Abstract
We study regularized deep neural networks (DNNs) and introduce a convex analytic framework to characterize the structure of the hidden layers. We show that a set of optimal hidden layer weights for a norm regularized DNN training problem can be explicitly found as the extreme points of a convex set. For the special case of deep linear networks, we prove that each optimal weight matrix aligns with the previous layers via duality. More importantly, we apply the same characterization to deep ReLU networks with whitened data and prove the same weight alignment holds. As a corollary, we also prove that norm regularized deep ReLU networks yield spline interpolation for one-dimensional datasets which was previously known only for two-layer networks. Furthermore, we provide closed-form solutions for the optimal layer weights when data is rank-one or whitened. The same analysis also applies to architectures with batch normalization even for arbitrary data. Therefore, we obtain a complete explanation for a recent empirical observation termed Neural Collapse where class means collapse to the vertices of a simplex equiangular tight frame.

1. Introduction
Deep neural networks (DNNs) have become extremely popular due to their success in machine learning applications. Even though DNNs are highly over-parameterized and non-convex, simple first-order algorithms, e.g., Stochastic Gradient Descent (SGD), can be used to successfully train them. Moreover, recent work has shown that highly over-parameterized networks trained with SGD obtain simple solutions that generalize well (Savarese et al., 2019; Parhi & Nowak, 2019; Ergen & Pilanci, 2020a,b). Where two-layer ReLU networks with the minimum Euclidean norm solution and zero training error are proven to fit a linear spline model in 1D regression. In addition, a recent series of work (Pilanci & Ergen, 2020; Ergen & Pilanci, 2021; Sahiner et al., 2021; Gupta et al., 2021) showed that regularized two-layer ReLU network training problems exhibit a convex loss landscape in a higher dimensional space, which was previously attributed to the benign impacts of overparameterization (Brutzkus et al., 2017; Li & Liang, 2018; Du et al., 2018b; Ergen & Pilanci, 2019). Therefore, regularizing the solution towards smaller norm weights might be the key to understand the generalization properties and loss landscape of DNNs. However, analyzing DNNs is still theoretically elusive even in the absence of nonlinear activations. To this end, we study norm regularized DNNs and develop a framework based on convex duality to characterize a set of optimal solutions to the training problem.

Deep linear networks have been the subject of extensive theoretical analysis due to their tractability. A line of research (Saxe et al., 2013; Arora et al., 2018a; Laurent & Brechi, 2018; Du & Hu, 2019; Shamir, 2018) focused on GD training dynamics, however, they lack the analysis of solution set and 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 and showed that linear networks trained with GD converge to minimum nuclear norm solutions. Later on, (Arora et al., 2018b; Du et al., 2018a) showed that gradient flow enforces the layer weights to align. Ji & Telgarsky (2019) further proved that each layer weight matrix is asymptotically rank-one. These results provide insights to characterize the structure of the optimal layer weights, however, they require multiple strong assumptions, e.g., linearly separable training data and strictly decreasing loss function, which makes the results impractical. Furthermore, (Zhang et al., 2019) provided some characterizations for nonstandard networks, which are valid for hinge loss with an uncommon regularization. Unlike these studies, we introduce a complete characterization for regularized deep network training problems without requiring such assumptions.

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1.1. Our contributions

Our contributions can be summarized as follows

- We introduce a convex analytic framework that characterizes a set of optimal solutions to regularized training problems as the extreme points of a convex set.
- For deep linear networks, we prove that each optimal layer weight matrix aligns with the previous layers via convex duality.
- For deep ReLU networks, we prove that the optimal regularization for the layer weights, β > 0 is a regularization parameter, \( \theta_t = \{ \{ W_{l,j} \} \}_{m=1}^m, m \) \( \theta = \{ \theta_t \}_{t=1}^t \). In the paper, for the sake of presentation simplicity, we illustrate the conventional training setup with squared loss and \( \ell_2^2 \)-norm regularization. However, our analysis is valid for arbitrary convex loss functions as proven in Appendix A.1.

Thus, we consider the following optimization problem

\[
P^* = \min_{\{ \theta_t \}_{t=1}^t} \mathcal{L}(f_{\theta,L}(X), y) + \frac{\beta}{2} \sum_{j=1}^m \sum_{l=1}^L \| W_{l,j} \|_F^2. \tag{2}
\]

Next, we show that the minimum \( \ell_2^2 \)-norm is equivalent to minimum \( \ell_1 \)-norm after a rescaling.

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

\[
\min_{\{ \theta_t \}_{t=1}^t} \mathcal{L}(f_{\theta,L}(X), y) + \frac{\beta}{2} \sum_{j=1}^m \sum_{l=1}^L \| W_{l,j} \|_F^2
= \min_{\{ \theta_t \}_{t=1}^t} \mathcal{L}(f_{\theta,L}(X), y) + \beta \| W \|_1
+ \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2;
\]

subject to \( w_{L-1,j} \in B_2, \| W_{l,j} \|_F \leq t_j, \forall l \in [L - 2] \)

Using Lemma 1.1\(^1\), 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 dual as a lower bound\(^2\)

\[
P^* \geq \mathcal{D}^* = \max_{\{ t_j \}_{j=1}^m} \min_{\{ \lambda \} \in \mathbb{R}} \lambda - \mathcal{L}^*(\lambda) + \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2
\]

subject to \( \| \mathcal{A}_{L-1,j}^T \lambda \|_\infty \leq \beta \).

To the best of our knowledge, the dual DNN characterization (3) is novel. Using this result, we first characterize a set of weights that minimize the objective via the optimality conditions and active constraints in (3). We then prove the optimality of these weights by proving strong duality, i.e., \( P^* = D^* \), for DNNs. We then show that, for deep linear networks, optimal weight matrices align with the previous layers.

More importantly, the same analysis and conclusions also apply to deep ReLU networks when the input is whitened and/or rank-one. Here, we even obtain closed-form solutions for the optimal layer weights. As a corollary, we show that deep ReLU networks fit a linear spline interpolation when the input is one-dimensional. We also provide an experiment in Figure 1 to verify this claim. Note that

\(^1\)The proof is presented in Appendix A.3

\(^2\)For the definitions and details see Appendix A.1 and A.2
this result was previously known only for two-layer networks (Savarese et al., 2019; Parhi & Nowak, 2019; Ergen & Plačnik, 2020a,b) and here we extend it to arbitrary depth $L$ (see Table 1 for details). We also show that the whitened/rank-one assumption can be removed by introducing batch normalization in between layers, which reflects the training setup in practice.

2. Warmup: Two-layer linear networks

As a warmup, we first consider the simple case of two-layer linear networks with the output $f_{\theta,2}(X) = XW_1w_2$ and the parameters as $\theta \in \Theta = \{ (W_1, w_2, m) | W_1 \in \mathbb{R}^{d \times m}, w_2 \in \mathbb{R}^m, m \in \mathbb{Z}_+ \}$. Motivated by recent results (Neyshabur et al., 2014; Savarese et al., 2019; Parhi & Nowak, 2019; Ergen & Plačnik, 2020a,b), we first focus on a minimum norm variant of (1) with squared loss, which can be written as

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

(4)

Using Lemma A.4, we equivalently have

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

(5)

which has the following dual form.

**Theorem 2.1.** The dual of the problem in (5) is given by

$$P^* \geq D^* = \max_{\chi \in \mathbb{R}^n} \chi^T y \text{ s.t. } \max_{w_1 \in B_2} \| \chi^T Xw_1 \|_1 \leq 1.$$  

(6)

For (5), $\exists m^* \leq n + 1$ such that strong duality holds, i.e., $P^* = D^*$, $\forall m \geq m^*$ and $W_1$ satisfies $\| (XW_1^T)^T \chi^* \|_\infty = 1$, where $\chi^*$ is the dual optimal parameter.

Using Theorem 2.1, we now characterize the optimal neurons as the extreme points of a convex set.

**Corollary 2.1.** By Theorem 2.1, the optimal neurons are extreme points which solve $\arg\max_{w_1 \in B_2} \| \chi^T Xw_1 \|$.

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**Definition 1.** We call the maximizers of the constraint in Corollary 2.1 extreme points throughout the paper.

From Theorem 2.1, we have the following dual problem

$$\max_{\lambda} \lambda^T y \text{ s.t. } \max_{w_1 \in B_2} | \lambda^T Xw_1 | \leq 1.$$  

(7)

Let $X = U_2 \Sigma_2 V_2^T$ be the singular value decomposition (SVD) of $X$. If we assume that there exists $w^*$ such that $Xw^* = y$ due to Proposition 2.1, then (7) is equivalent to

$$\max_{w^*} \lambda^T \Sigma_2 w^* \text{ s.t. } \| \Sigma_2 \lambda \|_2 \leq 1,$$  

(8)

where $\tilde{\lambda} = U_2^T \lambda$, $\tilde{w}^* = V_2^T w^*$, and we changed the constraint since the extreme point is achieved when $w_1 = X^T \lambda / \| X^T \lambda \|_2$. Given $\lambda_1(X) = r$, we have

$$\tilde{\lambda}^T \Sigma_2 \tilde{w}^* = \lambda^T \Sigma_2 \left[ \frac{I_r}{0_{r \times d-r}} - \frac{0_{r \times d-r}}{0_{d-r \times d-r}} \right] w^*$$

(9)

which shows that the maximum objective value is achieved when $\Sigma_2^T \tilde{\lambda} = c_1 \tilde{w}^*$. Thus, we have

$$w_1 = \frac{V_2 \Sigma_2^T \tilde{\lambda}}{\| V_2 \Sigma_2^T \tilde{\lambda} \|_2} = \frac{V_2 \tilde{w}^*}{\| V_2 \tilde{w}^* \|_2} = \frac{P_{X^T}(w^*)}{\| P_{X^T}(w^*) \|_2},$$

where $P_{X^T}(\cdot)$ projects its input onto the range of $X^T$. In the sequel, we first show that one can consider a planted model without loss of generality and then prove strong duality for (5).

**Proposition 2.1.** [Du & Hu, 2019] Given $w^*$, we have

$$\arg\min_{w_1} \| Xw - y \|_2 \text{, we have}$$

$$\arg\min_{w_1} \| Xw_1w_2 - Xw^* \|_2 = \arg\min_{w_1, w_2} \| Xw_1w_2 - y \|_2.$$  

**Theorem 2.2.** Let $\{ x, y \}$ be feasible for (5), then strong duality holds for finite width networks.

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

4All the equivalence lemmas are presented in Appendix A.3.

