Abstract

We study regularized deep neural networks and introduce an analytic framework to characterize the structure of the hidden layers. We show that a set of optimal hidden layer weight matrices for a norm regularized deep neural network training problem can be explicitly found as the extreme points of a convex set. For two-layer linear networks, we first formulate a convex dual program and prove that strong duality holds. We then extend our derivations to prove that strong duality also holds for certain deep networks. In particular, for linear deep networks, we show that each optimal layer weight matrix is rank-one and aligns with the previous layers when the network output is scalar. We also extend our analysis to the vector outputs and other convex loss functions. More importantly, we show that the same characterization can also be applied to deep ReLU networks with rank-one inputs, where we prove that norm regularization determines the complexity of layer weights by directly controlling the rank. Furthermore, we show that norm regularization enforces deep neural networks to achieve simple solutions, e.g., linear spline interpolation for one-dimensional datasets.

1. Introduction

Deep neural networks have become extremely popular due to their success in several machine learning applications. Even though deep neural networks are highly over-parametrized and non-convex, a simple first-order algorithm, e.g., Gradient Descent (GD), can be used to adequately train them. Moreover, it has been shown that these highly over-parametrized networks trained with GD obtain simple solutions that generalize well [Savarese et al., 2019; Parhi & Nowak, 2019; Maennel et al., 2018]. As an example, (Savarese et al., 2019] studied the function space characteristics for one-dimensional two-layer ReLU networks and proved that the linear spline interpolation is the minimum Euclidean norm solution among infinitely many possible solutions that perfectly fit the training data. Therefore, regularizing the training phase towards smaller norm solutions might be the key to understand the generalization properties of these architectures. Although there exist several studies on the effects of regularization for two-layer networks (Savarese et al., 2019; Maennel et al., 2018; Chizat & Bach, 2018; Wei et al., 2018; Parhi & Nowak, 2019), analyzing deeper networks is still theoretically elusive even in the absence of nonlinear activations.

To this end, we study norm regularized deep neural networks. Particularly, we develop a framework based on convex duality such that a set of optimal solutions to the training problem can be explicitly characterized as the extreme points of a convex set. Based on this characterization, we show that norm regularization determines the complexity of layer weights by directly controlling the rank. Furthermore, we show that norm regularization enforces deep neural networks to achieve simple solutions, e.g., linear spline interpolation for one-dimensional datasets.

1.1. Related work

Since deep linear networks are more amenable to analysis compared with deep nonlinear networks, they have been extensively studied in the recent literature. A line of research (Saxe et al., 2013; Arora et al., 2018a; Laurent & Brecht, 2018; Du & Hu, 2019; Shamir, 2018) particularly focused on GD training dynamics and convergence to a global optimum. Among these, (Saxe et al., 2013) studied the dynamics of learning and proved that linear networks have nonlinear training dynamics. In another study, (Shamir, 2018; Du & Hu, 2019) focused on the convergence of GD and proved the convergence to a global minimum. However, since these studies only focused on the training dynamics of GD, they are not quite useful to understand the generalization properties of deep networks.

Another line of research (Gunasekar et al., 2017; Arora et al., 2019; Bhojanapalli et al., 2016) studied the generalization properties via matrix factorization problems. In...
The authors proved that GD with sufficiently small step size and initialization converges to the minimum nuclear norm solution. This result shows that optimization variables, e.g., step size and initialization magnitude, act as a regularizer such that a two-layer network trained with GD can find a low complexity (in the nuclear norm sense) solution that generalizes well. Later on, (Arora et al., 2019) extended this work to deep linear networks and proved that GD has a tendency to find low-rank solutions without an exact characterization. In another study, (Gunasekar et al., 2018) proved that GD applied on a deep linear network converges to the maximum margin solution independent of depth. Then, (Arora et al., 2018b; Du et al., 2018) showed that gradient flow enforces the layer weights to align such that the squared Frobenius norm difference between any consecutive two layers remains invariant. (Ji & Telgarsky, 2019) further extended these results to show that deep linear networks trained with GD have aligned layer weights and each layer weight matrix is asymptotically rank-one. Moreover, in the case of logistic loss, the right singular vector of the first layer aligns with the maximum margin predictor defined by the data. These results are important since they completely characterize the structure of the optimal layer weights and provide a concrete relation between layer weight matrices and the input data. However, this study requires multiple strict assumptions, e.g., strictly decreasing loss function and linearity of integer from 1 to n as [n]. To denote Frobenius, operator, and nuclear norms, we use ∥·∥_F, ∥·∥_2, and ∥·∥, respectively. Furthermore, σ_{max}(·) and σ_{min}(·) represent the maximum and minimum singular values of their argument, respectively. We use B_2 to denote the unit ℓ_2 ball defined as B_2 = {u ∈ ℝ^d | ∥u∥_2 ≤ 1}.

1.3. Overview of our results

In this paper, we consider an L-layer network with layer weights W_l ∈ ℝ^{m_{l-1} × m_l}, ∀l ∈ [L], where m_0 = d and m_L = 1 are the input and output dimensions, respectively. Given n data samples, i.e., (x_i, y_i)_{i=1}^n, which are the rows of the data matrix X ∈ ℝ^{n × d}, the output is

\[ f_{\theta, L}(X) = A_{L-1} W_L, \quad A_l = g(A_{l-1} W_l) \forall l ∈ [L-1], \]

where A_0 = X and g(·) is the activation function. We then consider the following problem to estimate \( y \in ℝ^n \)

\[ \min_{\{\theta_l\}_{l=1}^L} \left\| f_{\theta, L}(X) - y \right\|^2_2 + \beta \sum_{l=1}^L \| W_l \|^2_F, \tag{1} \]

where \( \beta > 0 \) is a regularization parameter, \( \theta_l = \{W_l, m_l\}, \forall l ∈ [L-1] \) and \( \theta_L = \{W_L\} \). Motivated by recent results (Savarese et al., 2019; Chizat & Bach, 2018; Parhi & Nowak, 2019; Neyshabur et al., 2014), we first focus on a minimum norm variant of (1). Thus, we consider the following optimization problem

\[ P^* = \min_{\{\theta_l\}_{l=1}^L} \sum_{l=1}^L \| W_l \|^2_F \text{ s.t. } f_{\theta, L}(X) = y, \tag{2} \]

where we assume that the network is over-parameterized enough to reach zero training error. The next lemma shows that the minimum squared Euclidean norm is equivalent to minimum ℓ_1 norm after a suitable rescaling.

**Lemma 1.1.** The following problems are equivalent:

\[ \min_{\{\theta_l\}_{l=1}^L} \sum_{l=1}^L \| W_l \|^2_F = \min_{\{\theta_l\}_{l=1}^L, t} \| W_L \|_1 + (L-2)t^2 \]

s.t. \( f_{\theta, L}(X) = y, \forall W_{L-1,j} ∈ B_2 \),

s.t. \( f_{\theta, L}(X) = y, \| W_l \|_1 ≤ t, \forall l ∈ [L-2] \)

where \( W_{L-1,j} \) denotes the j-th column of \( W_{L-1} \).

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1Extension to other convex loss functions is presented in the supplementary material.

2Our derivations can also be applied to the vector outputs as detailed in the next sections.

3This corresponds to weak regularization, i.e., \( \beta → 0 \) in (1) (see e.g. (Wei et al., 2018)).

4This lemma is just for summarizing our results. The detailed version is restated and proved in the following sections.
Convex Duality of Deep Neural Networks

Figure 1: One dimensional interpolation using L-layer ReLU networks with 20 neurons in each hidden layer.

Using Lemma 1.1 we first take the dual with respect to the output layer weights \( w_L \) and then change the order of \( \min \)-\( \max \) to achieve the following lower bound

\[
P^* \geq D^* = \min_{\theta} \max_{\lambda} \min_{(\theta_j)_{j=1}^{L+1}} \lambda^T y + (L-2)t^2 \quad \text{s.t.} \quad \|A^T_{L-1} \lambda\|_{\infty} \leq 1, \forall \theta_{L-1,j} \in B_2, \\
\|w_l\|_F \leq t, \forall l \in [L-2].
\]

Using the above, we first characterize a set of weights that minimize the objective via active constraints in the dual objective. We then prove the optimality of these weights by proving strong duality, i.e., \( P^* = D^* \), for deep networks. We then show that each optimal hidden layer weight matrix is rank-one and aligns with the previous layer for a deep linear network with scalar output. We further extend this result to vector output networks to show that layer weights are aligned and their ranks are directly controlled by \( \beta \).

More importantly, we prove that strong duality also holds for deep ReLU networks with rank-one inputs, where the hidden layer weights are aligned and rank-one when the output is scalar. Furthermore, we show that an optimal network has kinks at the input data points. As a corollary of this fact, we prove that deep ReLU network learns the linear spline interpolation when the input is a one-dimensional dataset. Specifically, we consider the following problem for a one-dimensional dataset \( \{(x_i, y_i)\}_{i=1}^n \), \( x_i, y_i \in \mathbb{R} \),

\[
\min_{\{\theta_i\}_{i=1}^n} \sum_{i=1}^n \ell(f_{\theta,L}(x_i), y_i) + \beta R(\theta)
\]

where \( \ell(\cdot, \cdot) \) and \( R(\theta) \) are the loss function and regularization term, respectively. Then, the function learned by an L-layer ReLU network, i.e., \( f_{\theta,L}(x_i) \), is the linear spline interpolation for \( \{x_i, y_i\}_{i=1}^n \), \( \forall l \geq 2 \). We also provide a numerical experiment in Figure 1 to verify this claim. We emphasize that this result was previously known only for two-layer networks [Savarese et al. 2019, Parhi & Nowak 2019] and here we extend it to arbitrary \( L \).

2. Two-layer linear networks

In this section, we consider two-layer linear networks with the output as \( f_{\theta,2}(X) = Xw_1w_2 \). We define the parameter space as \( \Theta = \{ (W_1, w_2, m) \mid W_1 \in \mathbb{R}^{d \times m}, w_2 \in \mathbb{R}^m, m \in \mathbb{Z}_+ \} \). In the following, we first describe the training problem with equality constraint as in (2) and then extend our derivations to the original formulation in (1).

2.1. Training problem with equality constraints

The equality constrained training problem can be written as

\[
\min_{\theta \in \Theta} \|W_1\|_F^2 + \|w_2\|_2^2 \quad \text{s.t.} \quad f_{\theta,2}(X) = y.
\]

The next lemma shows that this problem can be reformulated as an \( \ell_1 \) problem norm after a suitable rescaling.

