(C)}{\lambda_j^j(D_1)}}
\]

where the first inequality follows from the fact stated above, the second inequality holds because \( S^{-1} = (X - Y^\top Z^{-1}Y)^{-1} \) is a principal submatrix of \( C'^{-1} \), and the second last equality holds because \( \lambda(C') = \lambda(C) \).
For each fixed $i$, pick $j = i, k = 1$, then we have

$$\lambda_i^j(M^j_2) \leq \frac{1}{1 + \frac{\lambda_i^j(C)}{\lambda_i^j(D)}} = \frac{1}{1 + \frac{\lambda_i^j(C)}{\lambda_i^j(D)}} = \frac{1}{1 + \frac{1}{d_{2,i}(1 + d_{2,i}^2)}} = \frac{d_{2,i}^2(1 + d_{2,i}^2)}{d_{2,i}^2(1 + d_{2,i}^2) + 1} \quad (61)$$

Thus

$$\lambda_i^j((I_p - M_2)^{-1}) = \frac{1}{1 - \lambda_i^j(M_2)} \leq \frac{1}{1 - \frac{d_{2,i}^2(1 + d_{2,i}^2)}{d_{2,i}^2(1 + d_{2,i}^2) + 1}} = d_{2,i}^2(d_{2,i}^2 + 1) + 1, \quad i = 1, 2, \ldots, r$$

$$\text{Tr}((I_p - M_2)^{-1}) = \sum_{i=1}^{p} \lambda_i^j((I_p - M_2)^{-1}) = \sum_{i=1}^{r} \frac{1}{1 - \lambda_i^j(M_2)} + \sum_{i=r+1}^{p} \frac{1}{1 - \lambda_i^j(M_2)} \leq \sum_{i=1}^{r} [d_{2,i}^2(1 + d_{2,i}^2) + 1] + (p - r) = p + \sum_{i=1}^{r} d_{2,i}^2(1 + d_{2,i}^2) \quad (62)$$

A.3 General $d$ hidden layers

A.3.1 Proof of Lemma 3.8

Proof. We prove this lemma by induction. Let $\mu_\ell = y\tilde{W_\ell} \cdots \tilde{W_1} \tilde{w_0}$, i.e. $\mu_\ell$ is the mean of $z_i$ under the marginal distribution, $\ell \in \{0, 1, \cdots, d\}$, and $\mu_0 = yw_0$. Note $\mu_{\ell+1} = \tilde{W}_{\ell+1}\mu_\ell$. The base cases for $d = 1$ and $d = 2$ are proved, as for the 1-layer network we have

$$p(z_0 | y; \tilde{W})p(z_1 | z_0; \tilde{W}) \propto \exp \left( -\frac{1}{2} (z_0 - \mu_0, z_1 - \mu_1) \top \kappa^{(1)}(z_0 - \mu_0, z_1 - \mu_1) \right) \quad (63)$$

and for the 2-layer network we have

$$p(z_0, z_1, z_2 | y; \tilde{w}_0, \tilde{w}_1, \tilde{w}_2) = p(z_0 | y; \tilde{W})p(z_1 | z_0; \tilde{W})p(z_2 | z_1; \tilde{W})$$

$$\propto \exp \left( -\frac{1}{2} (z_0 - \mu_0, z_1 - \mu_1, z_2 - \mu_2) \top \kappa^{(2)}(z_0 - \mu_0, z_1 - \mu_1, z_2 - \mu_2) \right) \quad (64)$$

Let the statement in the lemma be the inductive hypothesis (IH) and now we want to show the (IH) holds for $d + 1$ layers.

$$p(z_0, z_1, \cdots, z_d, z_{d+1} | y; \tilde{w}_0, \tilde{w}_1, \tilde{w}_2, \cdots, \tilde{w}_{d-1}, \tilde{w}_d, \tilde{w}_{d+1})$$

$$= p(z_0, z_1, \cdots, z_d | y; \tilde{w}_0, \tilde{w}_1, \tilde{w}_2, \cdots, \tilde{w}_{d-1}, \tilde{w}_d)p(z_{d+1} | z_d; \tilde{w}_{d+1}) \quad (IH)$$

$$\propto \exp \left( -\frac{1}{2} \left[ (z_0 - \mu_0, \cdots, z_d - \mu_d) \top \kappa^{(d)}(z_0 - \mu_0, \cdots, z_d - \mu_d) + (z_{d+1} - \tilde{w}_{d+1}z_d) \top \tilde{\Sigma}_{d+1}(z_{d+1} - \tilde{W}_{d+1}z_d) \right] \right) \quad (65)$$

Now want to show the RHS of (65) is proportional to the proposed density in Lemma 3.8. That is, we want to show that they have the same exponent. Note that
\[
\kappa^{(d+1)} = \begin{pmatrix}
\kappa^{(d)} & 0 \\
\vdots & \ddots & \ddots & \ddots & 0 \\
0 \cdots 0 & 0
\end{pmatrix} + \begin{pmatrix}
0 & \cdots & 0 & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots 0 & \tilde{\Sigma}_{d+1} \tilde{\Sigma}_{d+1} & \tilde{\Sigma}_{d+1} \\
0 & \cdots 0 & -\left(\tilde{\Sigma}_{d+1} \tilde{\Sigma}_{d+1}\right)^\top & \tilde{\Sigma}_{d+1}
\end{pmatrix}
= : \kappa_1^{(d+1)} + \kappa_2^{(d+1)}
\]