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**Width (m) | Assumption | Depth (L) | # of outputs (K)**

| (Savarese et al., 2019) | $\infty$ | 1D data (d = 1) | 2 | $K = 1$ |
| (Parhi & Nowak, 2019) | $\infty$ | 1D data (d = 1) | 2 | $K = 1$ |
| (Ergen & Plačnik, 2020a,b) | finite | rank-one/whitened | 2 | $K = 1$ |

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finite | rank-one/whitened or BatchNorm | $L \geq 2$ | $K = 1$ |

Figure 1 & Table 1: One dimensional interpolation using $L$-layer ReLU networks with 20 neurons in each hidden layer. As predicted by Corollary 2.1, the optimal solution is given by piecewise linear splines for any $L \geq 2$. Additionally, we provide a comparison with previous studies about this characterization.
2.1. Regularized training problem

In this section, we define the regularized version of (5) as

$$\min_{\theta \in \Theta} \frac{1}{2} \|f_{\theta,2}(X) - Y\|_F^2 + \beta \|w_2\|_1 \quad \text{s.t. } w_{1,j} \in \mathcal{B}_2, \quad (10)$$

which has the following dual form

$$\max_{\lambda} -\frac{1}{2} \|\lambda - \frac{1}{\beta} (\lambda^T X w_1)\|_2^2 \quad \text{s.t. } w_{1,j} \in \mathcal{B}_2.$$  

Then, an optimal neuron needs to satisfy the condition

$$w_1^* = \frac{X^T \mathcal{P}_{X,B}(y)}{\|X^T \mathcal{P}_{X,B}(y)\|_2}$$

where \(\mathcal{P}_{X,B}(\cdot)\) projects to \(\{u \in \mathbb{R}^n \mid \|X^T u\|_2 \leq \beta\}\). We now prove strong duality.

**Theorem 2.3.** Strong duality holds for (10) with finite width.

2.2. Training problem with vector outputs

Here, our model is \(f_{\theta,2}(X) = XW_1W_2\) to estimate \(Y \in \mathbb{R}^{n \times K}\), which can be optimized as follows

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

Using Lemma A.2, we reformulate (11) as

$$\min_{\theta \in \Theta} \sum_{j=1}^m \|w_{2,j}\|_2 \quad \text{s.t. } f_{\theta,2}(X) = Y, w_{1,j} \in \mathcal{B}_2, \quad (12)$$

which has the following dual with respect to \(W_2\)

$$\max_{\lambda} \text{tr}(\Lambda^T Y) \quad \text{s.t. } \|\Lambda^T X w_1\|_2 \leq 1, \forall w_1 \in \mathcal{B}_2. \quad (13)$$

Since we can assume \(Y = XW^*\) due to Proposition 2.1

$$\text{tr}(\Lambda^T Y) = \text{tr}(\Lambda^T X W^*) \leq \sigma_{\max}(\Lambda^T U_x \Sigma_x) \|W^*_r\|_* \quad (14)$$

where \(\sigma_{\max}(\Lambda^T X) \leq 1\) due to (13) and \(\tilde{W}_r = \left[\begin{array}{c} I_r \circ 0_{r \times d-r} \\ 0_{d-r \times r} \circ 0_{d-r \times d-r} \end{array}\right] V_x^T W^*\). Given the SVD of \(\tilde{W}_r^*\), i.e., \(U_w \Sigma_w V_w^*\), choosing

$$\Lambda^T U_x \Sigma_x = V_w \left[\begin{array}{c} I_r \circ 0_{r \times d-r} \\ 0_{K-r \times r} \circ 0_{K-r \times d-r} \end{array}\right] U_w^T$$

achieves the upper-bound above, where \(r_w = \text{rank}(\tilde{W}_r^*)\).

Thus, optimal neurons are a subset of the first \(r_w\) right singular vectors of \(\Lambda^T X\). We next prove strong duality.

**Theorem 2.4.** Let \((X, Y)\) be feasible for (12), then strong duality holds for finite width networks.

2.2.1. Regularized case

Here, we define the regularized version of (12) as follows

$$\min_{\theta \in \Theta} \frac{1}{2} \|f_{\theta,2}(X) - Y\|_F^2 + \beta \sum_{j=1}^m \|w_{2,j}\|_2 \quad \text{s.t. } w_{1,j} \in \mathcal{B}_2, \quad (15)$$

which has the following dual with respect to \(W_2\)

$$\max_{\lambda} -\frac{1}{2} \|\lambda - \frac{1}{\beta} (\lambda^T X w_1)\|_2^2 \quad \text{s.t. } \sigma_{\max}(\Lambda^T X) \leq \beta.$$  

Then, the optimal neurons are a subset of the maximal right singular vectors of \(\mathcal{P}_{X,B}(Y)^T X\), where \(\mathcal{P}_{X,B}(\cdot)\) projects its input to the set \(\{U \in \mathbb{R}^{n \times K} \mid \sigma_{\max}(U^T X) \leq \beta\}\).

**Remark 2.1.** Note that the optimal neurons are the right singular vectors of \(\mathcal{P}_{X,B}(Y)^T X\) that achieve \(\|\mathcal{P}_{X,B}(Y)^T X w_1\|_2 = \beta\), where \(\|w_1\|_2 = 1\). This implies that \(\|Y^T X w_1\|_2 \geq \beta\), therefore, the number of optimal neurons and rank \((W_1^*)\) are determined by \(\beta\).

**Remark 2.2.** The right singular vectors of \(\mathcal{P}_{X,B}(Y)^T X\) are not the only solutions. Consider \(u_1\) and \(u_2\) as the optimal right singular vectors. Then, \(u = \alpha_1 u_1 + \alpha_2 u_2\) with \(\alpha_1^2 + \alpha_2^2 = 1\) also achieves the upper-bound, thus, optimal.

3. Deep linear networks

We now consider an \(L\)-layer linear network with the output function \(f_{\theta,L}(X) = \sum_{j=1}^m XW_{1,j} \ldots W_{L,j}\), and the training problem

$$\min_{\{\theta_l\}_{l=1}^L} \frac{1}{2} \sum_{j=1}^m \sum_{l=1}^L \|W_{l,j}\|_F^2 \quad \text{s.t. } f_{\theta,L}(X) = y. \quad (15)$$

**Proposition 3.1.** First \(L - 2\) layer weight matrices in (15) have the same operator and Frobenius norms, i.e., \(t_j = \|W_{l,j}\|_F = \|W_{l,j}\|_2, \forall l \in [L - 2], \forall j \in [m]\).

This result shows that the layer weights obey an alignment condition. After using the scaling in Lemma A.3 and the same convex duality arguments, a set of optimal solutions to the training problem can be described as follows.

**Theorem 3.1.** Optimal layer weights for (15) are

$$W_{l,j}^* = \begin{cases} \frac{t_j}{\|t_j\|_2} V_{l,j}^* \rho_{l,j}^T & \text{if } l = 1 \\ t_j \rho_{l-1,j} \rho_{l,j}^T & \text{if } 1 < l \leq L - 2 \\ \rho_{L-2,j} & \text{if } l = L - 1 \end{cases}$$

where \(\rho_{l,j} \in \mathbb{R}^{m_l} \) such that \(\|\rho_{l,j}\|_2 = 1, \forall l \in [L - 2], \forall j \in [m]\) and \(\tilde{W}_r^*\) is defined in (9).

Next, we prove strong duality holds.
3.1. Regularized training problem

We now present the regularized training problem as follows:

$$\min_{\{\theta_l\}_{l=1}^L} \frac{1}{2} \|f_{\theta,L}(X) - y\|^2 + \frac{\beta}{2} \sum_{j=1}^L \sum_{l=1} \|W_{l,j}\|_F^2. \quad (16)$$

Next result provides a set of optimal solutions to (16).

**Theorem 3.3.** Optimal layer weights for (16) are

$$W_{l,j}^* = \begin{cases} t_s^x X^T \mathcal{P}_{X,\beta}(y) & \text{if } l = 1 \\ t_s^x \rho_{L-1,j}^T \theta_{L-1,j} & \text{if } 1 < l \leq L - 2 \\ \rho_{L-2,j} & \text{if } l = L - 1 \end{cases},$$

where $\mathcal{P}_{X,\beta}(\cdot)$ projects to $\{u \in \mathbb{R}^n \mid \|X^T u\|_2 \leq \beta t_s^{2-L}\}$.

**Corollary 3.2.** Theorem 3.2 also shows that strong duality holds for the training problem in (16).

3.2. Training problem with vector outputs

Here, we consider vector output deep networks with the output function $f_{\theta,L}(X) = \sum_{j=1}^m X W_{1,j} \ldots W_{L,j}$. In this case, we have the following training problem:

$$\min_{\{\theta_l\}_{l=1}^L} \sum_{j=1}^m \sum_{l=1}^L \|W_{l,j}\|_F^2 \quad \text{s.t. } f_{\theta,L}(X) = Y. \quad (17)$$

Using the scaling in Lemma [A.4] and the same convex duality arguments, optimal layer weight configurations for (17) are as follows.

**Theorem 3.4.** Optimal layer weights for (17) are

$$W_{l,j}^* = \begin{cases} t_s^x \hat{v}_{w,j} \rho_{l,j}^T & \text{if } l = 1 \\ t_s^x \rho_{l-1,j} \rho_{l,j}^T & \text{if } 1 < l \leq L - 2 \\ \rho_{L-2,j} & \text{if } l = L - 1 \end{cases},$$

where $j \in [K]$, $\hat{v}_{w,j}$ is the $j^{th}$ maximal right singular vector of $\Lambda^T x$ and $\{\rho_{l,j}\}_{l=1}^{L-2}$ are arbitrary unit norm vectors such that $\rho_{l,j}^T \rho_{l,k} = 0$, $\forall j \neq k$.

The next theorem formally proves that strong duality holds for the primal problem in (17).

**Theorem 3.5.** Let $(X, Y)$ be feasible for (17), then strong duality holds for finite width networks.

3.2.1. Regularized Case

We now examine the following regularized problem:

$$\min_{\{\theta_l\}_{l=1}^L} \frac{1}{2} \|f_{\theta,L}(X) - y\|^2 + \frac{\beta}{2} \sum_{j=1}^m \sum_{l=1}^L \|W_{l,j}\|_F^2. \quad (18)$$

Next result provides a set of optimal solutions to (18).