**Lemma 2.1.** ([Savarese et al. 2019, Neyshabur et al. 2014]) The following two problems are equivalent:

\[
\min_{\theta \in \Theta} \|W_1\|_F^2 + \|w_2\|_2^2 = \min_{\theta \in \Theta} \|w_2\|_1 \\
\quad \text{s.t.} \quad f_{\theta,2}(X) = y \quad \text{s.t.} \quad f_{\theta,2}(X) = y, \forall w_{1,j} \in B_2.
\]

Using Lemma 2.1, we equivalently have

\[
P^* = \min_{\theta \in \Theta} \|w_2\|_1 \quad \text{s.t.} \quad f_{\theta,2}(X) = y, \forall w_{1,j} \in B_2,
\]

which has the following dual form.

**Theorem 2.1.** The dual of the problem in (3) is given by

\[
D^* = \max_{\lambda \in \mathbb{R}^n} \lambda^T y \quad \text{s.t.} \quad |\lambda^TXw_1|_1 \leq 1, \forall w_1 \in B_2
\]

and we have \( P^* \geq D^* \). For finite width networks, there exists a finite \( m \) value such that we have strong duality, i.e., \( P^* = D^* \), and an optimal \( W_1 \) for (4) satisfies \( \|\lambda^TXw_1\|_1 \). where \( \lambda^* \) is dual optimal.

Based on Theorem 2.1, we can characterize the optimal neurons as the extreme points of a convex set as follows.

**Corollary 2.1.** Theorem 2.1 implies that the optimal neurons are extreme points which solve the following problem

\[
\arg\max_{w_1: \|w_1\|_2 \leq 1} |\lambda^TXw_1|.
\]

**Definition 1.** Throughout the paper, we use the term “extreme point” to denote the neurons that maximize the dual constraint, e.g., see Corollary 2.1.

From Theorem 2.1, we have the following dual problem

\[
\max_{\lambda} \lambda^T y \quad \text{s.t.} \quad |\lambda^TXw_1|_1 \leq 1, \forall w_1 \in B_2.
\]

Let \( \lambda = U \Sigma V^T \) be the singular value decomposition (SVD) of \( \lambda^* \). If we assume that there exists \( w^* \) such that \( Xw^* = y \) due to Proposition 2.1, then (6) is equivalent to

\[
\max_{\lambda} \lambda^T \Sigma_x \tilde{w}^* \quad \text{s.t.} \quad \|\Sigma_x^T \lambda\|_2 \leq 1,
\]

\footnote{All the proofs are presented in the supplementary material.}

\footnote{In this paper, we use full SVD unless otherwise stated.}
where $\hat{\lambda} = U_x^T \lambda$ and $\hat{w}^* = V_x^T w^*$. Notice that in (7), we use an alternative formulation for the constraint, i.e., $\|X^T \lambda\|_2 \leq 1$ instead of $|X^T \mathbf{w}_1| \leq 1$, $\forall \mathbf{w}_1 \in B_2$ since the extreme point is achieved when $w_1 = X^T \lambda / \|X^T \lambda\|_2$.

Given rank($X$) = $r \leq \min\{n, d\}$, we have

$$\hat{\lambda}^T \Sigma^* \hat{w} = \lambda^T \Sigma \begin{bmatrix} I_{d-r \times r} & 0_{d-r \times r} \\ 0_{r \times d-r} & 0_{r \times d-r} \end{bmatrix} \begin{bmatrix} \hat{w}^* \\ \hat{w} \end{bmatrix} \leq \|\Sigma^T \hat{\lambda}\|_2 \|\hat{w}^*\|_2 = \|\hat{w}^*\|_2,$$

which shows that the maximum objective value is achieved when $\Sigma^T \hat{\lambda} = c_1 \hat{w}^*$. Thus, an optimal neuron is

$$w^*_1 = \frac{V_x \Sigma^T \hat{\lambda}}{\|V_x \Sigma^T \hat{\lambda}\|_2} = \frac{V_x \hat{w}^*}{\|V_x \hat{w}^*\|_2} = \frac{P_{\mathcal{X}^T}(w^*)}{\|P_{\mathcal{X}^T}(w^*)\|_2}.$$

where $P_{\mathcal{X}^T}(\cdot)$ projects its input onto the range of $X^T$.

In the following results, we first prove that the planted model assumption can be used without loss of generality. Then, we show that strong duality holds for (4).

**Proposition 2.1.** ([Du & Hu 2019]) Assuming there exists a planted model parameter, i.e., $Xw^* = y$, does not change the solution to the following training problem

$$\min_{w_1, w_2} \|XW_1 w_2 - y\|_2^2.$$

**Theorem 2.2.** Let $\{X, y\}$ be a dataset such that (4) is feasible. Then, strong duality holds for (4).

### 2.2. Regularized training problem

In this section, we define the regularized version of (4) as

$$\min_{\theta \in \Theta} \beta \|W_2\|_2 + \frac{1}{2} \|f_{\theta,2}(X) - y\|_2^2 \text{ s.t. } \forall \mathbf{w}_{1,j} \in B_2, \quad (8)$$

which has the following dual form

$$\max_{\mathbf{\lambda}} \frac{1}{2} \mathbf{\lambda} - \|\mathbf{y}\|_2^2 + \frac{1}{2} \|\mathbf{y}\|_2^2 \text{ s.t. } |\lambda^T X \mathbf{w}_1| \leq \beta, \forall \mathbf{w}_1 \in B_2.$$

The next lemma provides an equivalent formulation for this problem.

**Lemma 2.2.** The following problems are equivalent

$$\max_{\mathbf{\lambda}} \frac{1}{2} \mathbf{\lambda} - \|\mathbf{y}\|_2^2 + \frac{1}{2} \|\mathbf{y}\|_2^2 \text{ s.t. } |\lambda^T X \mathbf{w}_1| \leq \beta, \forall \mathbf{w}_1 \in B_2 \quad \text{ s.t. } \|X^T X \mathbf{w}_1\|_2 \leq \beta.$$

Using Lemma 2.2, we write the problem as

$$\min_\mathbf{\hat{w}} \|\mathbf{\hat{s}} - \hat{w}^*\|_2^2 \text{ s.t. } \|\Sigma^T \mathbf{\hat{s}}\|_2 \leq \beta, \quad (9)$$

where $\hat{\mathbf{s}} = \Sigma_x V_x^T s$ and $\hat{w}^* = \Sigma_x V_x^T w^*$. Then, an optimal neuron can be described as

$$w^*_1 = \frac{V_x \Sigma^T \hat{\lambda}_{\beta} \hat{w}^*}{\|V_x \Sigma^T \hat{\lambda}_{\beta} \hat{w}^*\|_2} \text{ s.t. } P_{\mathcal{X}^T,\beta}(\cdot) \text{ projects its input to } \{u \in \mathbb{R}^d \|\Sigma^T_u u\|_2 \leq \beta\}, \quad (10)$$

where $P_{\mathcal{X}^T,\beta}(\cdot)$ projects its input onto the range of $X^T$.

**Theorem 2.3.** For any dataset $\{X, y\}$, strong duality holds for the two-layer linear network training problem in (3).

### 2.3. Training problem with vector outputs

Here, we modify our model as $f_{\theta,2}(X) = XW_1 W_2$ to estimate $Y \in \mathbb{R}^{n \times k}$. In the sequel, we examine the equality constrained and regularized version of the problem.

#### 2.3.1. Equality constrained case

In this case, we have the following primal problem

$$\min_{\theta \in \Theta} \|W_1\|_F^2 + \|W_2\|_F^2 \text{ s.t. } f_{\theta,2}(X) = Y, \quad (10)$$

which can be equivalently stated as follows.

**Lemma 2.3.** The following problems are equivalent:

$$\min_{\theta \in \Theta} \|W_1\|_F^2 + \|W_2\|_F^2 = \min_{\theta \in \Theta} \sum_{j=1}^m \|w_{2,j}\|_2 \text{ s.t. } f_{\theta,2}(X) = Y, \quad (11)$$

Using Lemma 2.3, we reformulate (10) as

$$\min_{\theta \in \Theta} \sum_{j=1}^m \|w_{2,j}\|_2 \text{ s.t. } f_{\theta,2}(X) = Y, \forall \mathbf{w}_{1,j} \in B_2.$$

which has the following dual with respect to $W_2$

$$\max_{\mathbf{\lambda}} \text{trace}(A^T Y) \text{ s.t. } \|A^T X \mathbf{w}_1\|_2 \leq 1, \forall \mathbf{w}_1 \in B_2. \quad (12)$$

Since we can assume that $Y = XW^*$ due to Proposition 2.1, where $W^* \in \mathbb{R}^{d \times k}$, we obtain the following bound

$$\text{trace}(A^T Y) = \text{trace}(A^T X W^*) \leq \sigma_{\max}(A^T U_x \Sigma_x \hat{W}^*_r) \|\hat{W}^*_r\|_2 \leq \|\hat{W}^*_r\|_2 \quad (13)$$

where $\sigma_{\max}(A^T X)$ is $\leq 1$ due to (12) and

$$\hat{W}^*_r = \begin{bmatrix} I_r & 0_{r \times d-r} \\ 0_{d-r \times r} & 0_{d-r \times d-r} \end{bmatrix} U_x^T W^*.$$

Given the SVD of $\hat{W}^*_r$, i.e., $U_w \Sigma_w \hat{W}^*_r$, choosing

$$A^T U_x \Sigma_x = V_w \begin{bmatrix} I_r & 0_{r \times d-r} \\ 0_{k-r \times r} & 0_{k-r \times d-r} \end{bmatrix} U_w^T$$

achieves the upper-bound above, where $r_w = \text{rank}(\hat{W}^*_r)$. Thus, optimal neurons can be formulated as a subset of the first $r_w$ right singular vectors of $A^T X$. Moreover, the next result shows that strong duality holds in this case as well.
Theorem 2.4. Let \( \{X, Y\} \) be a dataset such that \((11)\) is feasible. Then, strong duality holds for \((11)\).

2.3.2. Regularized Case

Here, we define the regularized version of \((11)\) as follows
\[
\min_{\emptyset \in \Theta} \frac{1}{2} \sum_{j=1}^{m} \|w_{2,j}\|^2 + \frac{1}{2} \|f_{\theta,2}(X) - Y\|^2 \quad \text{s.t. } \forall w_{1,j} \in B_2.
\]
which has the following dual with respect to \(W_2\)
\[
\max_{\lambda} \frac{1}{2} \|A - Y\|^2 + \frac{1}{2} \|Y\|^2 \quad \text{s.t. } \sigma_{\max}(\Lambda^T X) \leq \beta.
\]
In Lemma 2.2, this problem can be rewritten as
\[
\max_{\lambda} -\|S - W^*\|^2 \quad \text{s.t. } \sigma_{\max}(S^T \Sigma_x) \leq \beta, \quad (14)
\]
where \(S = \Sigma_x V^T \Sigma \) and \(W^* = \Sigma_x V^T W^*\). Then, the optimal neurons are a subset of the maximum right singular vectors of \(P_{\Sigma_x, \beta}(W^*)^T \Sigma_x V^T \), where \(P_{\Sigma_x, \beta}(\cdot)\) projects its input to the set \(\{U \in \mathbb{R}^{n \times k} : \sigma_{\max}(U^T \Sigma_x) \leq \beta\}\).