(66)

Thus the exponent of the proposed density in Lemma 3.8, ignoring the factor of \(-\frac{1}{2}\), is

\[
(z_0 - \mu_0, \cdots, z_{d+1} - \mu_{d+1})^\top \kappa^{(d+1)} (z_0 - y\tilde{w}_0, \cdots, z_{d+1} - y\tilde{w}_{d+1} \cdots \tilde{W}_1 \tilde{w}_0)
= (z_0 - \mu_0, \cdots, z_{d+1} - \mu_{d+1})^\top \kappa^{(d+1)} (z_0 - \mu_0, \cdots, z_{d+1} - \mu_{d+1})
\]

\[
= (z_0 - \mu_0, \cdots, z_d - \mu_d)^\top \kappa^{(d)} (z_0 - \mu_0, \cdots, z_d - \mu_d) + (z_{d+1} - \mu_{d+1})^\top \tilde{\Sigma}_{d+1} (z_{d+1} - \mu_{d+1})
\]

\[
- (z_d - \mu_d)^\top \tilde{\Sigma}_{d+1} (z_{d+1} - \mu_{d+1}) + (z_{d+1} - \mu_{d+1})^\top \tilde{\Sigma}_{d+1} (z_d - \mu_d)
\]

\[
= (z_0 - \mu_0, \cdots, z_{d-1} - \mu_{d-1})^\top \kappa^{(d)} (z_0 - \mu_0, \cdots, z_{d-1} - \mu_{d-1}) + (z_d - \mu_d)^\top \tilde{\Sigma}_{d+1} (z_{d+1} - \mu_{d+1})
\]

\[
- 2 (\tilde{W}_{d+1} z_d - \mu_d)^\top \tilde{\Sigma}_{d+1} (z_{d+1} - \mu_{d+1}) + (\tilde{W}_{d+1} z_d - \mu_d)^\top \tilde{\Sigma}_{d+1} (\tilde{W}_{d+1} z_d - \mu_d)
\]

\[
= (z_0 - \mu_0, \cdots, z_d - \mu_d)^\top \kappa^{(d)} (z_0 - \mu_0, \cdots, z_d - \mu_d) + (z_{d+1} \tilde{\Sigma}_{d+1} z_{d+1} - 2 \mu_{d+1} \tilde{\Sigma}_{d+1} z_{d+1} + \mu_{d+1} \tilde{\Sigma}_{d+1} \mu_{d+1})
\]

\[
- 2 (\tilde{W}_{d+1} z_d)^\top \tilde{\Sigma}_{d+1} z_{d+1} + 2 \mu_{d+1} \tilde{\Sigma}_{d+1} z_{d+1} + 2 (\tilde{W}_{d+1} z_d)^\top \tilde{\Sigma}_{d+1} \mu_{d+1} - 2 \mu_{d+1} \tilde{\Sigma}_{d+1} \mu_{d+1}
\]

\[
+ (\tilde{W}_{d+1} z_d)^\top \tilde{\Sigma}_{d+1} z_{d+1} + 2 (\tilde{W}_{d+1} z_d)^\top \tilde{\Sigma}_{d+1} \mu_{d+1} + \mu_{d+1} \tilde{\Sigma}_{d+1} \mu_{d+1}
\]

\[
= (z_0 - \mu_0, \cdots, z_d - \mu_d)^\top \kappa^{(d)} (z_0 - \mu_0, \cdots, z_d - \mu_d) + z_{d+1} \tilde{\Sigma}_{d+1} z_{d+1}
\]

\[
- 2 (\tilde{W}_{d+1} z_d)^\top \tilde{\Sigma}_{d+1} z_{d+1} + (\tilde{W}_{d+1} z_d)^\top \tilde{\Sigma}_{d+1} (\tilde{W}_{d+1} z_d)
\]

(67)

which is exactly the exponent of \(p(z_0, \cdots, z_d | y; \tilde{W}) p(z_{d+1} | z_d; \tilde{W})\), ignoring the factor of \(-\frac{1}{2}\), thus (IH) holds. \(\square\)

A.3.2 Proof of Lemma 3.9

Proof. We only need to show that the covariance of \(x|y; \tilde{W}\) is \(\sigma^2 (I_p - M_d)^{-1}\). Note that we are interested in \((\kappa^{(d)})_{d,d}^{-1}\), the \((d, d)\)-th block of the inverse of \(\kappa^{(d)}\), where \(\kappa^{(d)}\) is the precision matrix of \((z_0, z_1, z_2, \cdots, z_d) | y; \tilde{W}\). We will make use of the tri-diagonal block structure of \(\kappa^{(d)}\).