**Theorem 3.6.** Optimal layer weights for (18) are

$$W_{l,j}^* = \begin{cases} t_s^x \hat{v}_{x,j} \rho_{l,j}^T & \text{if } l = 1 \\ t_s^x \rho_{l-1,j} \rho_{l,j}^T & \text{if } 1 < l \leq L - 2 \\ \rho_{L-2,j} & \text{if } l = L - 1 \end{cases},$$

where $j \in [K]$, $\hat{v}_{x,j}$ is a maximal right singular vector of $\mathcal{P}_{X,\beta}(\cdot)^T X$ and $\mathcal{P}_{X,\beta}(\cdot)$ projects to $\{U \in \mathbb{R}^{n \times k} \mid \sigma_{max}(U^T X) \leq \beta t_s^{2-L}\}$. Additionally, $\rho_{l,j}$ is an orthonormal set. Therefore, the rank of each hidden layer is determined by $\beta$ as in Remark [2.7].

4. Deep ReLU networks

Here, we consider an $L$-layer ReLU network with the output function $f_{\theta,L}(X) = A_{L-1} W_l$, where $A_{l-1} = (A_{l-1,j} W_{l,j})_{+}$, $A_{0,j} = X$, $\forall l, j$, and $(x)_{+} = \max(0, x)$. Below, we first state the minimum norm training problem and then present our results:

$$\min_{\{\theta_l\}_{l=1}^L} \sum_{j=1}^m \sum_{l=1}^L \|W_{l,j}\|_F^2 \quad \text{s.t. } f_{\theta,L}(X) = y. \quad (19)$$

**Theorem 4.1.** Let $X$ be a rank-one matrix such that $X = ca_0^T$, where $c \in \mathbb{R}^n$ and $a_0 \in \mathbb{R}^d$, then strong duality holds and the optimal weights are

$$W_{l,j} = \frac{\phi_{l-1,j}}{\|\phi_{l-1,j}\|_2} \phi_{l,j}^T, \forall l \in [L - 2], \text{ } W_{L-1,j} = \frac{\phi_{L-2,j}}{\|\phi_{L-2,j}\|_2},$$

where $\phi_{0,j} = a_0$ and $\{\phi_l\}_{l=1}^{L-2}$ is a set of vectors such that $\phi_{l,j} \in \mathbb{R}^{n \times 1}$ and $\|\phi_{l,j}\|_2 = t_s^x$, $\forall l \in [L - 2], \forall j \in [m]$.

In the sequel, we first examine a two-layer training problem with bias and then extend this to multi-layer.

**Theorem 4.2.** Let $X$ be a matrix such that $X = ca_0^T$, where $c \in \mathbb{R}^n$ and $a_0 \in \mathbb{R}^d$. Then, when $L = 2$, a set of optimal solutions to (19) is $\{(w_i, b_i)\}_{i=1}^m$, where $w_i = s_i a_0 / \|a_0\|_2$, $b_i = -s_i c_i$, and $s_i = \pm 1, \forall i \in [m]$. Therefore, the optimal network output has kinks only at the input data points, i.e., the output function is in the following form: $f_{a_2}(x) = \sum_i (x_i - x_i)_+$. Hence, the network output becomes a linear spline interpolation.
We now extend the results in Theorem 4.2 and Corollary 4.1 to multi-layer ReLU networks.

**Proposition 4.1.** Theorem 4.1 still holds when we add a bias term to the last hidden layer, i.e., \( \sum_j (A_{L-2,j}w_{L-1,j} + 1_n b_j) \cdot w_{L,j} = y \).

**Corollary 4.2.** As a result of Theorem 4.2 and Proposition 4.1, for one dimensional data, i.e., \( x \in \mathbb{R}^n \), the optimal network output has kinks only at the input data points, i.e., the output function is in the following form:

\[
    f_{\theta,L}(x) = \sum_i (x_i - x_i)^}_+. \text{ Therefore, the optimal network output is a linear spline interpolation.}
\]

In Corollary 4.1 and 4.2, the optimal output function for multi-layer ReLU networks are linear spline interpolators for rank-one data, which generalizes the two-layer results for one-dimensional data in (Savarese et al. 2019) (Parhi & Nowak 2019) (Ergen & Pilanci 2020a, b) to arbitrary depth.

### 4.1. Regularized problem with vector outputs

We now extend the analysis to regularized training problems with \( K \) outputs, i.e., \( Y \in \mathbb{R}^{n \times K} \).

The result in Theorem 4.1 also holds for vector output multi-layer ReLU networks as shown below.

**Proposition 4.2.** Theorem 4.1 extends to deep ReLU networks with vector outputs, therefore, the optimal layer weights can be formulated as in Theorem 4.1.

Now, we extend our characterization to arbitrary rank whitened data matrices and fully characterize the optimal layer weights of a deep ReLU network with \( K \) outputs. We also note that one can even obtain closed-form solutions for all the layers weights as proven in the next result.

**Theorem 4.3.** Let \( \{X, Y\} \) be a dataset such that \( XX^T = I_n \) and \( Y \) is one-hot encoded, then a set of optimal solutions for the following regularized training problem

\[
    \min_{\theta \in \Theta} \frac{1}{2} \| f_{\theta,L}(X) - Y \|_F^2 + \frac{\beta}{2} \sum_{j=1}^m \sum_{l=1}^L \| W_{l,j} \|^2_F
\]

(20)

can be formulated as follows

\[
    W_{l,j} = \begin{cases} \frac{\phi_{0,j-1} + \phi_{l,j}}{\| \phi_{0,j} \|_2 + \beta} \phi_{l,j}^T, & \text{if } l \in [L-1] \\ \left( \| \phi_{0,j} \|_2 - \beta \right) \phi_{l-1,j} e_j^T, & \text{if } l = L \end{cases}
\]

where \( \phi_{0,j} = X^T y_j \), \( \{ \phi_{l,j} \}_{l=1}^{L-2} \) are vectors such that \( \phi_{l,j} \in \mathbb{R}_{+}^n \), \( \| \phi_{l,j} \|_2 = t_j \), and \( \phi_{l-1,j} \phi_{l,j} = 0 \), \( \forall i \neq j \). Moreover, \( \phi_{L-1,j} = e_j \) is the \( j \)-th ordinary basis vector.

**Remark 4.1.** We note that the whitening assumption \( XX^T = I_n \) necessitates that \( n \leq d \), which might appear to be restrictive. However, this case is common in few-shot classification problems with limited labels (Chen et al. 2018). Moreover, it is challenging to obtain reliable labels in problems involving high dimensional data such as in medical imaging (Hyan et al. 2020) and genetics (Singh & Yamada 2020), where \( n \leq d \) is typical. More importantly, SGD employed in deep learning frameworks, e.g., PyTorch and Tensorflow, operate in mini-batches rather than the full dataset. Therefore, even when \( n > d \), each gradient descent update can only be evaluated on small batches, where the batch size \( n_b \) satisfies \( n_b \ll d \). Hence, the \( n \leq d \) case implicitly occurs during the training phase.

**Remark 4.2.** We also note that the conditions in Theorem 4.3 are common in practical frameworks. As an example, for image classification, it has been shown that whitening significantly improves the classification accuracy of the state-of-the-art architectures, e.g., ResNets, on benchmark datasets such as ImageNet (Huang et al. 2018). Furthermore, the label matrix is one hot encoded in image classification. Therefore, in such cases, there is no need to train a deep ReLU network in an end-to-end manner. Instead one can directly use the closed-form formulas in Theorem 4.3.

### 4.2. Regularized problem with Batch Normalization

We now consider a more practical setting with an arbitrary \( L \)-layer network and batch normalization (Ioffe & Szegedy 2015). We first define batch normalization as follows. For the activation matrix \( A_{L-1} \in \mathbb{R}^{n \times m_{l-1}} \), batch normalization applies to each column \( j \) independently as follows

\[
    \text{BN}_{\gamma, \alpha}(A_{l-1,j}w_{l,j}) = \frac{(I_n - \frac{1}{n} 1_n 1_n^T) A_{l-1,j}w_{l,j}}{\| (I_n - \frac{1}{n} 1_n 1_n^T) A_{l-1,j}w_{l,j} \|_2} \gamma_j^{(l)} + \frac{1}{\sqrt{n}} \alpha_j^{(l)}
\]

where \( \gamma_j^{(l)} \) and \( \alpha_j^{(l)} \) scales and shifts the normalized value, respectively. The following theorem presents a complete characterization for the last two layers’ weights.

**Theorem 4.4.** Suppose \( Y \) is one hot encoded and the network is overparameterized such that the range of \( A_{L-2,j} \) is \( \mathbb{R}^d \), then an optimal solution to the following problem

\[
    \min_{\theta \in \Theta} \frac{1}{2} \left\| \sum_{j=1}^m \left( \text{BN}_{\gamma, \alpha}(A_{L-2,j}w_{L-1,j}) + w_{L,j} \right) - Y \right\|_F^2
\]

(20)

\[
    + \frac{\beta}{2} \sum_{j=1}^m \left( \gamma_j^{(L-1)} + \alpha_j^{(L-1)} + \| w_{L,j} \|_2^2 \right)
\]

where \( \gamma_j^{(l)} \) and \( \alpha_j^{(l)} \) scales and shifts the normalized value, respectively. The following theorem presents a complete characterization for the last two layers’ weights.

**Theorem 4.4.** Suppose \( Y \) is one hot encoded and the network is overparameterized such that the range of \( A_{L-2,j} \) is \( \mathbb{R}^d \), then an optimal solution to the following problem
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Figure 2: Verification of Remark 2.1. (a) Rank of the hidden layer weight matrix as a function of $\beta$ and (b) rank of the hidden layer weights for different regularization parameters, i.e., $\beta_1 < \beta_2 < \beta_3 < \beta_4$.

Figure 3: Verification of Proposition 3.1 and 4.1. (a) Evolution of the operator and Frobenius norms for the layer weights of a linear network and (b) Rank of the layer weights of a ReLU network with $K = 1$. One-hot encoding is one of the common strategies to convert categorical variables into a binary representation that can be processed by DNNs. Although (Papyan et al., 2020) empirically verified the emergence of certain patterns, termed Neural Collapse, for one-hot encoded labels trained with batch normalization, the theory behind these findings are still unknown. Therefore, we first define a new notion of simplex Equiangular Tight Frame (ETF) and then explain the Neural Collapse phenomenon where class means collapse to the vertices of a simplex ETF. We also note that all of our derivations hold for arbitrary convex loss functions, therefore, are also valid for the commonly adopted cross entropy loss as proven in Appendix A.1.

Definition 2. A standard simplex ETF is a set of points in $\mathbb{R}^K$ selected from the columns of the following matrix

$$S = \sqrt{\frac{K}{K-1}} \left( I_K - \frac{1}{K} 1_{K \times K} \right),$$

where we assume that samples are ordered, i.e., the first $n/K$ samples belong to class 1, next $n/K$ samples belong.
to class 2 and so on. Therefore, all the activations for a certain class k are the same and their mean is given by $\frac{(K/n)(e_k - 1_K/K)}{\sqrt{K}}$, which is the kth column of a general simplex ETF with $0.20 < 0.25 < 0.30$.