Remark 2.1. We note that the optimal neurons are the right singular vectors of \(P_{\Sigma_x, \beta}(W^*)^T \Sigma_x V^T \) that achieve the corresponding upper-bound of the set, i.e., \(\|P_{\Sigma_x, \beta}(W^*)^T \Sigma_x V^T w^*_1\|_2 = \beta\), where \(w^*_1\) is a normalized optimal neuron. This implies that the optimal neurons satisfy \(\|W^* \Sigma_x V^T w^*_1\|_2 \geq \beta\). Therefore, the number of optimal neurons and the rank of the optimal weight matrix, i.e., \(W_1\), are directly controlled by the value of \(\beta\).

Remark 2.2. There might exist optimal solutions other than the right singular vectors of \(P_{\Sigma_x, \beta}(W^*)^T \Sigma_x V^T \). As an example, consider \(u_1\) and \(u_2\) as the optimal right singular vectors. Then, any \(u = \alpha_1 u_1 + \alpha_2 u_2\) with \(\alpha_1^2 + \alpha_2^2 = 1\) also achieves the upper-bound, therefore, optimal.

3. Deep linear networks

Here, we consider an \(L\)-layer linear network with \(f_{\theta,L}(X) = XW_1 \ldots W_L\), where we examine the equality constrained and regularized versions of the problem.

3.1. Training problem with equality constraints

The training problem can be described as
\[
P^* = \min_{\{\theta_i\}_{i=1}^{L}} \sum_{l=1}^{L} \|W_l\|_F^2 \quad \text{s.t. } \quad f_{\emptyset,L}(X) = y, \quad (15)
\]
which can be equivalently stated as follows,

Lemma 3.1. The following problems are equivalent:
\[
\min_{\{\theta_i\}_{i=1}^{L}} \sum_{l=1}^{L} \|W_l\|_F^2 = \min_{\{\theta_i\}_{i=1}^{L} \in \Theta_{L-1}}, \sum_{l=1}^{L-2} \|W_l\|_F^2 + \sum_{l=1}^{L-2} t_l^2 \quad \text{s.t. } \quad f_{\emptyset,L}(X) = y, \quad \forall w_{L-1,j} \in B_2
\]
\[
\|W_l\|_F \leq t_l, \quad \forall l \in [L - 2]
\]

Proposition 3.1. First \(L - 2\) hidden layer weight matrices in \((13)\) have the same operator and Frobenius norms.

Using Lemma 3.1 and Proposition 3.1, we have the following dual problem for \((15)\)
\[
P^* = \min_{\{\theta_i\}_{i=1}^{L}} \max_{\lambda} \lambda^T y + (L - 2)t^2
\]
\[
\text{s.t. } \|XW_1 \ldots W_{L-1}\|^2 \lambda \leq 1, \quad \forall W_{L-1,j} \in B_2, \quad (16)
\]
\[
\|W_l\|_F \leq t_l, \quad \forall l \in [L - 2]
\]
Now, let us assume that the optimal Frobenius norm for each layer \(l \) is \(t^*\). Then, if we define \(\Theta_{L-1} = \{\theta_1, \ldots, \theta_{L-1}\} \|W_{L-1,j}\|^2 \leq 1, \forall j \in [m_{L-1}], \|W_l\|_F \leq t^*, \forall l \in [L - 2]\), (16) reduces to the following problem
\[
P^* \geq D^* = \max_{\lambda} \lambda^T y
\]
\[
\text{s.t. } \|XW_1 \ldots W_{L-1}\|^2 \lambda \leq 1, \quad \forall \theta_l \in \Theta_{L-1}, \forall l \quad (17)
\]
where we change the order of min-max to obtain a lower bound for \((16)\). The dual of the semi-infinite problem in \((17)\) is given by
\[
\min_{\mu} \|\mu\|_{TV}
\]
\[
\text{s.t. } \int_{\Theta_{L-1}} XW_1 \ldots W_{L-1} d\mu(\theta_1, \ldots, \theta_{L-1}) = y, \quad (18)
\]
where \(\mu\) is a signed Radon measure and \(\| \cdot \|_{TV}\) is the total variation norm. We emphasize that \((18)\) has infinite width in each layer, however, an application of Carathéodory’s theorem shows that the measure \(\mu\) in the integral can be represented by finitely many (at most \(n + 1\) Dirac delta functions \((Rosset et al. 2007)\)). Such selection of \(\mu\) yields the following problem
\[
P_m^* = \min_{\{\theta_i\}_{i=1}^{L}} \|W_L\|_F
\]
\[
\text{s.t. } \sum_{j=1}^{m_{L-1}} XW_1^T \ldots W_{L-1}^T w_{L,j} = y, \quad \theta_j \in \Theta_{L-1}, \forall l \quad (19)
\]
We first note that since the model in \((19)\) has multiple weight matrices for each layer, it has more expressive power than a regular network. Thus, we have \(P^* \geq P_m^*\). Since the dual of \((13)\) and \((19)\) are the same, we also have \(D_m^* = D^*\), where \(D_m^*\) is the optimal dual value for \((19)\).

We now apply the variable change in \((7)\) to \((17)\) as follows
\[
\max_{\lambda} \lambda^T \Sigma_x w^*_r
\]
\[
\text{s.t. } \|W_{L-2}^T \ldots W^T \Sigma_x \|_2 \leq 1, \quad \forall \theta_l \in \Theta_{L-1}, \forall l
\]
which shows that the maximum objective value is achieved when \(\Sigma_x^T \lambda = c_1 w^*_r\). Thus, the optimal layer weights can

\footnote{With this assumption, \((L - 2)t^2\) becomes constant so we ignore this term for the rest of our derivations.}
be found as the maximizers of the constraint when \( \Sigma_x^T \lambda = c_1 \tilde{w}_r^* \). To find the formulations explicitly, we first find an upper-bound for the constraint in (20) as follows
\[
\|W_{L-2}^T \cdots W_1^T V_x \Sigma_x^T \hat{\lambda}\|_2 = c_1 \|W_{L-2}^T \cdots W_1^T V_x \tilde{w}_r^*\|_2 \\
\leq c_1 \|W_{L-2}^T \cdots \|_2 \cdots \| V_x \tilde{w}_r^*\|_2 \\
\leq c_1 \| \tilde{w}_r^*\|_2,
\]
where the last inequality follows from the constraint on each layer weight’s norm and \( \gamma = t_s^{L-2} \). This upper-bound can be achieved when the layer weights are
\[
W_l^* = \begin{cases} 
 t_s^l \frac{V_x \tilde{w}_r^*}{\|V_x \tilde{w}_r^*\|_2} P^T_1 & \text{if } l = 1 \\
 t_s^l \rho_{l-1}^T P^T_1 & \text{if } 1 < l \leq L - 2 \\
 \rho_{L-2}^T & \text{if } l = L - 1 
\end{cases}
\]
where \( \| \rho_l \|_2 = 1, \forall l \in [L - 2] \). This shows that the weight matrices are rank-one and align with each other. Therefore, an arbitrary set of unit norm vectors, i.e., \( \{ \rho_l \}_{l=1}^{L-2} \) can be chosen to achieve the maximum dual objective.

We note that the layer weights in (21) are optimal for the relaxed problem in (19). However, since there exists a single possible choice for the left singular vector of \( W_1 \) and we can select an arbitrary set for \( \{ \rho_l \}_{l=1}^{L-2} \), we achieve \( D_{22}^* = D^* \) using the same layer weights. Therefore, the set of weights in (21) are also optimal for (15). The next theorem shows that strong duality holds in this case.

**Theorem 3.1.** Let \( \{ X, y \} \) be a dataset such that (15) is feasible. Then, strong duality holds for (15).

**Corollary 3.1.** As a consequence of the analysis above, a deep linear network achieves the desired output using the first hidden layer alone. Therefore, rest of the layers do not add any expressive power to the network.

### 3.2. Regularized training problem

Using Lemma 2.2 and Proposition 3.1, we have the following dual for the regularized version of (15)
\[
\max_{\Lambda} - \frac{1}{2} \|Xs - Xw^*\|_2^2 \\
s.t. \| (XW_1 \cdots W_{L-2})^T Xs \|_2^2 \leq \beta, \forall \theta_l \in \Theta_{L-1}, \forall l.
\]
Then, using the notation in (9), the weight matrices that maximize the value of the constraint can be described as
\[
W_l^* = \begin{cases} 
 t_s^l \frac{V_x \Sigma_x^T \hat{\lambda}}{\|V_x \Sigma_x^T \hat{\lambda}\|_2} P^{T}_1 & \text{if } l = 1 \\
 t_s^l \rho_{l-1}^T \rho_{l-2}^T & \text{if } 1 < l \leq L - 2 \\
 \rho_{L-2}^T & \text{if } l = L - 1 
\end{cases}
\]
where \( P_{\Sigma_x, \beta}(\cdot) \) projects its input to \( \{ u \in \mathbb{R}^d, \| \Sigma_x^T u \|_2^2 \leq \beta \gamma^{-1} \} \).

**Corollary 3.2.** The analysis above and Theorem 3.1 also show that strong duality holds for the regularized deep linear network training problem.

### 3.3. Training problem with vector outputs

Here, we consider vector output, i.e., \( m_L = k \), deep linear networks with the output \( f_{\theta, L}(X) = XW_1 \cdots W_L \).

#### 3.3.1. Equality constrained case

In this case, we have the following training problem
\[
\min_{\{ \theta_l \}_{l=1}^L} \sum_{l=1}^{L} \|W_l\|_F^2 \text{ s.t. } f_{\theta, L}(X) = Y, \tag{22}
\]
which has the equivalent form shown in the lemma below.