We will apply the block matrix inverse formula repeatedly. We start with the submatrix \(\kappa^{(d)}_{[0:1],[0:1]}\), which denotes \[
\begin{pmatrix}
\kappa^{(d)}_{0,0} & \kappa^{(d)}_{0,1} \\
\kappa^{(d)}_{1,0} & \kappa^{(d)}_{1,1}
\end{pmatrix}
\]

as defined in (11). We first look for the bottom right block in the inverse
of $\kappa_{[0:1],[0:1]}^{(d)}$, which we denote as $\left( \kappa_{[0:1],[0:1]}^{(d)} \right)_1^{-1}$. By the block matrix inverse formula, we know

$$
\left( \kappa_{[0:1],[0:1]}^{(d)} \right)_1^{-1} = \left( \kappa_{1,1}^{(d)} - \kappa_{1,0}^{(d)} \left( \kappa_{0,0}^{(d)} \right)_1^{-1} \kappa_{0,1}^{(d)} \right)_1^{-1}
$$

$$
= \left( \left( \mathbf{\Sigma}_1 + \mathbf{W}_2^\top \mathbf{\Sigma}_2 \mathbf{W}_2 \right) - \left( -\mathbf{\Sigma}_{i+1} \mathbf{W}_{i+1} \right) \left( \mathbf{\Sigma}_0 + \mathbf{W}_1^\top \mathbf{\Sigma}_1 \mathbf{W}_1 \right) \left( -\mathbf{\Sigma}_{i+1} \mathbf{W}_{i+1} \right)^\top \right)_1^{-1}
$$

$$
= \sigma^2 \left( \mathbf{I}_{n_1} + \mathbf{W}_2^\top \mathbf{W}_2 - \mathbf{M}_1 \right)_1^{-1}
$$

(68)

Now we start to make use of the tri-diagonal block structure of $\kappa^{(d)}$. We calculate $\left( \kappa_{[0:2],[0:2]}^{(d)} \right)_2^{-1}$ using $\left( \kappa_{[0:1],[0:1]}^{(d)} \right)_1^{-1}$:

$$
\left( \kappa_{[0:2],[0:2]}^{(d)} \right)_2^{-1} = \left( \kappa_{2,2}^{(d)} - \kappa_{2,1}^{(d)} \left( \kappa_{1,1}^{(d)} \right)_1^{-1} \kappa_{1,2}^{(d)} \right)_1^{-1}
$$

$$
= \left( \kappa_{2,2}^{(d)} - \kappa_{2,1}^{(d)} \left( \kappa_{1,1}^{(d)} \right)_1^{-1} \kappa_{1,2}^{(d)} \right)_1^{-1}
$$

$$
= \left( \mathbf{\Sigma}_2 + \mathbf{W}_3^\top \mathbf{\Sigma}_3 \mathbf{W}_3 \right) - \left( -\mathbf{\Sigma}_2 \mathbf{W}_2 \right) \sigma^2 \left( \mathbf{I}_{n_2} + \mathbf{W}_2^\top \mathbf{W}_2 - \mathbf{M}_1 \right)_1^{-1} \left( -\mathbf{\Sigma}_2 \mathbf{W}_2 \right)^\top_1^{-1}
$$

$$
= \sigma^2 \left( \mathbf{I}_{n_2} + \mathbf{W}_3^\top \mathbf{W}_3 - \mathbf{M}_2 \right)_2^{-1}
$$

(69)

where $\kappa_{2,[0:1]}^{(d)} = \begin{bmatrix} \kappa_{2,0}^{(d)} & \kappa_{2,1}^{(d)} \end{bmatrix}$ and $\kappa_{[0:1],2}^{(d)} = \begin{bmatrix} \kappa_{0,2}^{(d)} \\ \kappa_{1,2}^{(d)} \end{bmatrix}$, and the second equality follows from the fact that $\kappa_{2,0}^{(d)} = \mathbf{0}$ and $\kappa_{0,2}^{(d)} = \mathbf{0}$.

It is easy to see this pattern would hold for any general $\ell \in \{1, 2, \cdots, d - 1\}$, i.e.,

$$
\left( \kappa_{[0:\ell],[0:\ell]}^{(d)} \right)_\ell^{-1} = \sigma^2 \left( \mathbf{I}_{n_\ell} + \mathbf{W}_{\ell+1}^\top \mathbf{W}_{\ell+1} - \mathbf{M}_\ell \right)_\ell^{-1}
$$

(70)

Therefore, we have

$$
\left( \kappa_{[0:d-1],[0:d-1]}^{(d)} \right)_{d,d}^{-1} = \left( \kappa_{d,d}^{(d)} - \kappa_{d,d-1}^{(d)} \left( \kappa_{[0:d-1],[0:d-1]}^{(d)} \right)_{d-1,d-1}^{-1} \kappa_{d,d-1}^{(d)} \right)_{d,d}^{-1}
$$

$$
= \left( \kappa_{d,d}^{(d)} - \kappa_{d,d-1}^{(d)} \left( \kappa_{[0:d-1],[0:d-1]}^{(d)} \right)_{d-1,d-1}^{-1} \kappa_{d,d-1}^{(d)} \right)_{d,d}^{-1}
$$

$$
= \left( \mathbf{\Sigma}_d - \left( -\mathbf{\Sigma}_d \mathbf{W}_d \right) \sigma^2 \left( \mathbf{I}_{n_d} + \mathbf{W}_d^\top \mathbf{W}_d - \mathbf{M}_{d-1} \right)_{d-1,d-1}^{-1} \left( -\mathbf{\Sigma}_d \mathbf{W}_d \right)^\top_1^{-1}
$$

$$
= \sigma^2 \left( \mathbf{I}_{n_d} - \mathbf{M}_d \right)_d^{-1} = \sigma^2 \left( \mathbf{I}_p - \mathbf{M}_d \right)_d^{-1}
$$