5. Numerical experiments

Here, we present numerical results to verify our theoretical analysis. We first use synthetic datasets generated from a random data matrix with zero mean and identity covariance and the corresponding output vector is obtained via a random initialization of the teacher network.

![Graphs showing training and test performance on whitened and sampled datasets, where $(n, d) = (60, 90)$, $K = 10$, $L = 3, 4, 5$ with 50 neurons per layer and we use squared loss with one hot encoding. For Theory, we use the layer weights in Theorem 4.3, which achieves the optimal performance as guaranteed by Theorem 4.3.]

We also conduct an experiment for a five-layer ReLU network with $W_{1,j} \in \mathbb{R}^{10 \times 50}$, $W_{2,j} \in \mathbb{R}^{50 \times 40}$, $W_{3,j} \in \mathbb{R}^{40 \times 30}$, $W_{4,j} \in \mathbb{R}^{30 \times 20}$, and $W_{5,j} \in \mathbb{R}^{20 \times 1}$. Here, we use data such that $X = c a_k^T$, where $c \in \mathbb{R}^{d}$ and $a_k \in \mathbb{R}^d$. In Figure 3b, we plot the rank of each weight matrix, which converges to one as claimed in Proposition 4.1.

We also verify our theory on two real benchmark datasets, i.e., MNIST (LeCun) and CIFAR-10 (Krizhevsky et al. 2014). We first randomly undersample and whiten these datasets. We then convert the labels into one hot encoded form. Then, we consider a ten class classification/regression task using three multi-layer ReLU network architectures with $L = 3, 4, 5$. For each architecture, we use SGD with momentum for training and compare the training/test performance with the corresponding network constructed via the closed-form solutions (without any sort of training) in Theorem 4.3, i.e., denoted as “Theory”.

6. Concluding remarks

We studied regularized DNN training problems and developed an analytic framework to characterize the optimal so-
lutions. We showed that optimal 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 both deep linear and ReLU networks and provided a set of optimal solutions. We also extended our derivations to the vector outputs and many other loss functions. More importantly, our analysis shows that when the input data is whitened or rank-one, instead of training an $L$-layer deep ReLU network in an end-to-end manner, one can directly use the closed-form solutions provided in Theorem 4.1 and 4.3. Furthermore, we showed that whitening/rank-one assumptions can be removed via batch normalization (see Theorem 4.4). After our work, this was also realized by Ergen et al. [2021], where the authors proved that batch normalization effectively whitens the input data matrix. As a corollary, we uncovered theoretical reasons behind a recent empirical observation termed Neural Collapse [Papyan et al., 2020]. As another corollary, we proved that the kinks of ReLU occur exactly at the input data so that the optimal network outputs linear spline interpolations for one-dimensional datasets, which was previously known only for two-layer networks (Savarese et al., 2019; Parhi & Nowak, 2019; Ergen & Pilanci, 2020a;b).

As the limitation of this work, we note that for networks with more than two-layers (i.e., $L > 2$), we use a non-standard architecture, where each layer consists of $m$ weight matrices. Thus, we are able to achieve strong duality which is essential for our analysis. We leave the strong duality analysis of standard deep networks as an open research problem for future work.

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Appendix

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A. Appendix
Here, 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 also provide a table for notations below.

Table 2: Notations and variables in this paper.

| Notation | Description |
|----------|-------------|
| $X \in \mathbb{R}^{n \times d}$ | Data matrix |
| $y \in \mathbb{R}^n, Y \in \mathbb{R}^{n \times K}$ | Label vector and matrix |
| $W_{l,j} \in \mathbb{R}^{m_{l-1} \times m_l}$ | $l^{th}$ layer weight matrix |
| $A_l \in \mathbb{R}^{n \times m_l}$ | $l^{th}$ layer activation matrix |
| $\lambda \in \mathbb{R}^n, \Lambda \in \mathbb{R}^{n \times K}$ | Dual vector and matrix |
| $w^* \in \mathbb{R}^d, W^* \in \mathbb{R}^{d \times K}$ | Optimal weight vector and matrix |
| $r$ | Rank of $X$ |
| $U, \Sigma, V^T$ | $X$ SVD |
| $e_j$ | $j^{th}$ ordinary basis vector |
| $\mathcal{L}(-, y)$ | Arbitrary convex loss function |
| $f_{\theta,L}(X)$ | Output of an $L$-layer network |

A.1. General loss functions

In this section, we show that our extreme point characterization holds for arbitrary convex loss functions including cross entropy and hinge loss. We first restate the primal training problem after applying the rescaling in Lemma 1.1 as follows

$$\min_{\theta, t_j} \mathcal{L}(f_{\theta,L}(X), y) + \beta \|W_L\|_1 + \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2 \text{ s.t. } W_{L-1,j} \in \mathcal{B}_2, \|W_{l,j}\|_F \leq t_j, \forall l \in [L-2], \forall j \in [m],$$  \hspace{1cm} (21)

where $\mathcal{L}(-, y)$ is a convex loss function.

Theorem A.1. The dual of (21) is given by

$$\min_{t_j} \max_{\lambda} -\mathcal{L}^*(\lambda) + \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2 \text{ s.t. } \max_{W_{L-1,j} \in \mathcal{B}_2} \|A_{L-1}^T \lambda\|_\infty \leq \beta,$$
where $\mathcal{L}^*$ is the Fenchel conjugate function defined as
\[
\mathcal{L}^*(\lambda) = \max_z z^T \lambda - \mathcal{L}(z, y).
\]

**Proof of Theorem A.1** The proof directly follows from the dual derivation in Appendix A.2.

Theorem A.1 proves that our extreme point characterization applies to arbitrary loss function. Therefore, optimal parameters for (21) 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 also valid for all of these cases.

### A.2. Derivations for the dual problem in networks

We first restate the scaled primal problem in Lemma 1.1

\[
P^* = \min_{\{\theta_t\}_{t=1}^{L-1}, t_j} \max_{\hat{y}, y, L} \mathcal{L}(\hat{y}, y) + \beta \|w_L\|_1 + \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2 \\
\text{s.t. } w_{L-1,j} \in B_2, \|w_{l,j}\|_F \leq t_j, \forall l \in [L - 2], \forall j \in [m] \\
\hat{y} = f_{\theta,L}(X).
\]

Then, the corresponding Lagrangian is

\[
L(\lambda, \hat{y}, w_L) = \mathcal{L}(\hat{y}, y) - \lambda^T \hat{y} + \lambda^T f_{\theta,L}(X) + \beta \|w_L\|_1 + \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2.
\]

Based on the Lagrangian above, we now obtain the dual function as follows

\[
g(\lambda) = \min_{\hat{y}, w_L} L(\lambda, \hat{y}, w_L) \\
= \min_{\hat{y}, w_L} \mathcal{L}(\hat{y}, y) - \lambda^T \hat{y} + \lambda^T f_{\theta,L}(X) + \beta \|w_L\|_1 + \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2 \\
= \min_{\hat{y}, w_L} \mathcal{L}(\hat{y}, y) - \lambda^T \hat{y} + \lambda^T A_{L-1} w_L + \beta \|w_L\|_1 + \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2
\]

\[
= -\mathcal{L}^*(\lambda) + \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2 \text{ s.t. } \|A_{L-1}^T\|_\infty \leq \beta.
\]

where $\mathcal{L}^*$ is the Fenchel conjugate function defined as [Boyd & Vandenberghe 2004]

\[
\mathcal{L}^*(\lambda) = \max_z z^T \lambda - \mathcal{L}(z, y).
\]

Thus, taking the dual of (22) in terms of $w_L$ and $\hat{y}$ yield

\[
P^* = \min_{\{\theta_t\}_{t=1}^{L-1}, t_j} \max_{\lambda} g(\lambda) = \min_{\{\theta_t\}_{t=1}^{L-1}, t_j} \max_{\lambda} -\mathcal{L}^*(\lambda) + \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2 \text{ s.t. } \|A_{L-1}^T\|_\infty \leq \beta.
\]

To achieve the lower bound in the main paper, we now change the order of min (for the layer weights)-max as follows

\[
P^* \geq D^* = \min_{t_j} \max_{\lambda} \min_{\|w_{L-1,j}\|_F \leq t_j} -\mathcal{L}^*(\lambda) + \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2 \text{ s.t. } \|A_{L-1}^T\|_\infty \leq \beta
\]

\[
= \min_{t_j} \max_{\lambda} -\mathcal{L}^*(\lambda) + \frac{\beta}{2} (L - 2) \sum_{j=1}^m t_j^2 \text{ s.t. } \max_{\|w_{L-1,j}\|_F \leq t_j} \|A_{L-1}^T\|_\infty \leq \beta,
\]

which completes the derivation.
A.3. Equivalence (Rescaling) lemmas for the non-convex objectives

In this section, we present all the equivalence (scaling transformation) lemmas we used in the main paper and the the proofs are presented in Appendix A.6[A.7] and A.8[two-layer, deep linear, and deep ReLU networks, respectively. We also note that similar scaling techniques were also utilized in Neyshabur et al., 2014[Savarese et al., 2019]Ergen & Pilanci, 20192020a,b,c).

Lemma 1.1. The following problems are equivalent:

\[
\min_{\{\theta_i\}_{i=1}^L} \mathcal{L}(f_{\theta,L}(X), y) + \frac{\beta}{2} \sum_{j=1}^L \sum_{l=1}^m \|W_{l,j}\|_2^2 \\
= \min_{\{\theta_i\}_{i=1}^L, \{t_j\}_{j=1}^m} \mathcal{L}(f_{\theta,L}(X), y) + \beta \|W_L\|_1 \\
\quad + \frac{\beta}{2} (L-2) \sum_{j=1}^m t_j^2, \\
\text{s.t. } W_{L-1,j} \in \mathcal{B}_2, \|W_{l,j}\|_F \leq t_j, \forall l \in [L-2]
\]

Proof of Lemma 1.1. For any \(\theta \in \Theta\), we can rescale the parameters as \(\bar{w}_{L-1,j} = \alpha_j w_{L-1,j}\) and \(\bar{w}_{L,j} = w_{L,j}/\alpha_j\), for any \(\alpha_j > 0\). Then, the network output becomes

\[
f_{\theta,L}(X) = \sum_{j=1}^m \left( (XW_{1,j})_+ \cdots w_{L-1,j} \right) + \bar{w}_{L,j} = \sum_{j=1}^m \left( (XW_{1,j})_+ \cdots w_{L-1,j} \right) + w_{L,j} = f_{\theta,L}(X),
\]

which proves that this scaling does not change the output of the network. In addition to this, we have the following basic inequality

\[
\sum_{j=1}^m \sum_{l=1}^L \|W_{l,j}\|_F^2 \geq \sum_{j=1}^m \sum_{l=1}^{L-2} \|W_l\|_F^2 + 2 \sum_{j=1}^m |w_{L,j}| \|W_{L-1,j}\|_2,
\]

where the equality is achieved with the scaling choice \(\alpha_j = \left( \frac{|w_{L,j}|}{\|w_{L-1,j}\|_2} \right)^{\frac{1}{2}}\) is used. Since the scaling operation does not change the right-hand side of the inequality, we can set \(\|w_{L-1,j}\|_2 = 1, \forall j\). Therefore, the right-hand side becomes \(\|W_L\|_1\).