**Lemma 3.2.** The following problems are equivalent:
\[
\min_{\{ \theta_l \}_{l=1}^L} \sum_{l=1}^{L} \|W_l\|_F^2 \text{ s.t. } f_{\theta, L}(X) = Y, \forall \theta_{L-1} \in B_2 \\
s.t. f_{\theta, L}(X) = Y, \forall \theta_{L-1} \in B_2 \\
\|W_l\|_F \leq t_l, \forall l \in [L - 2]
\]

Using Proposition 3.1 and Lemma 3.2 we obtain the following dual problem
\[
\max_{\Lambda} \text{trace}(\Lambda^T Y) \tag{23}
\]
\[s.t. \sigma_{max}(\Lambda^T XW_1 \cdots W_{L-2}) \leq \lambda, \forall \theta_l \in \Theta_{L-1}.
\]

It is straightforward to show that the optimal layer weights are the extreme points of the constraint in (23), which achieves the following upper-bound
\[
\max_{\{ \theta_l \}_{l=1}^L \in \Theta_{L-1}} \sigma_{max}(\Lambda^T XW_1 \cdots W_{L-2}) \leq \sigma_{max}(\Lambda^T X) \gamma.
\]

This upper-bound is achieved when the first \( L - 2 \) layer weights are rank-one with the singular value \( t_s^l \) by Proposition 3.1. Additionally, the left singular vector of \( W_1 \) needs to align with one of the maximum right singular vectors of \( \Lambda^T X \). Since the upper-bound for the objective is achievable for any \( \Lambda \), we can maximize the objective value, as in (13), by choosing a matrix \( \Lambda \) such that
\[
\Lambda^T U_x \Sigma_x = V_w \left[ \begin{array}{cc}
\gamma^{-1} I_{r_w} & 0_{r_w \times d-r_w} \\
0_{k-r_w \times r_w} & 0_{k-r_w \times d-r_w}
\end{array} \right] U_w^T
\]
where \( W^*_w = U_w \Sigma_w V_w^T \). Thus, a set of optimal layer weights can be formulated as follows
\[
W_l^* = \begin{cases} 
 t_s^l \tilde{w}_{w,j} \rho_{l-1}^T & \text{if } l = 1 \\
 t_s^l \rho_{l-1}^T \rho_{l-2}^T & \text{if } 1 < l \leq L - 2 \\
 \rho_{L-2}^T & \text{if } l = L - 1 
\end{cases}
\]
where \( \tilde{w}_{w,j} \) is the \( j^{th} \) maximal right singular vector of \( \Lambda^T X \). However, notice that the layer weights in (24) are
feasible. Then, strong duality holds for Theorem 3.2.

Let (22) be a dataset such that \( X = c a_0^T \), where \( c \in \mathbb{R}_+^n \) and \( a_0 \in \mathbb{R}^m \), then the weight matrix for each layer can be formulated as follows

\[
W_l = \frac{a_{l-1}}{a_{l-2}} \phi_l^T, \forall l \in [L - 2], \quad w_{L-1} = \frac{a_{L-2}}{a_{L-2}}
\]

where \( a_l = (a_l^T W_l)^+ \), \( \forall l \in [L - 1] \), and \( \{ \phi_l \}_{l=1}^{L-2} \) is a set of vectors satisfying \( \| \phi_l \|_2 = t^* \), \( \forall l \in [L - 2] \).

Our derivations can also be extended to a case with bias term as illustrated in the next proposition.

**Proposition 4.1.** Theorem 4.1 still holds when we add a bias term to the last hidden layer of the problem in (28), i.e., the output network becomes \( (A_{L-2} W_{L-1} + 1_n b^T)^+ \) \( w_L = y \), where \( A_l = (A_l-1 W_l)^+ \), \( \forall l \in [L - 2] \).

Based on Proposition 4.1, we next prove that the optimal solution has kinks at the input data points.

**Corollary 4.1.** As a result of Proposition 4.1 and Theorem 4.1, the optimal solutions have kinks at the input data points so that the network output becomes linear spline interpolation for one-dimensional datasets.

**Corollary 4.2.** As a direct consequence of Theorem 4.1, several cases of strong duality also holds for deep ReLU networks.

**Remark 4.1.** Since the layer weights align with the previous layers as proved in Theorem 4.1, each weight matrix exhibits a rank-one structure. Therefore, adding more layers does not increase the expressive power of the network.

We note that all the results also hold for the regularized version of (28) since our characterization stays the same.

### 5. Numerical experiments

Here, we present numerical results to verify our theoretical analysis in the previous section.\(^8\) We first consider a two-layer linear network with the parameters \( W_1 \in \mathbb{R}^{20 \times 50} \) and \( W_2 \in \mathbb{R}^{50 \times 5} \). In order to prove our claim in Remark 2.1, we train the network using GD with different regularization parameters. In Figure 2a, we plot the rank of \( W_1 \) as a function of the regularization parameter \( \beta \), where we also plot the location of the singular values of \( \Sigma_x \Sigma_x^T \) using vertical red lines. This experiment clearly shows that the rank of the hidden layer changes when \( \beta \) is equal to one of

\( \Sigma \) is a maximal right singular vector of \( \mathcal{P}_{S_x, \beta} (W^*)^T \Sigma_x V_x^T \) and \( \mathcal{P}_{S_x, \beta} (\cdot) \) projects its input to the set \( \{ U \in \mathbb{R}^{n \times k} | \| u \|_2 \leq \beta \gamma^{-1} \} \). Additionally, \( \rho_{l,i,j} \)'s is an orthonormal set. Therefore, the rank of each hidden layer is determined by \( \beta \) as in Remark 2.1.

4. Deep ReLU networks

In this section, we consider an \( L \)-layer ReLU network with \( m_L = 1 \) and the output \( f_{\theta, L}(X) = A_{L-1} w_L \), where

\[
A_l = (A_{l-1} W_l)^+, \quad \forall l \in [L - 1], \quad A_0 = X, \quad \text{and} \quad (x)_+ = \max(0, x). \quad \text{The training problem is as follows}
\]

\[
\min \left\{ \sum_{l=1}^{m_L-1} \| W_{l,j} \|_2 \right\} \quad \text{s.t.} \quad \sum_{j=1}^{m_L-1} X W_{l,j} \cdots W_{L-1,j}^T = Y, \quad \forall \theta_l^T \in \Theta_{L-1}
\]

Using the optimal layer weights in (24), we have the following network output for the relaxed model

\[
\sum_{j=1}^{m_L-1} X W_{l,j} \cdots W_{L-1,j}^T = \gamma \sum_{j=1}^{m_L-1} q_{w,j} W_{L,j}^T
\]

Since we know that the objective value for (25) is a lower bound for (22), the layer weights that achieve the output above for the original problem in (22) is optimal. Thus, a set of optimal solutions to (25) can be formulated as follows

\[
W_l^T = \begin{cases}
\tau^* \sum_{j=1}^{m_{l-1}} \hat{v}_{x,j} \rho_{l,j}^T & \text{if } l = 1 \\
\tau^* \sum_{j=1}^{m_{l-1}} -\rho_{l-1,j} \rho_{l,j}^T & \text{if } 1 < l \leq L - 2 \\
\tau^* \sum_{j=1}^{m_{l-1}} \rho_{l-1,j} \rho_{l-2,j} & \text{if } l = L - 1
\end{cases}
\]

where \( \hat{v}_{x,j} \) is a maximal right singular vector of \( \mathcal{P}_{S_x, \beta} (W^*)^T \Sigma_x V_x^T \) and \( \mathcal{P}_{S_x, \beta} (\cdot) \) projects its input to the set \( \{ U \in \mathbb{R}^{n \times k} | \| U \|_2 \leq \beta \gamma^{-1} \} \). Additionally, \( \rho_{l,i,j} \)'s is an orthonormal set. Therefore, the rank of each hidden layer is determined by \( \beta \) as in Remark 2.1.

### 3.3.2. Regularized case

Using Lemma 2.2 and 3.2 and Proposition 3.1, we have the following dual for the regularized version of (22).

\[
\max -\frac{1}{2} \| \hat{S} - \hat{W}^* \|_F^2
\]

s.t. \( \| \Sigma_x V_x^T S \|_2 \leq \beta, \forall \theta_l \in \Theta_{L-1} \),

where \( \hat{S} = \Sigma_x V_x^T S \) and \( \hat{W}^* = \Sigma_x V_x^T W^* \). Then, as in (26), a set of optimal layer weights is

\[
W_l^T = \begin{cases}
\tau^* \sum_{j=1}^{m_{l-1}} \hat{v}_{x,j} \rho_{l,j}^T & \text{if } l = 1 \\
\tau^* \sum_{j=1}^{m_{l-1}} -\rho_{l-1,j} \rho_{l,j}^T & \text{if } 1 < l \leq L - 2 \\
\tau^* \sum_{j=1}^{m_{l-1}} \rho_{l-1,j} \rho_{l-2,j} & \text{if } l = L - 1
\end{cases}
\]

where \( \hat{v}_{x,j} \) is a maximal right singular vector of \( \mathcal{P}_{S_x, \beta} (W^*)^T \Sigma_x V_x^T \) and \( \mathcal{P}_{S_x, \beta} (\cdot) \) projects its input to the set \( \{ U \in \mathbb{R}^{n \times k} | \| U \|_2 \leq \beta \gamma^{-1} \} \). Additionally, \( \rho_{l,i,j} \)'s is an orthonormal set. Therefore, the rank of each hidden layer is determined by \( \beta \) as in Remark 2.1.

### 4. Deep ReLU networks

In this section, we consider an \( L \)-layer ReLU network with \( m_L = 1 \) and the output \( f_{\theta, L}(X) = A_{L-1} w_L \), where
Figure 2: Verification of our results on linear networks. (a) Rank of the hidden layer weight matrix as a function of $\beta$ and (b) rank of the hidden layer weights for four different regularization parameters, i.e., $\beta_1 < \beta_2 < \beta_3 < \beta_4$.

Figure 3: Evolution of the operator and Frobenius norms for the hidden layer weights of a deep linear network.

Figure 4: Rank of the hidden layer weights of a five-layer ReLU network with scalar output.

6. Concluding remarks

We have studied norm regularized deep neural network training problems and developed an analytic framework to characterize a set of optimal solutions. Particularly, we showed that optimal layer weights can be explicitly formulated as the extreme points of a convex set via the dual problem. We then proved that strong duality holds for deep linear networks and provided a set of optimal solutions to the training problem. We also extended our derivations to the vector outputs and arbitrary convex loss functions. More importantly, we also utilized our characterization to prove that strong duality holds for deep ReLU networks with rank-one input and scalar output. As a corollary, we further proved that the kinks of ReLU activations occur exactly at the input data points so that the optimized network yields simple solutions, e.g., linear spline interpolation for one-dimensional datasets. We conjecture that a similar characterization can also be applied to any deep ReLU network to explain their extraordinary generalization performance in practice.
References


A. Supplementary Material

In this file, we present additional materials and proofs of the main results that are not included in the main paper due to the page limit. We also restate each result before the corresponding proof for the convenience of the reader. We refer to the equations in the main paper as [Main Paper, (#)] (except for the restatements of the theoretical results in the main paper) to prevent ambiguities.