(71)

which is the desired result. □
### A.3.3 Proof of Lemma 3.10

**Proof.** Similar to the proof of Lemma 3.5, we use the fact that

\[
\mathbb{KL}(P_{(x,y)\mid \mathbf{w}} \mid \mathcal{Q}) = \sum_{y \in \{-1, +1\}} \int p(x, y) \log \frac{p(x, y)}{q(x, y)} dx
\]

\[
= \frac{1}{2} \mathbb{KL}(P_{x \mid y = -1} \mid \mathcal{W} \mid N(0, \tau^2 I_p)) + \frac{1}{2} \mathbb{KL}(P_{x \mid y = +1} \mid \mathcal{W} \mid N(0, \tau^2 I_p))
\]

\[
= \frac{1}{2} \frac{\sigma^2}{\tau^2} \text{Tr}((I_p - \mathbf{M}_d)^{-1}) + \frac{1}{2} \left((\mathbf{W}_d \mathbf{W}_{d-1} \cdots \mathbf{W}_1 \mathbf{W}_0)^\top (\tau^2 I_p)^{-1} (\mathbf{W}_d \mathbf{W}_{d-1} \cdots \mathbf{W}_1 \mathbf{W}_0)\right)
\]

\[
+ \frac{1}{2} \ln \left(\frac{\det(\tau^2 I_p)}{\det(\text{Cov}(x \mid y))}\right) = \frac{p}{2}
\]

(72)

For term I, the base case is proved in Lemma 3.2 and Lemma 3.5. Now we prove the inductive case for the general \(d\)-layer setting. From Lemma 3.7, we know when \(d = 2\),

\[
i = 1, 2, \ldots, r : \lambda_i^1((I_p - \mathbf{M}_2)^{-1}) = \frac{1}{1 - \lambda_i^2(M_2)} \leq d_{2,i}^2 (d_{1,1}^2 + 1) + 1 = m_{2,i} + 1
\]

\(i = r + 1, r + 2, \ldots, p : \lambda_i^1((I_p - \mathbf{M}_2)^{-1}) = 1
\]

(73)

We defined the constants \(m_{d,i}\) recursively in (13), and we let the inductive hypothesis (IH) be:

\[
\forall i \in \{1, 2, \ldots, r\} : \lambda_i^1((I_p - \mathbf{M}_d)^{-1}) \leq m_{d,i} + 1
\]

(74)

and we see (IH) holds for \(d = 2\). Now suppose (IH) holds for any \(d \geq 2\), and we want to show it holds for \(d + 1\) as well.

Recall

\[
\mathbf{M}_{d+1} := \mathbf{W}_{d+1} (\mathbf{I}_{n_d} + \mathbf{W}_{d+1}^\top \mathbf{W}_{d+1} - \mathbf{M}_d)^{-1} \mathbf{W}_{d+1}^\top \\
\mathbf{M}'_{d+1} := (\mathbf{I}_{n_d} + \mathbf{W}_{d+1}^\top \mathbf{W}_{d+1} - \mathbf{M}_d)^{-1} \mathbf{W}_{d+1}^\top \mathbf{W}_{d+1}
\]

Follow the similar reasoning as in Lemma 3.7 equations (51) - (58),

\[
\forall i \in \{1, 2, \ldots, r\} : \forall j, k \in \{1, 2, \ldots, r\} \text{ s.t. } j + k = i + 1, \lambda_i^1(M_{d+1}') \leq \frac{1}{1 + \frac{1}{\lambda_j^2((I_p - \mathbf{M}_d)^{-1})} \lambda_i^1(W_{d+1} W_{d+1})}
\]

\[
\forall i \in \{r + 1, r + 2, \ldots, p\} : \lambda_i^1(M_{d+1}') = 0
\]

(75)
For each \( i \in \{1, 2, \cdots, r \} \), pick \( j = i \) and \( k = 1 \), get
\[
\lambda_i^\downarrow (M^{d+1}_d) \leq \frac{1}{1 + \lambda_i^\downarrow ((I_p - M_d)^{-1})\lambda_i^\downarrow (W^{d+1}_{d+1}W_{d+1})} \leq \frac{1}{1 + \frac{1}{(m_{d,1}+1)\lambda_i^\downarrow (W^\top_{d+1}W_{d+1})}} = \frac{1}{1 + \frac{1}{(m_{d,1}+1)d_{d+1}^2}} = \frac{1}{1 + (m_{d,1}+1)d_{d+1}^2}.
\]
(76)

Therefore, for \( i \in \{1, 2, \cdots, r \} \)
\[
\lambda_i^\downarrow ((I_p - M^{d+1}_d)^{-1}) = \frac{1}{1 - \lambda_i^\downarrow (M^{d+1}_d)} \leq \frac{1}{1 - \frac{(m_{d,1}+1)d_{d+1}^2}{1 + (m_{d,1}+1)d_{d+1}^2}} = \frac{1}{1 - \frac{(m_{d,1}+1)d_{d+1}^2}{1 + (m_{d,1}+1)d_{d+1}^2}} = d_{d+1,i}^2(1 + m_{d,1} + 1 = m_{d+1,i} + 1.
\]
(77)

which says (IH) is true for all \( d \geq 2 \), and
\[
\forall i \in \{r + 1, r + 2, \cdots, p \} : \lambda_i^\downarrow ((I_p - M^{d+1}_d)^{-1}) = 1
\]
(78)

Therefore
\[
I = \text{Tr} \left((I_p - M_d)^{-1}\right) = \sum_{i=1}^{p} \lambda_i^\downarrow ((I_p - M_d)^{-1}) = \sum_{i=1}^{r} \frac{1}{1 - \lambda_i^\downarrow (M_d)} + \sum_{i=r+1}^{p} \frac{1}{1 - 0}
\]
(79)

It is easy to see that \( II = \frac{1}{\pi^2} \|\hat{W}_d \hat{W}_{d-1} \cdots \hat{W}_1 \hat{W}_0\|_2^2 \).