Now, let us consider a modified version of the problem, where the unit norm equality constraint is relaxed as \(\|w_{L-1,j}\|_2 \leq 1\). Let us also assume that for a certain index \(j\), we obtain \(\|w_{L-1,j}\|_2 < 1\) with \(w_{L,j} \neq 0\) as an optimal solution. This shows that the unit norm inequality constraint is not active for \(w_{L-1,j}\), and hence removing the constraint for \(w_{L-1,j}\) will not change the optimal solution. However, when we remove the constraint, \(\|w_{L-1,j}\|_2 \rightarrow \infty\) reduces the objective value since it yields \(w_{L,j} = 0\). Therefore, we have a contradiction, which proves that all the constraints that correspond to a nonzero \(w_{L,j}\) must be active for an optimal solution. This also shows that replacing \(\|w_{L-1,j}\|_2 = 1\) with \(\|w_{L-1,j}\|_2 \leq 1\) does not change the solution to the problem.

Then, we use the epigraph form for the sum of the norm of the first \(L-2\) layers to achieve the equivalence, i.e., we introduce \(\|W_{l,j}\|_F \leq t_j\) constraint and replace \(\sum_{j=1}^{L-2} \|W_{l,j}\|_F^2\) with \((L-2)t_j^2\) in the objective. We also note that since the optimal layer weights have the same Frobenius norm as proven in Proposition 3.1, we can replace the Frobenius norm of each layer weight matrix with the same variable \(t\) without loss of generality.

Lemma A.1. The following two problems are equivalent:

\[
\min_{\theta \in \Theta} \|W_1\|_F^2 + \|w_2\|_2^2 = \min_{\theta \in \Theta} \|w_2\|_1 \\
\text{s.t. } f_{\theta,2}(X) = y \\
\text{s.t. } f_{\theta,2}(X) = y, w_{1,j} \in \mathcal{B}_2.
\]
Proof of Lemma A.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

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

which proves \( f_{\theta,2}(X) = \bar{f}_{\theta,2}(X) \). 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 \( \alpha_j = (\frac{|w_{2,j}|}{\|w_{1,j}\|_2})^2 \) is used. Since the scaling operation does not change the right-hand side of the inequality, we can set \( \|w_{1,j}\|_2 = 1, \forall j \). Therefore, the right-hand side becomes \( \|w_2\|_1 \).

Now, let us consider a modified version of the problem, where the unit norm equality constraint is relaxed as \( \|w_{1,j}\|_2 \leq 1 \). Let us also assume that for a certain index \( j \), we obtain \( \|w_{1,j}\|_2 < 1 \) 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, \( \|w_{1,j}\|_2 \to \infty \) 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 \( \|w_{1,j}\|_2 = 1 \) with \( \|w_{1,j}\|_2 \leq 1 \) does not change the solution to the problem. \( \square \)

Lemma A.2. The following problems are equivalent:

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

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

Proof of Lemma A.2 The proof directly follows from Proof of Lemma A.1 using the following inequality

\[
\frac{1}{2} \sum_{j=1}^{m} (\|w_{2,j}\|^2_2 + \|w_{1,j}\|^2_2) \geq \sum_{j=1}^{m} (\|w_{2,j}\|_2 \|w_{1,j}\|_2).
\]

Then, if we set \( \|w_{1,j}\|_2 = 1, \forall j \), the right-hand side becomes \( \sum_{j=1}^{m} \|w_{2,j}\|_2 \).

Lemma A.3. The following problems are equivalent:

\[
\min_{\{\theta_i\}_{i=1}^{L}} \frac{1}{2} \sum_{j=1}^{m} \sum_{t=1}^{L} \|W_{t,j}\|^2_F = \min_{\{\theta_i\}_{i=1}^{L}, (t_j)_{j=1}^{m}} \|W_L\|_1 + \frac{1}{2} (L - 2) \sum_{j=1}^{m} t_j^2 \quad \text{s.t.} \quad f_{\theta,L}(X) = y, w_{L-1,j} \in B_2, \|W_{t,j}\|_F \leq t_j, \forall t \in [L - 2], \forall j \in [m]
\]

Proof of Lemma A.3 Applying the rescaling in Lemma A.1 to the last two layers of the \( L \)-layer network in [15] gives

\[
\min_{\{\theta_i\}_{i=1}^{L}} \|W_L\|_1 + \frac{1}{2} \sum_{j=1}^{m} \sum_{t=1}^{L-2} \|W_{t,j}\|^2_F \quad \text{s.t.} \quad \|W_{L-1,j}\|_2 \leq 1, \forall j \in [m], \sum_{j=1}^{m} \sum_{L-1}^{L} j w_{L-j} = y
\]

Then, we use the epigraph form for the norm of the first \( L - 2 \) to achieve the equivalence. \( \square \)
Lemma A.4. The following problems are equivalent:

\[
\min_{\{\theta_l\}_{l=1}^L} \frac{1}{2} \sum_{j=1}^m \sum_{l=1}^L \|W_{l,j}\|_F^2 = \min_{\{\theta_l\}_{l=1}^L, \{\gamma_j\}_{j=1}^m} \frac{1}{2} \sum_{j=1}^m \|w_{L,j}\|_2 + \frac{1}{2} (L - 2) \sum_{j=1}^m t_j^2.
\]

s.t. \(f_{\theta,L}(X) = Y\) s.t. \(f_{\theta,L}(X) = Y, w_{L-1,j} \in \mathcal{B}_2, \|W_{l,j}\|_F \leq t_j, \forall l \in [L - 2], \forall j \in [m]\)

Proof of Lemma A.4. Applying the rescaling in Lemma A.1 to the last two layer of the L-layer network in (17) gives

\[
\min_{\{\theta_l\}_{l=1}^L} \sum_{j=1}^m \|W_{L,j}\|_2 + \frac{1}{2} \sum_{j=1}^m \sum_{l=1}^L \|W_l\|_F^2
\]

s.t. \(\|w_{L-1,j}\|_2 \leq 1, \forall j \in [m], \sum_{j=1}^m X_{1,j} \cdots w_{L-1,j}w_{L,j}^T = Y\)

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

\[\square\]

A.4. Regularization in Theorem 4.4

In this section, we prove that regularizing the all the parameters do not alter the claims in Theorem 4.4. We first state the primal problem, where all the parameters are regularized, as follows

\[
P^{**}_r = \min_{\theta \in \Theta} \frac{1}{2} \sum_{j=1}^m (\text{BN}_{\gamma_j, \alpha_j} (A_{L-2,j}w_{L-1,j}))_+ w_{L,j}^T - Y \|_F^2 + \frac{\beta}{2} \sum_{j=1}^m \sum_{l=1}^L \left( \|\gamma_j\|_2^2 + \|\alpha_j\|_2^2 + \|W_{l,j}\|_F^2 \right),
\]

where we use \(\gamma^{(L)} = \alpha^{(L)} = 0\) as dummy variables for notational simplicity. Now, we rewrite (23) as

\[
P^{**}_r = \min_{t \geq 0} \min_{\theta \in \Theta} \frac{1}{2} \sum_{j=1}^m (\text{BN}_{\gamma_j, \alpha_j} (A_{L-2,j}w_{L-1,j}))_+ w_{L,j}^T - Y \|_F^2 + \frac{\beta}{2} \sum_{j=1}^m \sum_{l=1}^L \left( \|\gamma_j\|_2^2 + \|\alpha_j\|_2^2 + \|W_{l,j}\|_F^2 \right) + \frac{\beta}{2} t
\]

s.t. \(\sum_{j=1}^m \sum_{l=1}^L \left( \|\gamma_j\|_2^2 + \|\alpha_j\|_2^2 + \|W_{l,j}\|_F^2 \right) + \|W_{L-1}\|_F^2 \leq t\).

After applying the scaling between \(W_L\) and \((\gamma^{(L-1)}, \alpha^{(L-1)})\) as in Lemma A.1, we take the dual with respect to \(W_L\) to obtain the following problem

\[
P^*_r \geq D^*_r = \max_{t \geq 0} \max_{A \in \mathbb{R}} -\frac{1}{2} \|A - Y\|_F^2 + \frac{1}{2} \|Y\|_F^2 + \frac{\beta}{2} t
\]

s.t. \(\max_{\theta \in \Theta_r} \|A^T (\text{BN}_{\gamma_j, \alpha_j} (A_{L-2,j}w_{L-1,j}))_+ \|_2 \leq \beta\),

where \(\Theta_r = \{\theta \in \Theta : \gamma_j^{(L-1)} + \alpha_j^{(L-1)} = 1, \forall j \in [m], \sum_{l=1}^{L-2} \left( \|\gamma_j\|_2^2 + \|\alpha_j\|_2^2 + \|W_{l,j}\|_F^2 \right) + \|W_{L-1}\|_F^2 \leq t\}\).

Since

\[
\text{BN}_{\gamma_j, \alpha_j} (A_{L-2,j}w_{L-1,j}) = \frac{(I_n - \frac{1}{n} 1_{n \times n})A_{L-2,j}w_{L-1,j} - \gamma_j^{(L-1)} + \frac{1}{n} \sqrt{n} \gamma_j^{(L-1)}}{h(\theta')},
\]

where \(\theta'\) denotes all the parameters except \(\gamma^{(L-1)}, \alpha^{(L-1)}, W_L\). Then, independent of the value \(t\), \(h(\theta')\) is always a unit norm vector. Therefore, the maximization constraint in (24) is independent of the norms of the parameters in \(\theta'\), which also proves that regularizing the weights in \(\theta'\) does not affect the dual characterization in (24).
A.5. Additional numerical results

Here, we present additional numerical results that are not included in the main paper. 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 2.4. 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.