A.1. General loss functions

In this section, we show that our extreme point characterization holds for arbitrary convex loss functions.

\[ \min_{\theta \in \Theta} \ell(f_{\theta,2}(X), y) + \beta \|w_2\|_1 \quad \text{s.t.} \quad \forall w_{1,j} \in B_2, \quad (29) \]

where \( \ell(\cdot, y) \) is a convex loss function.

**Theorem A.1.** The dual of (29) is given by

\[ \max_{\lambda} -\ell^*(\lambda) \quad \text{s.t.} \quad \|X^T\lambda\|_2 \leq \beta, \]

where \( \ell^* \) is the Fenchel conjugate function defined as

\[ \ell^*(\lambda) = \max_{z} z^T \lambda - \ell(z, y). \]

Theorem A.1 proves that our extreme point characterization in Corollary 2.1 applies to arbitrary loss function. Therefore, optimal parameters for (3) and (8) are a subset of the same extreme point set, i.e., determined by the input data matrix \( X \), independent of loss function.

**Remark A.1.** Since our characterization is generic in the sense that it holds for vector output, deep linear and deep ReLU networks (see the main paper for details), Theorem A.1 is valid for all of our derivations.

A.2. Additional numerical results

Here, we present numerical results that are not included in the main paper due to the page limit. In Figure 5a, we perform an experiment to check whether the hidden neurons of a two-layer linear network align with the proposed right singular vectors. For this experiment, we select a certain \( \beta \) such that \( W_1 \) becomes rank-two. After training, we first normalize each neuron to have unit norm, i.e., \( \|w_{1,j}\|_2 = 1, \forall j \), and then compute the sum of the projections of each neuron onto each right singular vector, i.e., denoted as \( v_i \). Since we choose \( \beta \) such that \( W_1 \) is a rank-two matrix, most of the neurons align with the first two right singular vectors as expected. Therefore, this experiment verifies our analysis and claims in Remark 2.1. We also provide the histogram of the projections for this experiment in Figure 6. Furthermore, as an alternative to Figure 2a, we plot the singular values of \( W_1 \) with respect to the regularization parameter \( \beta \) in Figure 5b.

A.3. Proofs of the main results

**Lemma 2.1.** ([Savarese et al., 2019] [Neyshabur et al., 2014]) The following two problems are equivalent:

\[ \min_{\theta \in \Theta} \|W_1\|_F^2 + \|w_2\|_2^2 \quad \text{s.t.} \quad f_{\theta,2}(X) = y \]

\[ \min_{\theta \in \Theta} \|w_2\|_1 \quad \text{s.t.} \quad f_{\theta,2}(X) = y, \forall w_{1,j} \in B_2. \]

**Proof of Lemma 2.1** For any \( \theta \in \Theta \), we can rescale the parameters as \( \bar{w}_{1,j} = \alpha_j w_{1,j} \) and \( \bar{w}_{2,j} = w_{2,j}/\alpha_j \), for any \( \alpha_j > 0 \). Then, the network output becomes

\[ f_{\theta,2}(X) = \sum_{j=1}^{m} \bar{w}_{2,j}X\bar{w}_{1,j} = \sum_{j=1}^{m} \frac{w_{2,j}}{\alpha_j} \alpha_j Xw_{1,j} = \sum_{j=1}^{m} w_{2,j}Xw_{1,j}, \]

which proves \( f_{\theta,2}(X) = f_{\bar{\theta},2}(X) \). In addition to this, we have the following basic inequality

\[ \frac{1}{2} \sum_{j=1}^{m} (w_{2,j}^2 + \|w_{1,j}\|_2^2) \geq \sum_{j=1}^{m} (|w_{2,j}| \|w_{1,j}\|_2), \]
where the equality is achieved with the scaling choice \( \alpha_j = \left( \frac{1}{\|w_{1,j}\|} \right)^2 \) is used. Since the scaling operation does not change the right-hand side of the inequality, we can set \( \|w_{1,j}\| = 1, \forall j \). Therefore, the right-hand side becomes \( \|w_2\| \).

Now, let us consider a modified version of the problem, where the unit norm equality constraint is relaxed as \( \|w_{1,j}\| \leq 1 \). Let us also assume that for a certain index \( j \), we obtain \( \|w_{1,j}\| < 1 \) with \( w_{2,j} \neq 0 \) as an optimal solution. This shows that the unit norm inequality constraint is not active for \( w_{1,j} \), and hence removing the constraint for \( w_{1,j} \) will not change the optimal solution. However, when we remove the constraint, \( \|w_{1,j}\| \to \infty \) reduces the objective value since it yields \( w_{2,j} = 0 \). Therefore, we have a contradiction, which proves that all the constraints that correspond to a nonzero \( w_{2,j} \) must be active for an optimal solution. This also shows that replacing \( \|w_{1,j}\| = 1 \) with \( \|w_{1,j}\| \leq 1 \) does not change the solution to the problem.

**Theorem 2.1.** The dual of the problem in (4) is given by

\[
D^* = \max_{\lambda \in \mathbb{R}^n} \lambda^T y \text{ s.t. } \|\lambda^T Xw_1\| \leq 1 \forall w_1 \in B_2
\]

and we have \( P^* \geq D^* \). For finite width networks, there exists a finite \( m \) value such that we have strong duality, i.e., \( P^* = D^* \), and an optimal \( W_1 \) for (4) satisfies \( \|(XW_1)^T \lambda^*\|_\infty = 1 \), where \( \lambda^* \) is dual optimal.

**Corollary 2.1.** Theorem 2.1 implies that the optimal neurons are extreme points which solve the following problem

\[
\arg\max_{w_1: \|w_1\| \leq 1} |\lambda^*^T Xw_1|.
\]

**Proof of Theorem 2.1 and Corollary 2.1** We first note that the dual of [Main Paper, (4)] with respect to \( w_2 \) is

\[
\min_{\theta \in \Theta \setminus \{w_2\}} \max_{\lambda} \lambda^T y \text{ s.t. } \|(XW_1)^T \lambda\|_\infty \leq 1, \|w_{1,j}\| \leq 1, \forall j.
\]

Then, we can reformulate the problem as follows

\[
P^* = \min_{\theta \in \Theta \setminus \{w_2\}} \max_{\lambda} \lambda^T y + \mathcal{I}(\|(XW_1)^T \lambda\|_\infty \leq 1), \text{ s.t. } \|w_{1,j}\| \leq 1, \forall j.
\]

where \( \mathcal{I}(\|(XW_1)^T \lambda\|_\infty \leq 1) \) is the characteristic function of the set \( \|(XW_1)^T \lambda\|_\infty \leq 1 \), which is defined as

\[
\mathcal{I}(\|(XW_1)^T \lambda\|_\infty \leq 1) = \begin{cases} 
0 & \text{if } \|(XW_1)^T \lambda\|_\infty \leq 1 \\
-\infty & \text{otherwise}
\end{cases}
\]

Since the set \( \|(XW_1)^T \lambda\|_\infty \leq 1 \) is closed, the function \( \Phi(\lambda, W_1) = \lambda^T y + \mathcal{I}(\|(XW_1)^T \lambda\|_\infty \leq 1) \) is the sum of a linear function and an upper-semicontinuous indicator function and therefore upper-semicontinuous. The constraint on \( W_1 \)
is convex and compact. We use $P^*$ to denote the value of the above min-max program. Exchanging the order of min-max we obtain the dual problem given in [Main Paper, (5)], which establishes a lower bound $D^*$ for the above problem:

$$
P^* \geq D^* = \max_{\lambda} \min_{\theta \in \Theta \setminus \{w_2\}} \lambda^T y + \mathcal{I}(\|Xw_1\|_\infty \leq 1), \text{ s.t. } \|w_{1,j}\|_2 \leq 1, \forall j,
$$

$$
= \max_{\lambda} \lambda^T y, \text{ s.t. } \|Xw_1\|_\infty \leq 1 \forall w_{1,j} : \|w_{1,j}\|_2 \leq 1, \forall j,
$$

$$
= \max_{\lambda} \lambda^T y, \text{ s.t. } \|Xw_1\|_\infty \leq 1 \forall w_1 : \|w_1\|_2 \leq 1,
$$

We now show that strong duality holds for infinite size NNs. The dual of the semi-infinite program in [Main Paper, (5)] is given by (see Section 2.2 of [Goberna & López-Cerdá, 1998] and also [Bach, 2017])

$$
\min \|\mu\|_{TV} \text{ s.t. } \int_{w_1 \in B_2} Xw_1 d\mu(w_1) = y,
$$

where TV is the total variation norm of the Radon measure $\mu$. This expression coincides with the infinite-size NN as given in [Bach, 2017], and therefore strong duality holds. Next we invoke the semi-infinite optimality conditions for the dual problem in [Main Paper, (5)], in particular we apply Theorem 7.2 of [Goberna & López-Cerdá, 1998]. We first define the set

$$
K = \text{cone} \left\{ \left( \begin{array}{c} sXw_1 \\ 1 \end{array} \right), w_1 \in B_2, s \in \{-1, +1\}; \left( \begin{array}{c} 0_n \\ -1 \end{array} \right) \right\}.
$$

Note that $K$ is the union of finitely many convex closed sets, since the function $Xw_1$ can be expressed as the union of finitely many convex closed sets. Therefore the set $K$ is closed. By Theorem 5.3 [Goberna & López-Cerdá, 1998], this implies that the set of constraints in [Main Paper, (5)] forms a Farkas-Minkowski system. By Theorem 8.4 of [Goberna & López-Cerdá, 1998], this implies that the set of constraints in [Main Paper, (5)] forms a Farkas-Minkowski system. By Theorem 8.4 of [Goberna & López-Cerdá, 1998], this implies that the set of constraints in [Main Paper, (5)] forms a Farkas-Minkowski system.
primal and dual values are equal, given that the system is consistent. Moreover, the system is discretizable, i.e., there exists a sequence of problems with finitely many constraints whose optimal values approach to the optimal value of \cite{[Main Paper, (5)]}. The optimality conditions in Theorem 7.2 \cite{[Main Paper, (5)]} implies that \(y = XW_1^*w_2^*\) for some vector \(w_2^*\). Since the primal and dual values are equal, we have \(\lambda^+T\, y = \lambda^+T\, XW_1^*w_2^* = \|w_2^*\|_1\), which shows that the primal-dual pair \((\{w_2^*, W_1^*\}, \lambda^*)\) is optimal. Thus, the optimal neuron weights \(W_1^*\) satisfy \(\|(XW_1^*)^T\, \lambda^*\|_\infty = 1\).