Now we provide an upper bound on term \( III \), where the last inequality follows from (76)
\[
III = \ln \left(\frac{\det(\tau^2 I_p)}{\det(\text{Cov}(x|y))}\right) = p \ln \left(\frac{\tau^2}{\sigma^2}\right) + \ln \left(\det(I_p - M_d)\right)
\]
\[
= p \ln \left(\frac{\tau^2}{\sigma^2}\right) + \ln \left(\prod_{i=1}^{p} (1 - \lambda_i(M_d))\right) \leq p \ln \left(\frac{\tau^2}{\sigma^2}\right)
\]
(80)

\[\Box\]

### A.4 Sample complexity lower bound for the exact recovery of the network parameters

Below we provide Fano’s inequality and a well known fact about mutual information and KL divergence. \[12\] \[14\]

**Theorem** A.1 (Fano’s inequality). For any hypothesis \( \hat{f} \in \mathcal{F} \), consider the data generating process \( f \rightarrow S \rightarrow \hat{f} \), where the dataset \( S = \{(x_i, y_i)\}_{i=1}^{n} \), \( (x_i, y_i) \) i.i.d., and the true hypothesis \( f \) is chosen by nature uniformly at random from \( \mathcal{F} \), then we have:
\[
P(\hat{f} \neq f) \geq 1 - \frac{\mathbb{I}(\hat{f}; S) + \log 2}{\log |\mathcal{F}|}
\]
Lemma A.2. Consider a hypothesis class $\mathcal{F}$, a true hypothesis $\tilde{f} \in \mathcal{F}$ that is chosen by nature uniformly at random from $\mathcal{F}$, and a data point $(x, y)$. Then for any prior distribution $Q$ of $(x, y)$

$$\mathbb{I}(\tilde{f}; (x, y)) \leq \frac{1}{|\mathcal{F}|} \sum_{f \in \mathcal{F}} \text{KL}(P(x, y) || Q) \quad (81)$$

A.4.1 Proof of Lemma 3.11

Proof. It is known that $\mathbb{I}(\tilde{W}; \{(x_1, y_1), \cdots, (x_n, y_n)\})$ is concave in $n$, which implies $\mathbb{I}(\tilde{W}; (x_n, y_n)|((x_1, y_1), \cdots, (x_{n-1}, y_{n-1}))) \leq \mathbb{I}(\tilde{W}; (x_n, y_n))$ ([7], [3]). By the chain rule of mutual information we have

$$\mathbb{I}(\tilde{W}; S) = \mathbb{I}(S; \tilde{W}) = \mathbb{I}((x_1, y_1), \cdots, (x_n, y_n); \tilde{W})$$

$$= \sum_{i=1}^{n} \mathbb{I}((x_i, y_i); \tilde{W}|(x_1, y_1), \cdots, (x_{i-1}, y_{i-1}))$$

$$\leq \sum_{i=1}^{n} \mathbb{I}(\tilde{W}; (x_i, y_i)) = n\mathbb{I}(\tilde{W}; (x, y)) \quad (82)$$

A.4.2 Proof of Lemma 3.12

Proof. Recall $y \sim \text{Unif}\{-1, +1\}$,

$$\mathbb{I}(\tilde{W}; (x, y)) = \sum_{y \in \{-1, +1\}} \int_{x} \int_{\tilde{W}} p(\tilde{W}, x, y) \log \frac{p(\tilde{W}, x, y)}{p(\tilde{W})p(x, y)} d\tilde{W} dx$$

$$= \sum_{y \in \{-1, +1\}} \int_{x} \int_{\tilde{W}} p(\tilde{W})p(y)p(x|y, \tilde{W}) \log \frac{p(y)p(x|y, \tilde{W})}{p(y)p(x|y)} d\tilde{W} dx$$

$$= \frac{1}{2} \int_{x} \int_{\tilde{W}} p(\tilde{W})p(x|y = -1, \tilde{W}) \log \frac{p(x|y = -1, \tilde{W})}{p(x|y = -1)} d\tilde{W} dx +$$

$$\frac{1}{2} \int_{x} \int_{\tilde{W}} p(\tilde{W})p(x|y = +1, \tilde{W}) \log \frac{p(x|y = +1, \tilde{W})}{p(x|y = +1)} d\tilde{W} dx \quad (83)$$

and note that

$$\mathbb{I}(\tilde{W}; x|y = -1) = \int_{x} \int_{\tilde{W}} p(\tilde{W}, x|y = -1) \log \frac{p(\tilde{W}, x|y = -1)}{p(\tilde{W}|y = -1)p(x|y = -1)} d\tilde{W} dx$$

$$= \int_{x} \int_{\tilde{W}} p(\tilde{W}, x|y = -1) \log \frac{p(\tilde{W})p(x|\tilde{W}, y = -1)}{p(\tilde{W})p(x|y = -1)} d\tilde{W} dx \quad (84)$$

and similar result holds for $(\tilde{W}; x|y = +1)$, which proves the desired result. □
A.4.3 Proof of Theorem 3.13

Proof. Now we calculate the matrix \((I_p - M_d)^{-1}\) under the assumption A1, which is important in the calculation of the KL divergence and the expected risk.