![Graph 5a](image1.png) ![Graph 5b](image2.png)

Figure 5: (a) Projection of the hidden neurons to the right singular vectors claimed in Remark 2.4 and (b) singular values of $W_1$ with respect to $\beta$.

![Graph 6a](image1.png) ![Graph 6b](image2.png)

Figure 6: Training and test performance of full batch SGD (4 initializations) on the CIFAR-100 datasets for a four class classification tasks, where $(n,d) = (2000,3072)$, $K = 4$, $L = 2$ with 100 neurons and we use squared loss with one hot encoding. For Theory, we use the layer weights in Theorem 4.4, which achieves the optimal performance as guaranteed by Theorem 4.4. We also use a marker to denote the time required to compute the closed-form solution.

We also conduct an experiment on CIFAR-100 (Krizhevsky et al., 2014) datasets, for which we consider a four class classification task. In order to verify our results in Theorem 4.4, we train a two-layer regularized ReLU networks with batch normalization using four different initializations and then plot the results with respect to wall-clock time. As demonstrated in Figure 6, our closed form solution, i.e., denoted as Theory, achieves lower objective value as proven in Theorem 4.4 and higher test accuracy.
A.6. Proofs for two-layer networks

**Theorem 2.1.** The dual of the problem in (5) is given by

$$P^* \geq D^* = \max_{\lambda \in \mathbb{R}^n} \lambda^T y \quad \text{s.t.} \quad \max_{w_i \in B_2} |\lambda^T X w_i| \leq 1. \quad (6)$$

For (6), \(\exists m^* \leq n + 1\) such that strong duality holds, i.e., \(P^* = D^*, \forall m \geq m^*\) and \(W_1^*\) satisfies \(\|(XW_1^*)^T \lambda^*\|_\infty = 1\), where \(\lambda^*\) is the dual optimal parameter.

**Corollary 2.1.** By Theorem 2.1, the optimal neurons are extreme points which solve argmax\(_{w_i \in B_2}\) \(|\lambda^*^T X w_i|\).

**Proof of Theorem 2.1 and Corollary 2.1** We first note that the dual of [5] with respect to \(w_i\) is

$$\min_{\theta \in \Theta \setminus \{w_i\}} \max_{\lambda} \lambda^T y \quad \text{s.t.} \quad \|(XW_1)^T \lambda\|_\infty \leq 1, \|w_{1,j}\|_2 \leq 1, \forall j.$$ 

Then, we can reformulate the problem as follows

$$P^* = \min_{\theta \in \Theta \setminus \{w_i\}} \max_{\lambda} \lambda^T y + I(\|(XW_1)^T \lambda\|_\infty \leq 1), \text{s.t.} \|w_{1,j}\|_2 \leq 1, \forall j,$$

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

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

Since the set \(\|(XW_1)^T \lambda\|_\infty \leq 1\) is closed, the function \(\Phi(\lambda, W_1) = \lambda^T y + I(\|(XW_1)^T \lambda\|_\infty \leq 1)\) 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 (6), which establishes a lower bound \(D^*\) for the above problem:

$$P^* \geq D^* = \max_{\lambda} \min_{\theta \in \Theta \setminus \{w_i\}} \lambda^T y + I(\|(XW_1)^T \lambda\|_\infty \leq 1), \text{s.t.} \|w_{1,j}\|_2 \leq 1, \forall j,$$

where

$$= \max_{\lambda} \lambda^T y, \quad \text{s.t.} \quad \|(XW_1)^T \lambda\|_\infty \leq 1 \forall w_{1,j}, \quad \|w_{1,j}\|_2 \leq 1, \forall j,$$

$$= \max_{\lambda} \lambda^T y, \quad \text{s.t.} \quad \|(XW_1)^T \lambda\|_\infty \leq 1 \forall w_1 : \|w_1\|_2 \leq 1.$$ 

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

$$\min_{\mu} \|\mu\|_{TV} \quad \text{s.t.} \quad \int_{w_i \in B_2} X w_i d\mu(w_i) = y,$$

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. We also note that although the above formulation involves an infinite dimensional integral form, by Caratheodory’s theorem, the integral can be represented as a finite summation of at most \(n + 1\) Dirac delta functions ([Rosset et al., 2007]). Next we invoke the semi-infinite optimality conditions for the dual problem in (6), in particular we apply Theorem 7.2 of [Goberna & López-Cerdá, 1998]. We first define the set

$$K = \text{cone} \left\{ \left( sXw_1 \right)_1, w_1 \in B_2, s \in \{-1, +1\}; \left( 0_n, -1 \right) \right\}.$$ 

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 (6) forms a Farkas-Minkowski system. By Theorem 8.4 of (Goberna & López-Cerdá, 1998), 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 the optimal value of (6). The optimality conditions in Theorem 7.2 (Goberna & López-Cerdá, 1998) 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. ([Du & Hu 2019]) Given $w^* = \arg\min_w \|Xw - y\|_2$, we have
\[
\arg\min_{W_1, w_2} \|X W_1 w_2 - X w^*\|_2^2 = \arg\min_{W_1, w_2} \|X W_1 w_2 - y\|_2^2.
\]

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
\[
f(w) = \|Xw - Xw^* + Xw^* - y\|_2^2
\]
\[
= \|Xw - Xw^*\|_2^2 + 2(w - w^*)^T X^T(Xw^* - y) + \|Xw^* - y\|_2^2
\]
\[
= \|Xw - Xw^*\|_2^2 + \|Xw^* - y\|_2^2.
\]
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 [5].

Theorem 2.2. Let $\{X, y\}$ be feasible for (5), then strong duality holds for finite width networks.

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 [5] with $W_1 = w_e$ is
\[
D_e^* = \max_{\lambda} \lambda^T y \text{ s.t. } ||(Xw_e)^T\lambda||_\infty \leq 1.
\] (25)

Then, we have
\[
P^* = \min_{\theta \in \Theta \setminus \{w_e\}} \max_{\lambda} \lambda^T y \geq \max_{\lambda} \min_{\theta \in \Theta \setminus \{W_2\}} \lambda^T y
\]
\[
s.t. \|(XW_1)^T\lambda\|_\infty \leq 1, \|w_{1,j}\|_2 \leq 1, \forall j \quad \text{s.t. } \|(XW_1)^T\lambda\|_\infty \leq 1, \|w_{1,j}\|_2 \leq 1, \forall j
\]
\[
= \max_{\lambda} \lambda^T y
\]
\[
s.t. \|(Xw_e)^T\lambda\|_\infty \leq 1
\]
\[
= D_e^* = D^*
\] (26)

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
\[
P_e^* = \min_{\theta \in \Theta \setminus \{W_{1,m}\}} |w_2| \geq P^* = \min_{\theta \in \Theta} \|w_2\|_1
\] (27)
\[
s.t. \ Xw_e w_2 = y \quad \text{s.t. } XW_1 w_2 = y, \|w_{1,j}\|_2 \leq 1, \forall j.
\]
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 (27) 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 (26), we prove that strong duality holds for a finite width NN, i.e., $P_e^* = P^* = D^* = D_e^*$.
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 (10) with \( W_1 = w_e \)

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

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

Theorem 2.4. Let \( \{X, Y\} \) be feasible for (12), then strong duality holds for finite width networks.

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 (12) with \( W_1 = W_e \)

\[
D_* = \max_{\lambda} \text{tr}(\Lambda^T Y) \text { s.t. } \|\Lambda^T X w_{e,j}\|_2 \leq 1, \forall j \in [r_w].
\]

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

A.7. Proofs for deep linear networks

Proposition 3.1. First \( L - 2 \) layer weight matrices in (15) have the same operator and Frobenius norms, i.e., \( t_j = \|W_{l,j}\|_F = \|W_{l,j}\|_2, \forall l \in [L - 2], \forall j \in [m] \).

Proof of Proposition 3.1 Let us first rescale the first \( L - 2 \) layer weights as \( W_{l,j} = \frac{t_{l,j}}{\|W_{l,j}\|_F} W_{l,j} \), where \( t_{l,j} > 0 \). Defining \( t_{l-2}^L = \prod_{l=1}^{L-2} \|W_{l,j}\|_F \), if \( t_{l,j}'s \) are chosen such that \( \prod_{l=1}^{L-2} t_{l,j} = t_{L-2}^L \), then the rescaling does not alter the output of the network, i.e., \( f_{\theta,L}(X) = f_{\theta,L}(X) \). Therefore, we can optimize \( \{t_{l,j}\}_{l=1}^{L-2} \) as follows

\[
\min_{\{t_{l,j}\}_{l=1}^{L-2}} \frac{1}{2} \sum_{l=1}^{L-2} t_{l,j}^2 \text { s.t. } \prod_{l=1}^{L-2} t_{l,j} = t_{L-2}^L,
\]

for each \( j \in [m] \). Apparently, the optimal scaling parameters obey \( t_{1,j} = t_{2,j} = \ldots = t_{L-2,j} = t_j \). We also note that the optimal layer weights satisfy \( t_j = \|W_{l,j}\|_2 = \|W_{l,j}\|_F, \forall l \in [L - 2], \forall j \in [m] \), since the upper-bound is achieved when the matrices are rank-one (see (34)).

Theorem 3.1. Optimal layer weights for (15) are

\[
W_{l,j}^* = \begin{cases} 
\frac{t_j}{\|w_{l,j}\|_2} \rho_{l,j}^T & \text{if } l = 1 \\
\frac{t_j}{\|w_{l,j}\|_2} \rho_{l-1,j}^T & \text{if } 1 < l \leq L - 2 \\
\rho_{L-2,j} & \text{if } l = L - 1
\end{cases}
\]

where \( \rho_{l,j} \in \mathbb{R}^{m_j} \) such that \( \|\rho_{l,j}\|_2 = 1, \forall l \in [L - 2], \forall j \in [m] \) and \( w_{l,j}^* \) is defined in (9).