**Proposition 2.1.** \cite{[Du & Hu 2019]} Assuming there exists a planted model parameter, i.e., \(Xw^* = y\), does not change the solution to the following training problem

\[
\min_{w_1, w_2} \|Xw_1 w_2 - y\|_2^2.
\]

*Proof of Proposition 2.1* Let us first define a variable \(w^*\) that minimizes the following problem

\[
w^* = \min_w \|Xw - y\|_2^2.
\]

Thus, the following relation holds

\[
X^T (Xw^* - y) = 0_d.
\]

Then, for any \(w \in \mathbb{R}^d\), we have

\[
f(w) = \|Xw - Xw^* + Xw^* - y\|_2^2 = \|Xw - Xw^*\|_2^2 + 2(w - w^*)^T \underbrace{X^T (Xw^* - y)}_{=0_d} + \|Xw^* - y\|_2^2
\]

Notice that \(\|Xw^* - y\|_2^2\) does not depend on \(w\), thus, the relation above proves that minimizing \(f(w)\) is equivalent to minimizing \(\|Xw - Xw^*\|_2^2\), where \(w^*\) is the planted model parameter. Therefore, the planted model assumption does not change solution to the linear network training problem in \cite{[Main Paper, (5)]}.

**Theorem 2.2.** Let \(\{X, y\}\) be a dataset such that \(\{4\}\) is feasible. Then, strong duality holds for \(\{4\}\).

*Proof of Theorem 2.2* Since there exists a single extreme point, we can construct a weight vector \(w_e \in \mathbb{R}^d\) that is the extreme point. Then, the dual of [Main Paper, (4)] with \(W_1 = w_e\) is

\[
D_e^* = \max_{\lambda} \lambda^T y \text{ s.t. } \|(Xw_e)^T \lambda\|_\infty \leq 1. \tag{30}
\]

Then, we have

\[
P^* = \min_{\theta \in \Theta \setminus \{w_2\}} \max_{\lambda} \lambda^T y \geq \max_{\lambda} \min_{\theta \in \Theta \setminus \{w_2\}} \lambda^T y \text{ s.t. } \|(XW_1)^T \lambda\|_\infty \leq 1, \|w_1, j\|_2 \leq 1, \forall j
\]

\[
\geq \max_{\lambda} \lambda^T y \text{ s.t. } \|(Xw_e)^T \lambda\|_\infty \leq 1
\]

\[
= D_e^* = D^* \tag{31}
\]

where the first inequality follows from changing order of min-max to obtain a lower bound and the equality in the second line follows from Corollary 2.1.

From the fact that an infinite width NN can always find a solution with the objective value lower than or equal to the objective value of a finite width NN, we have

\[
P_e^* = \min_{\theta \in \Theta \setminus \{w_1, m\}} |w_2| \geq P^* = \min_{\theta \in \Theta} \|w_2\|_1 \text{ s.t. } Xw_e w_2 = y, \left\|w_1, j\right\|_2 \leq 1, \forall j. \tag{32}
\]
where $P^*$ is the optimal value of the original problem with infinitely many neurons. Now, notice that the optimization problem on the left hand side of (32) is convex since it is an $\ell_1$-norm minimization problem with linear equality constraints. Therefore, strong duality holds for this problem, i.e., $P^*_e = D^*_e$. Using this result along with (31), we prove that strong duality holds for a finite width NN, i.e., $P^*_e = P^* = D^* = D^*_e$.

**Lemma 2.2.** The following problems are equivalent

\[
\max_{\lambda} -\frac{1}{2}\|\lambda - y\|^2_2 + \frac{1}{2}\|y\|^2_2 \quad \text{s.t.} \quad |\lambda^T X w_1| \leq \beta, \quad \forall w_1 \in \mathcal{B}_2
\]

\[
\max_{s} -\frac{1}{2}\|Xs - Xw^*\|^2_2 \quad \text{s.t.} \quad \|X^T Xs\|_2 \leq \beta
\]

**Proof of Lemma 2.2.** We first note that the dual parameter can be written as $\lambda = Xs + \lambda^\perp$, where $s \in \mathbb{R}^d$ and $\lambda^\perp \perp \mathcal{R}(X)$ (equivalently $\lambda^\perp \in \mathcal{N}(X^T)$). Using this representation, the constraint can be written as

\[
|\lambda^T X w_1| = |(Xs + \lambda^\perp)^T X w_1| = |(Xs + \lambda^\perp) X w_1| = |s^T X^T X w_1| \leq \beta,
\]

where the extreme point is $w^*_1 = \frac{X^T X s}{\|X^T X s\|^2_2}$. Then the constraint becomes $\|X^T X s\|_2 \leq \beta$. The same approach can also be utilized to show that $\|\lambda - X w^*\|_2 = \|Xs + \lambda^\perp - X w^*\|_2^2 = \|Xs - X w^*\|_2^2$. Therefore, using the new constraint and objective, the problem can be equivalently described as

\[
\max_{s} -\frac{1}{2}\|Xs - Xw^*\|^2_2 \quad \text{s.t.} \quad \|X^T Xs\|_2 \leq \beta.
\]

**Theorem 2.3.** For any dataset $\{X, y\}$, strong duality holds for the two-layer linear network training problem in (8).

**Proof of Theorem 2.3.** Since there exists a single extreme point, we can construct a weight vector $w_e \in \mathbb{R}^d$ that is the extreme point. Then, the dual of [Main Paper, (8)] with $W_1 = w_e$

\[
D_e^* = \max_{\lambda} -\frac{1}{2}\|\lambda - y\|^2_2 + \frac{1}{2}\|y\|^2_2 \quad \text{s.t.} \quad |\lambda^T X w_e| \leq \beta.
\]

Then the rest of the proof directly follows Proof of Theorem 2.2.

**Theorem A.1.** The dual of (29) is given by

\[
\max_{\lambda} -\ell^*(\lambda) \quad \text{s.t.} \quad \|X^T \lambda\|_2 \leq \beta,
\]

where $\ell^*$ is the Fenchel conjugate function defined as

\[
\ell^*(\lambda) = \max_{z} z^T \lambda - \ell(z, y).
\]

**Proof of Theorem A.1.** The proof follows from classical Fenchel duality [Boyd & Vandenberghe, 2004]. We first describe (29) in an equivalent form as follows

\[
\min_{z, \theta \in \Theta} \ell(z, y) + \beta\|w_2\|_1 \quad \text{s.t.} \quad z = XW_1 w_2, \quad \|w_1,j\|_2 \leq 1, \forall j.
\]

Then the dual function is

\[
g(\lambda) = \min_{z, \theta \in \Theta} \ell(z, y) - \lambda^T z + \lambda^T X W_1 w_2 + \beta\|w_2\|_1 \quad \text{s.t.} \quad \|w_1,j\|_2 \leq 1, \forall j.
\]

Therefore, using the classical Fenchel duality [Boyd & Vandenberghe, 2004] yields the claimed dual form.
Lemma 2.3. The following problems are equivalent:

\[
\begin{align*}
\min_{\theta \in \Theta} & \quad \|W_1\|_F^2 + \|W_2\|_F^2 \\
\text{s.t.} & \quad f_{\theta,2}(X) = Y
\end{align*}
\]

\[
\begin{align*}
\min_{\theta \in \Theta} & \quad \sum_{j=1}^m \|w_{2,j}\|_2 \\
\text{s.t.} & \quad f_{\theta,2}(X) = Y, \forall w_{1,j} \in B_2
\end{align*}
\]

Proof of Lemma 2.3. The proof directly follows from Proof of Lemma 2.1.

Theorem 2.4. Let \{X, Y\} be a dataset such that (\(\Pi\)) is feasible. Then, strong duality holds for (\(\Pi\)).

Proof of Theorem 2.4. Since there exist \(r_w\) possible extreme points, we can construct a weight matrix \(W_e \in \mathbb{R}^{d \times r_w}\) that consists of all the possible extreme points. Then, the dual of [Main Paper, (\(\Pi\))] with \(W_1 = W_e\)

\[
D_e^* = \max_{\Lambda} \text{trace}(\Lambda^T Y) \quad \text{s.t.} \quad \|\Lambda^T Xw_{e,j}\|_2 \leq 1, \forall j \in [r_w].
\]

Then the rest of the proof directly follows Proof of Theorem 2.2.

Lemma 3.1. The following problems are equivalent:

\[
\begin{align*}
\min_{\{\theta_l\}_{l=1}^L} & \quad \sum_{l=1}^L \|W_l\|_F^2 \\
\text{s.t.} & \quad f_{\theta,L}(X) = Y
\end{align*}
\]

\[
\begin{align*}
\min_{\{\theta_l\}_{l=1}^{L-2},\{t_l\}_{l=1}^{L-2}} & \quad \|W_L\|_1 + \sum_{l=1}^{L-2} t_l^2 \\
\text{s.t.} & \quad \|W_{L-1,j}\|_2 \leq 1, \forall j \in [m_{L-1}] \\
& \quad XW_1 \ldots W_{L-1}W_L = Y
\end{align*}
\]

Proof of Lemma 3.1. Applying the scaling trick in Lemma 2.1 to the last two layers of the \(L\)-layer network in [Main Paper, (15)] gives

\[
\begin{align*}
\min_{\{\theta_l\}_{l=1}^{L-2},\{t_l\}_{l=1}^{L-2}} & \quad \|W_L\|_1 + \sum_{l=1}^{L-2} \|W_l\|_F^2 \\
\text{s.t.} & \quad \|W_{L-1,j}\|_2 \leq 1, \forall j \in [m_{L-1}] \\
& \quad XW_1 \ldots W_{L-1}W_L = Y
\end{align*}
\]

Then, we use the epigraph form for the norm of the first \(L - 2\) to achieve the equivalence.

Proposition 3.1. First \(L - 2\) hidden layer weight matrices in (15) have the same operator and Frobenius norms.