Note that our choice of \(A_1\) gives us

\[
\hat{W}_i^T \hat{W}_i = \hat{W}_i \hat{W}_i^T = \begin{bmatrix} I_r & 0 \\ 0 & c^2 I_{p-r} \end{bmatrix}
\]

(85)

Thus, by easy calculation, the matrices \(M_i\) defined in Lemma 3.9 become

\[
M_1 = \hat{W}_1 (I_p + \hat{W}_1^T \hat{W}_1)^{-1} \hat{W}_1^T = \begin{bmatrix} 2I_r & 0 \\ 0 & \frac{c^2}{1 + c^2} I_{p-r} \end{bmatrix}
\]

\[
M_2 = \hat{W}_2 (I_p + \hat{W}_2^T \hat{W}_2 - M_1)^{-1} \hat{W}_2^T = \begin{bmatrix} 2I_r & 0 \\ 0 & \frac{c^2}{1 + \sum_{j=1}^d c_j^2} I_{p-r} \end{bmatrix}
\]

\[
\vdots
\]

\[
M_d = \hat{W}_d (I_{n_p} + \hat{W}_d^T \hat{W}_d - M_{d-1})^{-1} \hat{W}_d^T = \begin{bmatrix} d+1 & 0 \\ 0 & \frac{\sum_{j=1}^d c_j^2}{1 + \sum_{j=1}^d c_j^2} I_{p-r} \end{bmatrix}
\]

(86)

which in turn gives the exact values of the eigenvalues of \((I_p - M_d)^{-1}\),

\[
\lambda_i^\dagger (M_d) = \begin{cases} \frac{d}{d+1}, & i \in \{1, 2, \ldots, r\} \\ \frac{\sum_{j=1}^d c_j^2}{1 + \sum_{j=1}^d c_j^2}, & i \in \{r+1, r+2, \ldots, p\} \end{cases}
\]

\[
\Rightarrow \lambda_i^\dagger (I_p - M_d)^{-1} = \begin{cases} d + 1, & i \in \{1, 2, \ldots, r\} \\ 1 + \sum_{j=1}^d c_j^2, & i \in \{r+1, r+2, \ldots, p\} \end{cases}
\]

(87)

Therefore, together with the assumptions A1 and A2, we calculate a tighter KL divergence upper bound than in Lemma 3.10:

\[
KL(P_{(x,y)}; \hat{W} || Q) = \frac{1}{2} KL(P_{(x|y=-1)}; \hat{W} || N(0, \tau^2 I_p)) + \frac{1}{2} KL(P_{(x|y=+1)}; \hat{W} || N(0, \tau^2 I_p)) = KL(P_{(x|y=-1)}; \hat{W} || N(0, \tau^2 I_p))
\]

\[
= \frac{1}{2} \sigma^2 \text{Tr} \left( (I_p - M_d)^{-1} \right) + \frac{1}{2} \left( \frac{\text{det} (\tau^2 I_p)}{\text{det} (\text{Cov}(x|y))} - \frac{p}{2} \right)
\]

\[
+ \frac{1}{2} \ln \left( \frac{\text{det} (\tau^2 I_p)}{\text{det} (\text{Cov}(x|y))} \right) \right) - \frac{p}{2}
\]

\[
\leq \frac{1}{2} \left( r \cdot (d + 1) + (p-r) \cdot \left( 1 + \sum_{j=1}^d c_j^2 \right) \right) + \frac{1}{2} \left( \frac{\text{det} (\tau^2 I_p)}{\text{det} (\text{Cov}(x|y))} - \frac{p}{2} \right)
\]

\[
\leq \frac{1}{2} \left( r \cdot d + (p-r) \cdot \left( \frac{d}{\sum_{j=1}^d c_j^2} \right) + \frac{1}{\sigma^2} \right)
\]

(88)
where the inequality follows from A2, eqn (57) and that \( \hat{\mathbf{W}}_d \hat{\mathbf{W}}_{d-1} \cdots \hat{\mathbf{W}}_1 = \begin{bmatrix} I_r & 0 \\ 0 & c^d I_{p-r} \end{bmatrix} \).

Now our choice of \( c \) in Assumption A3, \( c = \frac{p-r+1}{r^2} \), further improves our KL divergence upper bound. Observe \( \sum_{j=1}^d c^j < \frac{c^d}{1-c} \), and by setting \( \frac{c^d}{1-c} = \frac{1}{2r} \) we get \( c = \frac{1}{2r+1} \).