Proof of Theorem 3.1 Using Lemma A.3 and Proposition 3.1 we have the following dual problem for (15)

\[
P^* = \min_{\{\theta_l\}_{l=1}^{L-1}, \{t_j\}_{j=1}^m} \max_{\lambda} \lambda^T y + \frac{1}{2} (L - 2) \sum_{j=1}^m t_j^2 \text { s.t. } |(X W_{1,j} \ldots w_{L-1,j})^T \lambda| \leq 1, \|W_{l,j}\|_F \leq t_j, \forall l \in [L - 2], \forall j \in [m].
\]

Now, let us assume that the optimal Frobenius norm for each layer \( l \) is \( t_j^* \).9 Then, if we define \( \Theta_{L-1} = \{\theta_1, \ldots, \theta_{L-1} | \|W_{L-1,j}\|_2 \leq 1, \|W_{l,j}\|_F \leq t_j, \forall l \in [L - 2], \forall j \in [m]\} \), (28) reduces to the following problem

\[
P^* \geq D^* = \max_{\lambda} \lambda^T y \text { s.t. } |(X W_{1,j} \ldots w_{L-1,j})^T \lambda| \leq 1, \forall \theta_l \in \Theta_{L-1}, \forall l,
\]

9With this assumption, \( (L - 2) \sum_{j=1}^m t_j^2 \) becomes constant so we ignore this term for the rest of our derivations.
We now apply the variable change in (8) to (29) as follows for (31).

We note that an upper-bound for the constraint in (32) can be achieved as follows have

\[ P^* = \min_{\{\theta_l\}_{l=1}^n} \|W_l\|_1 \text{ s.t. } \sum_{j=1}^{m^*} XW_{1,j} \ldots w_{L-1,j} w_{L,j} = y, \ \theta_l \in \Theta_{L-1}, \ \forall l \]

(31)

We first note that since the model in (31) has the same expressive power with the network in (15) as long as \( m \geq m^* \), we have \( P^* = P^*_m \). Since the dual of (15) and (31) are the same, we also have \( D^*_m = D^* \), where \( D^*_m \) is the optimal dual value for (31).

We now apply the variable change in (8) to (29) as follows

\[ \max_{\lambda} \lambda^T \Sigma_x \tilde{w}^*_x \text{ s.t. } \|W_{L-2,j}^T \ldots W_{1,j}^T V_x \Sigma_x^T \tilde{\lambda} \|_2 \leq 1, \ \forall \theta_l \in \Theta_{L-1}, \ \forall l. \]  

(32)

We note that an upper-bound for the constraint in (32) can be achieved as follows

\[ \|W_{L-2,j}^T \ldots W_{1,j}^T V_x \Sigma_x^T \tilde{\lambda} \|_2 \leq \|W_{L-2,j}^T \|_2 \ldots \|W_{1,j}^T \|_2 \|V_x \Sigma_x^T \tilde{\lambda} \|_2 \leq t_j^{L-2} \| \Sigma_x^T \tilde{\lambda} \|_2, \]

where the last inequality follows from the constraint on each layer weight’s norm, i.e., \( \|W_{l,j}\|_F \leq t_j^* \). The equality can be reached when the layer weights are

\[ W_l = t_j^* \rho_{l-1,j} \rho_{l,j}^T \in [L-2], \]

where \( \{\rho_{l,j}\}_{l=1}^{L-2} \) is a set of arbitrary unit norm vectors and \( \rho_0 = V_x \Sigma_x^T \tilde{\lambda} / \|V_x \Sigma_x^T \tilde{\lambda} \|_2 \). Hence, we can rewrite (32) as

\[ \max_{\lambda} \lambda^T \Sigma_x \tilde{w}^*_x \text{ s.t. } t_j^{L-2} \| \Sigma_x^T \tilde{\lambda} \|_2 \leq 1, \ \forall j \in [m]. \]  

(33)

Therefore, the maximum objective value is achieved when \( \Sigma_x^T \tilde{\lambda} = c_1 \tilde{w}^*_x \) for some \( c_1 > 0 \), which yields the following set of optimal layer weight matrices

\[ W_{l,j}^* = \begin{cases} 
  t_j^* V_x \tilde{w}^*_x / \| V_x \tilde{w}^*_x \|_2 \rho_{l,j}^T & \text{if } l = 1 \\
  t_j^* \rho_{l-1,j} \rho_{l,j}^T & \text{if } 1 < l \leq L - 2 \\
  \rho_{L-2,j} & \text{if } l = L - 1
\end{cases}, \]

(34)

where \( \rho_{l,j} \in \mathbb{R}^{m_l} \) such that \( \| \rho_{l,j} \|_2 = 1, \ \forall l \in [L-2], \forall j \in [m] \). This shows that the weight matrices are rank-one and align with each other. Therefore, an arbitrary set of unit norm vectors, i.e., \( \{\rho_{l,j}\}_{l=1}^{L-2} \) can be chosen to achieve the maximum dual objective.

**Theorem 3.2.** Let \( \{X, y\} \) be feasible for (15), then strong duality holds for finite width networks.

**Proof of Theorem 3.2.** We first select a set of unit norm vectors, i.e., \( \{\rho_{l,j}\}_{l=1}^{L-2} \), to construct weight matrices \( \{W_{l,j}^*\}_{l=1}^{L-1} \) that satisfies (34). Then, the dual of (15) can be written as

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

s.t. \( |(XW_{1,j}^T \ldots w_{L-1,j}^T) \lambda| \leq 1, \ \forall j \in [m]. \)
Then, we have
\[
P^* = \min_{\{\theta_l\}_{l=1}^L} \max_{\lambda} \lambda^T y \quad \geq \quad \max_{\lambda} \lambda^T y \quad (35)
\]
s.t. \( |(XW_1 \ldots w_{L-1})^T \lambda| \leq 1 \)
\[
P^* = \min_{\{\theta_l\}_{l=1}^L} \|w_L\|_1 \quad \geq \quad P^* = \min_{\{\theta_l\}_{l=1}^L} \|w_L\|_1 \quad (36)
\]
s.t. \( \sum_{j=1}^m Xw^{i,j} \ldots w^L_{L-1}w_{L,j} = y \)
\[
\text{s.t. } \sum_{j=1}^m Xw^{i,j} \ldots w^L_{L-1}w_{L,j} = y,
\]
where the inequality follows from changing the order of min-max to obtain a lower bound and the first equality follows from the fact that \( \{W^c_i\}_{l=1}^{L-1} \) maximizes the dual problem. Furthermore, we have the following relation between the primal problems
\[
P^*_c = \min_{w_L} \|w_L\|_1 \quad \geq \quad P^* = \min_{\{\theta_l\}_{l=1}^L} \|w_L\|_1
\]
s.t. \( \sum_{j=1}^m Xw^{i,j} \ldots w^L_{L-1}w_{L,j} = y \)
\[
\text{s.t. } \sum_{j=1}^m Xw^{i,j} \ldots w^L_{L-1}w_{L,j} = y,
\]
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 \( \ell_1 \)-norm minimization problem with linear equality constraints. Therefore, strong duality holds for this problem, i.e., \( P^*_c \geq P^* \geq P^*_m \geq D^* = D^* = D^*_m \). Using this result along with (35), we prove that strong duality holds, i.e., \( P^*_c = P^* = P^*_m = D^* = D^*_m \).

**Corollary 3.1.** Theorem 3.1 implies that deep linear networks can obtain a scaled version of \( y \) using only the first layer, i.e., \( XW_1 \rho_1 = cy \), where \( c > 0 \). Therefore, the remaining layers do not contribute to the expressive power of the network.

**Proof of Corollary 3.1.** The proof directly follows from (34). \( \square \)

**Theorem 3.3.** Optimal layer weights for (16) are
\[
W^*_{i,j} = \begin{cases} 
\sum_{j | X^T P_{X,\beta}(y)} \rho^T_{i,j} & \text{if } l = 1 \\
\sum_{j \rho_{i-1,j}} \rho^T_{i,j} & \text{if } 1 < l \leq L - 2 \\
\rho_{L-2,j} & \text{if } l = L - 1 
\end{cases}
\]
where \( P_{X,\beta}(\cdot) \) projects to \( \{ u \in \mathbb{R}^n | \|X^T u\|_2 \leq \beta t^{2-L}_j \} \).

**Proof of Theorem 3.3.** Using Lemma A.3 and Proposition 3.1 we have the following dual for (16)
\[
\max_{\lambda} -\frac{1}{2} \|\lambda - y\|_2^2 + \frac{1}{2} \|y\|_2 \text{ s.t. } \|XW_{1,j} \ldots W_{L-2,j}\|_2 \leq \beta, \forall \theta_l \in \Theta_{L-1}, \forall l, j
\]
where \( \Theta_{L-1} = \{ \theta_1, \ldots, \theta_{L-1} | \|w_{L-1,j}\|_2 \leq 1, \|w_{i,j}\|_F \leq t^*_j, \forall l \in [L-2], \forall j \in [m] \} \). Then, the weight matrices that maximize the value of the constraint can be described as
\[
W^*_{i,j} = \begin{cases} 
\sum_{j | X^T P_{X,\beta}(y)} \rho^T_{i,j} & \text{if } l = 1 \\
\sum_{j \rho_{i-1,j}} \rho^T_{i,j} & \text{if } 1 < l \leq L - 2 \\
\rho_{L-2,j} & \text{if } l = L - 1 
\end{cases}
\]
where \( P_{X,\beta}(\cdot) \) projects its input to \( \{ u \in \mathbb{R}^n | \|X^T u\|_2 \leq \beta t^{2-L}_j \} \). \( \square \)

**Corollary 3.2.** Theorem 3.2 also shows that strong duality holds for the training problem in (16).
Proof of Corollary 3.2  The proof directly follows from the analysis in this section and Theorem 3.2.

Theorem 3.4. Optimal layer weight for (17) are

$$W^*_l,j = \begin{cases} t_j^r \nu_{w,j} \rho_{l,j}^T & \text{if } l = 1 \\ t_j^r \rho_{l-1,j} \rho_{l,j}^T & \text{if } 1 < l \leq L - 2 \\ \rho_{L-2,j} & \text{if } l = L - 1 \end{cases},$$

where $j \in [K]$, $\nu_{w,j}$ is the $j$th maximal right singular vector of $A^T X$ and $\{\rho_{l,j}\}_{l=1}^{L-2}$ are arbitrary unit norm vectors such that $\rho_{l,j} \rho_{l,k} = 0$, $\forall j \neq k$.

Proof of Theorem 3.4 Using Proposition 3.1 and Lemma 3.4, we obtain the following dual problem

$$D = \max_{\Lambda} \text{tr}(A^T Y) \text{ s.t. } \|A^T X W_{1,j} \ldots W_{L-2,j} W_{L-1,j}\|_2 \leq 1, \forall \theta_l \in \Theta_L, \forall j \in [m]$$

$$= \max_{\Lambda} \text{tr}(A^T Y) \text{ s.t. } \sigma_{\max}(A^T X W_{1,j} \ldots W_{L-2,j}) \leq 1, \forall \theta_l \in \Theta_L, \forall j \in [m],$$

(37)

where $\Theta_L = \{\theta_1, \ldots, \theta_L \mid \|W_{L-1,j}\|_2 \leq 1, \|W_{l,j}\|_F \leq t_j^r, \forall l \in [L-2], \forall j \in [m]\}$.