Proof of Proposition 3.1. Let us first denote the sum of the norms for the first \(L - 2\) layer as \(t\), i.e., \(t = \sum_{l=1}^{L-2} t_l\), where \(t_l = \|W_l\|_2 = \|W_l\|_F\) since the upper-bound is achieved when the matrices are rank-one (see [Main Paper, (21)]). Then, to find the extreme points, we need to solve the following problem

\[
\max_{\{\theta_l\}_{l=1}^{L-2}} \|W_{L-2}\|_2 \ldots \|W_1\|_2 \|W_L^*\|_2.
\]

We can equivalently rewrite this problem using the variables \(\{t_l\}_{l=1}^{L-2}\) as follows

\[
\max_{\{t_l\}_{l=1}^{L-2}} \prod_{l=1}^{L-2} t_l = \max_{\{t_l\}_{l=1}^{L-3}} \left( t - \sum_{l=1}^{L-3} t_l \right) \prod_{j=1}^{L-3} t_l
\]

s.t. \(\sum_{l=1}^{L-3} t_l \leq t, \ t_l \geq 0\)
If we take the derivative of the objective function of the latter problem, i.e., denoted as \( f(t_1, \ldots, t_{L-3}) \), with respect to \( t_k \), we obtain the following

\[
\frac{\partial f(t_1, \ldots, t_{L-3})}{\partial t_k} = t \prod_{l \neq k}^{L-3} t_l - 2 \prod_{l=1}^{L-3} t_l - \sum_{l \neq k}^{L-3} t_l \prod_{l=1}^{L-3} t_l.
\]

Then, equating the derivative to zero yields the following relation

\[
t_k^* = t - \sum_{l=1}^{L-3} t_l^*
\]

where \( t_k^* \) denotes the optimal operator norm for the \( k \)th layer's weight matrix. We also note that these solutions satisfy the constraints in the optimization problem above. Since by definition \( t - \sum_{l=1}^{L-3} t_l^* = t_{L-2}^* \), we have \( t_{L-1}^* = t_{L-2}^* = \ldots = t_2^* = t_1^* \).

**Theorem 3.1.** Let \( \{X, y\} \) be a dataset such that (15) is feasible. Then, strong duality holds for (15).

**Proof of Theorem 3.1.** We first select a set of unit norm vectors, i.e., \( \{\rho_l\}_{l=1}^{L-2} \), to construct weight matrices \( \{W_l\}_{l=1}^{L-1} \) that satisfies [Main Paper, (21)]. Then, the dual of [Main Paper, (15)] can be written as

\[
D_c^* = \max_{\lambda} \lambda^T y
\]

s.t. \(|(XW_1 \ldots W_{L-1})^T \lambda| \leq 1\) \hspace{1cm} (33)

Then, we have

\[
P^* = \min_{\{\theta_l\}_{l=1}^{L-1} \in \Theta_{L-1}} \max_{\lambda} \lambda^T y \geq \max_{\lambda} \lambda^T y
\]

s.t. \(|(XW_1 \ldots W_{L-1})^T \lambda| \leq 1\)

\[
= \max_{\lambda} \lambda^T y
\]

s.t. \(|(XW_1 \ldots W_{L-1})^T \lambda| \leq 1\)

\[
= D_c^* = D^* = D_m^*
\]

where the first inequality follows from changing the order of min-max to obtain a lower bound and the first equality follows from the fact that \( \{W_l\}_{l=1}^{L-1} \) maximizes the dual problem. Furthermore, we have the following relation between the primal problems

\[
P_c^* = \min_{W_L} \|W_L\|_1 \geq P^* = \min_{\{\theta_l\}_{l=1}^{L-1} \in \Theta_{L-1}} \|W_L\|_1
\]

s.t. \(W_1 \ldots W_{L-1}W_L = y\)

s.t. \(W_1 \ldots W_{L-1}W_L = y\)

where the inequality follows from the fact that the original problem has infinite width in each layer. Now, notice that the optimization problem on the left hand side of (34) is convex since it is an \( \ell_1 \)-norm minimization problem with linear equality constraints. Therefore, strong duality holds for this problem, i.e., \( P_c^* = D_c^* \) and we have \( P_c^* \geq P^* \geq P_m^* \geq D_c^* = D^* = D_m^* \). Using this result along with (33), we prove that strong duality holds, i.e., \( P_c^* = P^* = P_m^* = D_c^* = D^* = D_m^* \).

**Corollary 3.1.** As a consequence of the analysis above, a deep linear network achieves the desired output using the first hidden layer alone. Therefore, rest of the layers do not add any expressive power to the network.

**Proof of Corollary 3.1.** The proof directly follows from [Main Paper, 21].

**Corollary 3.2.** The analysis above and Theorem 3.1 also show that strong duality holds for the regularized deep linear network training problem.
Proof of Corollary 3.2. The proof directly follows from the analysis in this section and Theorem 3.1.

Lemma 3.2. The following problems are equivalent:

\[
\min_{\{\theta_i\}_{i=1}^L} \sum_{l=1}^L \|W_l\|_F^2 \quad \text{s.t.} \quad f_{\theta,L}(X) = Y
\]

\[
\min_{\{\theta_i\}_{i=1}^L, \{t_i\}_{i=1}^{L-2}} \sum_{j=1}^{m_{L-1}} \|W_{L,j}\|_2 + \sum_{l=1}^{L-2} \|W_l\|_F^2 \\
\text{s.t.} \quad f_{\theta,L}(X) = Y, \quad \forall w_{L-1,j} \in B_2 \\
\|W_l\|_F \leq t_l, \quad \forall l \in [L-2]
\]

Proof of Lemma 3.2. Applying the scaling trick in Lemma 2.1 to the last two layers of the $L$-layer network in [Main Paper, (22)] gives

\[
\min_{\{\theta_i\}_{i=1}^L, \{t_i\}_{i=1}^{L-2}} \sum_{j=1}^{m_{L-1}} \|W_{L,j}\|_2 + \sum_{l=1}^{L-2} \|W_l\|_F^2 \\
\text{s.t.} \quad \|W_{L-1,j}\|_2 \leq 1, \forall j \in [m_{L-1}] \\
XW_0 \ldots W_{L-1}W_L = Y
\]

Then, we use the epigraph form for the norm of the first $L-2$ to achieve the equivalence.

Theorem 3.2. Let \{X, y\} be a dataset such that (22) is feasible. Then, strong duality holds for (22).

Proof of Theorem 3.2. We first select a set of unit norm vectors, i.e., \{\rho_{i,j}\}_{i=1}^{L-2}, to construct weight matrices \{W_{i,j}\}_{i=1}^{L-1} that satisfies [Main Paper, (24)]. Then, the dual of [Main Paper, (22)] can be written as

\[
D_e^* = \max_{\Lambda} \text{trace}(\Lambda^T Y) \\
\text{s.t.} \quad \sigma_{\max}(\Lambda^T X W_1 \ldots W_{L-2}) \leq 1, \forall j
\]

Then, we have

\[
P^* = \min_{\{\theta_i\}_{i=1}^L} \max_{\Lambda} \text{trace}(\Lambda^T Y) \quad \geq \quad \max_{\Lambda} \text{trace}(\Lambda^T Y) \quad \text{(35)}
\]

\[
\text{s.t.} \quad \sigma_{\max}(\Lambda^T X W_1 \ldots W_{L-2}) \leq 1 \quad \text{s.t.} \quad \sigma_{\max}(\Lambda^T X W_1 \ldots W_{L-2}) \leq 1, \forall \theta_i \in \Theta_{L-1}
\]

\[
= \max_{\Lambda} \text{trace}(\Lambda^T Y) \\
\text{s.t.} \quad \sigma_{\max}(\Lambda^T X W_1 \ldots W_{L-2}) \leq 1, \forall j
\]

\[
D_e^* = D^* = D_m^*
\]

where the first inequality follows from changing the order of min-max to obtain a lower bound and the first equality follows from the fact that \{W_{i,j}\}_{i=1}^{L-1} maximizes the dual problem. Furthermore, we have the following relation between the primal problems

\[
P_e^* = \min_{W_L} \sum_{j=1}^{m_{L-1}} \|W_{L,j}\|_2 \quad \geq \quad P^* = \min_{\{\theta_i\}_{i=1}^L} \sum_{j=1}^{m_{L-1}} \|W_{L,j}\|_2 \quad \text{(36)}
\]

\[
\text{s.t.} \quad \sum_{j=1}^{m_{L-1}} W_{1,j} \ldots W_{L-1,j} W_L = Y \quad \text{s.t.} \quad W_1 \ldots W_{L-1}W_L = Y
\]

where the inequality follows from the fact that the original problem has infinite width in each layer. Now, notice that the optimization problem on the left hand side of (36) is convex since it is an $\ell_2$-norm minimization problem with linear equality constraints. Therefore, strong duality holds for this problem, i.e., $P_e^* = D_e^*$ and we have $P_e^* \geq P^* \geq P_m^* \geq D_e^* = D^* = D_m^*$. Using this result along with (35), we prove that strong duality holds, i.e., $P_e^* = P^* = P_m^* = D_e^* = D^* = D_m^*$. 

\qed
Convex Duality of Deep Neural Networks

**Theorem 4.1.** Let \( X \) be a rank-one data matrix such that \( X = ca_0^T \), where \( c \in \mathbb{R}^n_+ \) and \( a_0 \in \mathbb{R}^d \), then the weight matrix for each layer can be formulated as follows

\[
W_l = \frac{a_{l-1}}{\|a_{l-1}\|_2} \phi_l^T, \quad \forall l \in [L-2], \quad w_{L-1} = \frac{a_{L-2}}{\|a_{L-2}\|_2},
\]

where \( a_l^T = (a_{l-1}^T W_l)_+ \), \( \forall l \in [L-1] \), and \( \{ \phi_l \}_{l=1}^{L-2} \) is a set of vectors satisfying \( \|\phi_l\|_2 = t^*, \quad \forall l \in [L-2] \).

**Proposition 1.** First \( L-2 \) hidden layer weight matrices in [Main Paper, (28)] have the same operator and Frobenius norms.

**Proof of Proposition 1** Let us first denote the sum of the norms for the first \( L-2 \) layer as \( t \), i.e., \( t = \sum_{l=1}^{L-2} t_l \), where \( t_l = \|W_l\|_2 = \|W_l\|_F \) since the upper-bound is achieved when the matrices are rank-one. Then, to find the extreme points (see the details in Proof of Theorem 4.1), we need to solve the following problem

\[
\text{argmax}_{\{\theta_l\}_{l=1}^{L-2} \in \Theta_{L-1}} |\lambda^T c| \|a_{L-2}\|_2 = \text{argmax}_{\{\theta_l\}_{l=1}^{L-2} \in \Theta_{L-1}} |\lambda^T c| \|a_{L-3}^T W_{L-2}\|_2
\]

where we use \( a_{L-2} = (a_{L-1}^T W_{L-2})_+ \). Since \( \|W_{L-2}\|_F = t_{L-2} = t - \sum_{l=1}^{L-3} t_l \), the objective value above becomes

\[
|\lambda^T c| \|a_{L-3}\|_2 \left( t - \sum_{l=1}^{L-3} t_l \right).
\]

Applying this step to all the remaining layer weights gives the following problem

\[
\text{argmax}_{\{\theta_l\}_{l=1}^{L-2} \in \Theta_{L-1}} |\lambda^T c| \|a_0\|_2 \left( t - \sum_{l=1}^{L-3} \prod_{j=1}^{L-3} t_j \right. \text{ s.t. } \sum_{l=1}^{L-3} t_l \leq t, \quad t_l \geq 0.
\]

Then, the proof directly follows from Proof of Proposition 3.1.