Under A3, the upper bound of \( \text{KL}(P_{(x,y)\hat{\mathbf{W}}}||Q) \) becomes

\[
\text{KL}(P_{(x,y)\hat{\mathbf{W}}}||Q) \leq \frac{1}{2} \left( r \cdot d + 1 + \frac{1}{\sigma^2} \right) \tag{89}
\]

By Lemma 3.10 3.11 3.12 and A.2 for a \( d \)-layer network with true parameter \( \mathbf{W}^* = (\hat{\mathbf{W}}_d, \ldots, \hat{\mathbf{W}}_1, \hat{\mathbf{w}}_0) \) from hypothesis class \( \mathcal{F} \), we have

\[
\mathbb{I}(\hat{\mathbf{W}}^*; S) \leq n \mathbb{I}(\hat{\mathbf{W}}^*; (x, y)) = \frac{n}{2} (\mathbb{I}(\hat{\mathbf{W}}^*; x|y = -1) + \mathbb{I}(\hat{\mathbf{W}}^*; x|y = +1)) \\
\leq \frac{n}{2|\mathcal{F}|} \sum_{\mathbf{w} \in \mathcal{F}} \text{KL}(P_{(x|y=-1)\hat{\mathbf{w}}}||Q) + \text{KL}(P_{(x|y=+1)\hat{\mathbf{w}}}||Q) \\
= \frac{n}{|\mathcal{F}|} \sum_{\mathbf{w} \in \mathcal{F}} \text{KL}(P_{(x,y)\hat{\mathbf{w}}}||Q) \tag{90}
\]

where \( S = \{(x_i, y_i)\}_{i=1}^n \) is a dataset of size \( n \) of i.i.d. observations generated as in (10), and \( Q \) is a prior distribution defined in Lemma 3.10.

Therefore, together with assumptions A1 , A2 and A3, and eqn (89), we have

\[
\mathbb{I}(\hat{\mathbf{W}}^*; S) \leq \frac{n}{|\mathcal{F}|} \sum_{\mathbf{w} \in \mathcal{F}} \text{KL}(P_{(x,y)\mathbf{w}}}||Q) \leq \frac{n}{2|\mathcal{F}|} \sum_{\mathbf{w} \in \mathcal{F}} \left[ r \cdot d + 1 + \frac{1}{\sigma^2} \right] \tag{91}
\]

By Fano’s inequality (Theorem A.1), for any hypothesis \( \mathbf{W} \in \mathcal{F} \),

\[
P(\mathbf{W} \neq \hat{\mathbf{W}}^*) \geq 1 - \frac{\mathbb{I}(\hat{\mathbf{W}}^*; S) + \log 2}{\log |\mathcal{F}|} \\
\geq 1 - \frac{\log 2}{\log |\mathcal{F}|} - \frac{n/(2|\mathcal{F}|)}{\log |\mathcal{F}|} \sum_{\mathbf{w} \in \mathcal{F}} \left[ r \cdot d + 1 + \frac{1}{\sigma^2} \right] \\
\geq 1 - \frac{n}{2|\mathcal{F}|} \sum_{\mathbf{w} \in \mathcal{F}} \left[ r \cdot d + 1 + \frac{1}{\sigma^2} \right] \tag{92}
\]

Thus, combined with (18), the sample complexity lower bound is

\[
P(\mathbf{W} \neq \hat{\mathbf{W}}^*) \geq \frac{1}{2} \iff n \leq \frac{|\mathcal{F}| \log |\mathcal{F}|}{d \left( \sum_{i=1}^r \log(i) + o(1) + \frac{1}{2} (\log \frac{2p}{r} + \log(r)) + r \log \frac{2r}{\sqrt{3}} + (p-r) \log(2) - \log(4) \right)} \\
\]

meaning that if the number of samples is of order \( \Omega(\frac{p}{r \cdot d} + \log r) \), then the probability of identifying the truth \( \mathbf{W}^* \) is less than half. \( \square \)
A.5 Sample complexity lower bound for the expected risk

A.5.1 Proof of Lemma 3.14

Proof. Let \( u := y \hat{\w}^\top x \), then \( u \) is normally distributed with mean \( \hat{\w}^\top \hat{\w}^\ast \) and variance \( \sigma^2 \hat{\w}^\top (I_p - M_d)^{-1} \hat{\w} \), where \( M_d \) is defined in terms of \( \hat{\W}^\ast \). Thus the risk is

\[
R(\hat{\W}) = P_u [u \leq 0] = P_{z \sim N(0,1)} \left[ z \leq \frac{-\hat{\w}^\top \hat{\w}^\ast}{\sqrt{\sigma^2 \hat{\w}^\top (I_p - M_d)^{-1} \hat{\w}}} \right]
\]

\[
= \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{-\hat{\w}^\top \hat{\w}^\ast}{\sqrt{2\sigma^2 \hat{\w}^\top (I_p - M_d)^{-1} \hat{\w}}} \right) \right]
\]

(94)

As shown in eqn (86), we know that \( (I_p - M_d)^{-1} = \begin{bmatrix} (d + 1)I_r & 0 \\ 0 & (1 + \sum_{j=1}^d c^{2j}) I_{p-r} \end{bmatrix} \) where \( c = \frac{1}{p-r+1} \). Therefore we can calculate the denominator of \( R(\hat{\W}) \) exactly:

\[
\hat{\w}^\top (I_p - M_d)^{-1} \hat{\w} = (d + 1) \sum_{k=1}^r (\hat{\w}_k)^2 + \left( 1 + \sum_{j=1}^d c^{2j} \right) \sum_{k=r+1}^p (\hat{\w}_k)^2
\]

\[
= (d + 1) \sum_{k=1}^r (\hat{\w}_0)^2 + \left( 1 + \sum_{j=1}^d c^{2j} \right) \sum_{k=r+1}^p \left( c^d (\hat{\w}_0)_k \right)^2
\]

\[
= \frac{d + 1}{2} + \frac{c^{2d}}{2} \left( 1 + \sum_{j=1}^d c^{2j} \right)
\]

(95)

\[
= \frac{1}{2} \left[ (d + 1) + \frac{c^{2d} - c^{2(2d+1)}}{1 - c^2} \right]
\]

due to our choice of \( \hat{\W} \) and \( \hat{\w}_0 \) - the first \( r \) entries of \( \hat{\w}_0 \) only get permuted and never get scaled, while the last \( (p - r) \) entries of \( \hat{\w}_0 \) never get permuted but always get scaled \( d \) times.
Therefore, for all $\tilde{W}^* \in \mathcal{F}$, we have

$$R(\tilde{W}^*) = \frac{1}{2} \left[ 1 - \text{erf} \left( \frac{\|\tilde{w}^*\|^2}{2 \sqrt{\sigma^2 [d + 1 + \frac{c^{2d}(d^2 + 2)}{1 - c^2}]} \right) \right]$$

$$= \frac{1}{2} \left[ 1 - \text{erf} \left( \frac{1 + c^{2d}}{2 \sqrt{\sigma^2 [d + 1 + \frac{c^{2d}(d^2 + 2)}{1 - c^2}]} \right) \right]$$

where $\|\tilde{w}^*\|^2 = \sum_{k=1}^r (\tilde{w}_0)_k^2 + \sum_{k=r+1}^p (c^d (\tilde{w}_0)_k)^2 = \frac{1}{2} + \frac{c^{2d}}{2}$ by our choice of $\mathcal{F}$.

Now consider the following two cases for $R(\tilde{W}) - R(\tilde{W}^*)$ for $\tilde{W} \neq \tilde{W}^*$.

**Case 1:** $\tilde{w}^T \tilde{w}^* > 0$

Note $R(\tilde{W})$ is minimized when the numerator inside the erf function is maximized, that is, when $\tilde{w}^T \tilde{w}^*$ is maximized, as erf is a monotone increasing function. It is easy to see that $\tilde{w}^T \tilde{w}^*$ is maximized when $\tilde{w} = \tilde{w}^*$, thus $R(\tilde{W}) \geq R(\tilde{W}^*)$.

**Case 2:** $\tilde{w}^T \tilde{w}^* \leq 0$

By the same reasoning as in Case 1, $R(\tilde{W})$ is minimized when $\tilde{w}^T \tilde{w}^*$ is maximized, which means that $\tilde{w}^T \tilde{w}^* = 0$. Thus

$$R(\tilde{W}) - R(\tilde{W}^*) \geq \frac{1}{2} |1 - \text{erf}(0)| - \frac{1}{2} \left[ 1 - \text{erf} \left( \frac{1 + c^{2d}}{2 \sqrt{\sigma^2 [d + 1 + \frac{c^{2d}(d^2 + 2)}{1 - c^2}]} \right) \right]$$

$$= \frac{1}{2} \cdot \text{erf} \left( \frac{1 + c^{2d}}{2 \sqrt{\sigma^2 [d + 1 + \frac{c^{2d}(d^2 + 2)}{1 - c^2}]} \right) > 0$$

**A.5.2 Proof of Theorem 3.15**

**Proof.** By Theorem 3.13 we know that

$$n \leq \frac{d \left( \sum_{i=1}^r \log(i) + o(1) + \frac{1}{2} \left( \log \frac{3r}{2} + \log(r) \right) + r \log \frac{2}{\sqrt{\pi}} + (r - p) \log(2) - \log 4 \right)}{r \cdot d + 1 + \frac{1}{\sigma^2}}$$

$$\Rightarrow P(\tilde{W} \neq \tilde{W}^*) \geq \frac{1}{2}$$

By Lemma 3.14 we know that

$$\tilde{W} = \tilde{W}^* \Rightarrow R(\tilde{W}) - R(\tilde{W}^*) \geq \frac{1}{2} \cdot \text{erf} \left( \frac{1 + c^{2d}}{2 \sqrt{\sigma^2 [d + 1 + \frac{c^{2d}(d^2 + 2)}{1 - c^2}]} \right)$$

$$\text{(99)}$$
Therefore,

\[
n \leq \frac{d(\sum_{i=1}^{r} \log(i)) + o(1) + \frac{1}{2} \left( \log \frac{2\pi}{\lambda} + \log(r) \right) + r \log \frac{2}{\sqrt{3}} + (p - r) \log(2) - \log(4)}{r \cdot d + 1 + \frac{1}{\sigma^2}}
\]

\[
P \left( R(\mathbf{W}) - R(\mathbf{W}^*) \geq \mathbf{1} \{ \mathbf{w}^{\top} \mathbf{w}^* \leq 0 \} \cdot \frac{1}{2} \cdot \text{erf} \left( \frac{1 + c^{2d}}{2 \sqrt{\sigma^2 [(d + 1) + \frac{c^{2d}}{1-c^2}]} \left[ (d + 1) + \frac{c^{2d}}{1-c^2} \right]} \right) \right)
\]  

\[\geq P(\mathbf{W} \neq \mathbf{W}^*) \geq \frac{1}{2}
\]  

(100)