**Proof of Theorem 4.1** Using Lemma 3.1 and Proposition 1, this problem can be equivalently stated as

\[
\min_{\{\theta_l\}_{l=1}^{L-1} \in \Theta_{L-1}} \|w_L\|_1 \text{ s.t. } A_l = (A_{l-1} W_l)_+, \quad \forall l \in [L-1], \quad A_{L-1} W_L = y,
\]

which also has the following dual form

\[
P^* = \min_{\{\theta_l\}_{l=1}^{L-1} \in \Theta_{L-1}} \max_{\lambda} \lambda^T y \quad \text{s.t. } \|A_{L-1}^T \lambda\|_\infty \leq 1
\]

Notice that we remove the recursive constraint in (38) for notational simplicity, however, \( A_{L-1} \) is still a function of all the layer weights except \( w_L \). Changing the order of min-max in (38) gives

\[
P^* \geq D^* = \max_{\lambda} \lambda^T y \quad \text{s.t. } \|A_{L-1}^T \lambda\|_\infty \leq 1, \quad \forall \theta_l \in \Theta_{L-1}, \quad \forall l \in [L-1].
\]

The dual of the semi-infinite problem in (39) is given by

\[
\min \|\mu\|_{TV} \quad \text{s.t. } \int_{\{\theta_l\}_{l=1}^{L-1} \in \Theta_{L-1}} (A_{L-2} w_{L-1})_+ d\mu(\theta_1, \ldots, \theta_{L-1}) = y,
\]

where \( \mu \) is a signed Radon measure and \( \|\cdot\|_{TV} \) is the total variation norm. We emphasize that (40) has infinite width in each layer, however, an application of Carathéodory’s theorem shows that the measure \( \mu \) in the integral can be represented by finitely many (at most \( n+1 \)) Dirac delta functions [Rosset et al. 2007]. Thus, we choose

\[
\mu = \sum_{j=1}^{m_{L-1}} \delta(W_1 - W_1^j, \ldots, W_{L-1} - W_{L-1}^j),
\]
where \( \delta(\cdot) \) is the Dirac delta function and the superscript indicates a particular choice for the corresponding layer weight. This selection of \( \mu \) yields the following problem

\[
P^*_m = \min_{\{\theta_l\}_{l=1}^{mL-1}} \|w_L\|_1
eq mL-1
\]

\[
s.t. \sum_{j=1}^{L} (A_{L-2}^j w_{L-1,j})_+ w_{L,j} = y, \theta_l^i \in \Theta_{L-1}, \forall l \in [L-1]. \tag{41}
\]

Here, we first note that even though the model in (41) has the same layer widths with regular deep ReLU networks, it has more expressive power since it allows us to choose multiple weight matrices for each layer. Based on this observation, we have \( P^* \geq P^*_m \).

As a consequence of (39), we can characterize the optimal layer weights for (41) as the extreme points that solve

\[
\arg\max_{\{\theta_l\}_{l=1}^{L-2} \in \Theta_{L-1}} |\lambda^T (A_{L-2} w_{L-1})_+|
\]

where \( \lambda^* \) is the optimal dual parameter. Since we assume that \( X = c a_0^T \) with \( c \in \mathbb{R}^l_+ \), we have \( A_{L-2} = c a_{L-2}^T \), where \( a_i^j = (a_{L-1}^j w_i)_+ \), \( a_i \in \mathbb{R}^m_+ \) and \( \forall l \in [L-1] \). Based on this observation, we have \( w_{L-1} = a_{L-2}/\|a_{L-2}\|_2 \), which reduces (42) to the following

\[
\arg\max_{\{\theta_l\}_{l=1}^{L-2} \in \Theta_{L-1}} |\lambda^T c| \|a_{L-2}\|_2 \tag{43}
\]

We then apply the same approach to all the remaining layer weights. However, notice that each neuron for the first \( L-2 \) layers must have bounded Frobenius norms due to the norm constraint. If we denote the optimal \( \ell_2 \) norms vector for the neuron in the \( l^{th} \) layer as \( \phi^l \in \mathbb{R}^m_+ \), then we have the following formulation for the layer weights that solve (42)

\[
W_l = \frac{a_{l-1}}{\|a_{l-1}\|_2} \phi_l^T, \forall l \in [L-2], \quad w_{L-1} = \frac{a_{L-2}}{\|a_{L-2}\|_2},
\]

where \( \{\phi_l\}_{l=1}^{L-2} \) is a set of vectors satisfying \( \|\phi_l\|_2 = \mu^* \), \( \forall l \in [L-2] \).

We note that the layer weights in (44) are optimal for the relaxed problem in (41). However, since there exists a single possible choice for the left singular vector of \( W_1 \) and we can select an arbitrary set for \( \{\mu_l\}_{l=1}^{L-2} \), the dual problems coincide for [Main Paper, (28)] and (41), i.e., we achieve \( D^*_m = D^* \) using the same layer weights, where \( D^*_m \) is the optimal dual objective value for (41). Therefore, the set of weights in (44) are also optimal for [Main Paper, (28)].

**Proposition 4.1.** Theorem 4.7 still holds when we add a bias term to the last hidden layer of the problem in (28), i.e., the output network becomes \( (A_{L-2} W_{L-1} + 1_a b^T)_+ w_L = y \), where \( A_1 = (A_{L-1} W_i)_+ \), \( \forall l \in [L-2] \).

**Proof of Proposition 4.1.** Here, we add biases to the neurons in the last hidden layer of [Main Paper, (28)]. For this case, all the equations in (37)-(39) hold except notational changes due to the bias term. Thus, (42) changes as

\[
\arg\max_{\{\theta_l\}_{l=1}^{L-2} \in \Theta_{L-1}, b} |\lambda^T (A_{L-2} w_{L-1} + b 1_n)_+| = \arg\max_{\{\theta_l\}_{l=1}^{L-2} \in \Theta_{L-1}, b} |\lambda^T (c a_{L-2}^T w_{L-1} + b 1_n)_+|
\]

\[
= \arg\max_{\{\theta_l\}_{l=1}^{L-2} \in \Theta_{L-1}, b} \sum_{i=1}^{n} \lambda_i^* (c_i a_{L-2}^T w_{L-1} + b)^+_i \tag{45}
\]

which can also be written as

\[
\arg\max_{\{\theta_l\}_{l=1}^{L-2} \in \Theta_{L-1}, b} \sum_{i \in S} \lambda_i^* c_i a_{L-2}^T w_{L-1} + \sum_{i \in S^c} \lambda_i^* b \text{ s.t. } \begin{cases} c_i a_{L-2}^T w_{L-1} + b \geq 0, \forall i \in S \\ c_i a_{L-2}^T w_{L-1} + b \leq 0, \forall j \in S^c \end{cases},
\]

where \( S \) and \( S^c \) are the indices for which ReLU is active and inactive, respectively. This shows that \( w_{L-1} \) must be

\[
w_{L-1} = \begin{cases} \frac{a_{L-2}}{\|a_{L-2}\|_2} & \text{if } \sum_i \in S \lambda_i^* c_i \geq 0 \\ \frac{-a_{L-2}}{\|a_{L-2}\|_2} & \text{otherwise} \end{cases}
\]

and\( b^* = \begin{cases} \min_{j \in S^c} (-s_j \lambda_i^* c_i) & \text{if } \sum_i \lambda_i^* c_i \geq 0 \\ \max_{i \in S} (-s_j \lambda_i^* c_i) & \text{otherwise} \end{cases} \quad (46)

where \( s_{\lambda^*} = \text{sign}(\sum_{i \in S} \lambda^*_i c_i) \). This result reduces (45) to the following problem

\[
\arg \max_{(\theta_l)_{l=1}^{L-2} \in \Theta_{L-1}} |C(\lambda^*, \mathbf{c})| \| \mathbf{a}_{L-2} \|_2,
\]

where \( C(\lambda^*, \mathbf{c}) \) is constant scalar independent of \( \{\mathbf{W}_l\}_{l=1}^{L-2} \). Hence, this problem and its solutions are the same with (43) and (44), respectively.

\[\square\]

**Corollary 4.1.** As a result of Proposition 4.1 and Theorem 4.1, the optimal solutions have kinks at the input data points so that the network output becomes linear spline interpolation for one-dimensional datasets.

**Proof of Corollary 4.1.** Let us particularly consider the input sample \( \mathbf{a}_0 \). Then, the activations of the network defined by (44) and (46) are

\[
\begin{align*}
\mathbf{a}_1^T &= (\mathbf{a}_0^T \mathbf{W}_1)_+ = \left( \mathbf{a}_0^T \frac{\mathbf{a}_0}{\| \mathbf{a}_0 \|_2} \phi_1^T \right)_+ = \| \mathbf{a}_0 \|_2 \phi_1^T \\
\mathbf{a}_2^T &= (\mathbf{a}_1^T \mathbf{W}_2)_+ = \left( \mathbf{a}_1^T \frac{\mathbf{a}_1}{\| \mathbf{a}_1 \|_2} \phi_2^T \right)_+ = \| \mathbf{a}_0 \|_2 \| \phi_1 \|_2 \phi_2^T \\
&\vdots \\
\mathbf{a}_{L-2}^T &= (\mathbf{a}_{L-3}^T \mathbf{W}_{L-2})_+ = \left( \mathbf{a}_{L-3}^T \frac{\mathbf{a}_{L-3}}{\| \mathbf{a}_{L-3} \|_2} \phi_{L-2}^T \right)_+ = \| \mathbf{a}_0 \|_2 \| \phi_1 \|_2 \cdots \| \phi_{L-3} \|_2 \phi_{L-2}^T \\
\mathbf{a}_{L-1} &= (\mathbf{a}_{L-2}^T \mathbf{w}_{L-1} + \mathbf{b})_+ = (\| \mathbf{a}_{L-2} \|_2 - \| \mathbf{a}_{L-2} \|_2)_+ = 0.
\end{align*}
\]

Thus, if we feed \( c_i \mathbf{a}_0 \) to the network, we get \( \mathbf{a}_{L-1} = (c_i \| \mathbf{a}_{L-2} \|_2 - c_i \| \mathbf{a}_{L-2} \|_2)_+ = 0 \), where we use the fact that optimal biases are in the form of \( \mathbf{b} = -c_i \| \mathbf{a}_{L-2} \|_2 \) as proved in (46). This analysis proves that the kink of each ReLU activation occurs exactly at one of the data points. \(\square\)

**Corollary 4.2.** As a direct consequence of Theorem 3.1 and 4.1, strong duality also holds for deep ReLU networks.

**Proof of Corollary 4.2.** The proof directly follows from Theorem 3.1 and 4.1. \(\square\)