It is straightforward to show that the optimal layer weights are the extreme points of the constraint in (37), which achieves the following upper-bound

$$\max_{\{\theta_l\}_{l=1}^{L-2} \in \Theta_L} \sigma_{\max}(A^T X W_{1,j} \ldots W_{L-2,j}) \leq \sigma_{\max}(A^T X t_j^{L-2}.$$  

This upper-bound is achieved when the first $L-2$ layer weights are rank-one with the singular value $t_j^r$ by Proposition 3.1. Additionally, the left singular vector of $W_{1,j}$ needs to align with one of the maximum right singular vectors of $A^T X$. Since the upper-bound for the objective is achievable for any $\Lambda$, we can maximize the objective value, as in (14), by choosing a matrix $\Lambda$ such that

$$\Lambda^T U_x \Sigma_x = V_w \begin{bmatrix} t_j^{2-L} I_{r_w} & 0_{r_x \times d-r_w} \\ 0_{d-r_w \times r_x} & 0_{k-r_w \times d-r_w} \end{bmatrix} U_w \Lambda^T,$$

where $W^*_r = V^T w W^*_r = U_w \Sigma_w V^T w$. Thus, a set of optimal layer weights can be formulated as follows

$$W^*_l,j = \begin{cases} t_j^r \nu_{w,j} \rho_{l,j}^T & \text{if } l = 1 \\ t_j^r \rho_{l-1,j} \rho_{l,j}^T & \text{if } 1 < l \leq L - 2 \\ \rho_{L-2,j} & \text{if } l = L - 1 \end{cases},$$

(38)

where $\nu_{w,j}$ is the $j$th maximal right singular vector of $A^T X$ and we select a set of unit norm vectors $\{\rho_{l,j}\}_{l=1}^{L-2}$ such that $\rho_{l,j} \rho_{l,k} = 0$, $\forall j \neq k$.

Theorem 3.5. Let $\{X, Y\}$ be feasible for (17), then strong duality holds for finite width networks.

Proof of Theorem 3.5 We first select a set of unit norm vectors, i.e., $\{\rho_{l,j}\}_{l=1}^{L-2}$, to construct weight matrices $\{W^*_l,j\}_{l=1}^{L-1}$ that satisfies (38). Then, we have

$$P^* = \min_{\{\theta_l\}_{l=1}^{L-1} \in \Theta_L} \max_{\Lambda} \text{tr}(A^T Y) \geq \max_{\Lambda} \text{tr}(A^T Y)$$

s.t. $\sigma_{\max}(A^T X W_{1,j} \ldots W_{L-2,j}) \leq 1, \forall j$  

s.t. $\sigma_{\max}(A^T X W_{1,j} \ldots W_{L-2,j}) \leq 1, \forall j, \forall \theta_l \in \Theta_L$  

s.t. $\sigma_{\max}(A^T X W^*_1 \ldots W^*_{L-2,j}) \leq 1, \forall j$  

$$D^*_e = D^* = D^*_m,$$
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 \( \{W_{i,j}^e\}_{i=1}^{L-1} \) maximizes the dual problem. Furthermore, we have the following relation between the primal problems

\[
P_e^* = \min_{W_l} \sum_{j=1}^{m} \|W_{L,j}\|_2 \quad \geq \quad P^* = \min_{\{\theta_l\}_{l=1}^{L-1}} \sum_{j=1}^{m} \|W_{L,j}\|_2
\]

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 (40) is convex since it is an \( \ell_2 \)-norm minimization problem with linear equality constraints. Therefore, strong duality holds for this problem, i.e., \( P_e^* \geq P^* = P_m^* = D_e^* = D^* = D_m^* \). Using this result along with (39), we prove that strong duality holds, i.e., \( P_e^* = P^* = P_m^* = D_e^* = D^* = D_m^* \).

**Theorem 3.6.** Optimal layer weights for (18) are

\[W_{l,j}^* = \begin{cases} t_j^* \tilde{v}_{x,j} \rho_{1,j}^T & \text{if } l = 1 \\ t_j^* \theta_{l-1,j} \rho_{l,j}^T & \text{if } 1 < l \leq L - 2 \\ \rho_{L-2,j} & \text{if } l = L - 1 \end{cases} \]

where \( j \in [K] \), \( \tilde{v}_{x,j} \) is a maximal right singular vector of \( P_{X,\beta}(Y)^T X \) and \( P_{X,\beta}(\cdot) \) projects to \( \{U \in \mathbb{R}^{n \times k} | \sigma_{max}(U^T X) \leq \beta t_j^{2^l-1}\} \). Additionally, \( \theta_{l,j} \)'s is an orthonormal set. Therefore, the rank of each hidden layer is determined by \( \beta \) as in Remark 2.7.

**Proof of Theorem 3.6** Using Lemma A.4 and Proposition 3.1, we have the following dual for (18)

\[
\max_{\Lambda} \left(-\frac{1}{2} \|\Lambda - Y\|_F^2 + \frac{1}{2} \|Y\|_F^2\right) \text{ s.t. } \sigma_{max}(\Lambda^T XW_{1,j} \cdots W_{L-2,j}) \leq \beta, \forall \theta_l \in \Theta_{L-1}, \forall j \in [m],
\]

where we define \( \Theta_{L-1} = \{\theta_1, \ldots, \theta_{L-1} | \|W_{L-1,j}\|_2 \leq 1, \|W_{l,j}\|_F \leq t_j^*, \forall l \in [L-2], \forall j \in [m]\} \). Then, as in (38), a set of optimal layer weights is

\[W_{l,j}^* = \begin{cases} t_j^* \tilde{v}_{x,j} \rho_{1,j}^T & \text{if } l = 1 \\ t_j^* \theta_{l-1,j} \rho_{l,j}^T & \text{if } 1 < l \leq L - 2 \\ \rho_{L-2,j} & \text{if } l = L - 1 \end{cases} \]

where \( \tilde{v}_{x,j} \) is a maximal right singular vector of \( P_{X,\beta}(Y)^T X \) and \( P_{X,\beta}(\cdot) \) projects its input to the set \( \{U \in \mathbb{R}^{n \times k} | \sigma_{max}(U^T X) \leq \beta t_j^{2^l-1}\} \). Additionally, \( \theta_{l,j} \)'s is an orthonormal set.

**A.8. Proofs for deep ReLU networks**

**Theorem 4.1.** Let \( X \) be a rank-one matrix such that \( X = c a_0^T \), where \( c \in \mathbb{R}^n_+ \) and \( a_0 \in \mathbb{R}^d \), then strong duality holds and the optimal weights are

\[W_{l,j} = \frac{\phi_{l-1,j}}{\|\phi_{l-1,j}\|_2} \phi_{l,j}^T, \forall l \in [L-2], W_{L-1,j} = \frac{\phi_{L-2,j}}{\|\phi_{L-2,j}\|_2},\]

where \( \phi_{0,j} = a_0 \) and \( \{\phi_{l,j}\}_{l=1}^{L-2} \) is a set of vectors such that \( \phi_{l,j} \in \mathbb{R}^{m_l} \) and \( \|\phi_{l,j}\|_2 = t_j^*, \forall l \in [L-2], \forall j \in [m] \).

**Proposition 1.** First \( L - 2 \) hidden layer weight matrices in (19) 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 \( t_j \), i.e., \( t_j = \sum_{l=1}^{L-2} t_{l,j} \), where \( t_{l,j} = \|W_{l,j}\|_F \) 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

$$\arg\max_{\{a_t\}_{t=1}^L} |\lambda^T c| \|a_{L-2}\|_2 = \arg\max_{\{a_t\}_{t=1}^L \in \Theta_{L-1}} |\lambda^T c| \|(a_{L-3,j}^T W_{L-2,j})_+\|_2$$

where we use $a_{L-2,j}^T = (a_{L-3,j}^T W_{L-2,j})_+$. Since $\|W_{L-2,j}\|_F = t_{L-2,j} = t_j - \sum_{l=1}^{L-3} t_{l,j}$, the objective value above becomes $|\lambda^T c| \|(a_{L-3,j}^T)_+ \left( t_j - \sum_{l=1}^{L-3} t_{l,j} \right)$. Applying this step to all the remaining layer weights gives the following problem

$$\arg\max_{\{a_t\}_{t=1}^L} |\lambda^T c| \|a_0\|_2 \left( t_j - \sum_{l=1}^{L-3} t_{l,j} \right) \prod_{j=1}^{L-3} t_{l,j} \text{ s.t. } \sum_{l=1}^{L-3} t_{l,j} \leq t_j, \ t_{l,j} \geq 0.$$  

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

**Proof of Theorem 4.1** Using Lemma A.3 and Proposition 1, this problem can be equivalently stated as

$$\min_{\{A_l\}_{l=1}^L} \|w_L\|_1 \text{ s.t. } A_{l,j} = (A_{l-1,j} W_{l,j})_+, \ \forall l \in [L-1], \forall j \in [m],$$

$$A_{L-1} w_L = y$$

which also has the following dual form

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

(42)

Notice that we remove the recursive constraint in (42) 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 (42) gives

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

(43)

The dual of the semi-infinite problem in (43) is given by

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

(44)

where $\mu$ is a signed Radon measure and $\|\cdot\|_{TV}$ is the total variation norm. We emphasize that (44) has infinite width in each layer, however, an application of Caratheodory’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

$$\mu = \sum_{j=1}^m \delta(W_{1,j}, \ldots, w_{L-1,j} - w_{L-1,j}) w_{L,j},$$

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

$$P_m^* = \min_{\{\theta_l\}_{l=1}^L} \|w_L\|_1 \text{ s.t. } \sum_{j=1}^m (A_{L-2,j} w_{L-1,j})_+ w_{L,j} = y, \ \theta_l \in \Theta_{L-1}, \ \forall l \in [L-1].$$

(45)

Here, we note that the model in (45) has the same expressive power with ReLU networks, thus, we have $P^* = P_m^*$.  

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Revealing the Structure of Deep Neural Networks via Convex Duality
As a consequence of (43), we can characterize the optimal layer weights for (45) as the extreme points that solve
\[
\arg\max_{\{\theta_i\}_{l=1}^{L-2} \in \Theta_{L-1}} |\lambda^T (A_{L-2,j} w_{L-1,j})_+|
\] (46)
where \( \lambda^* \) is the optimal dual parameter. Since we assume that \( X = ca_0^T \) with \( c \in \mathbb{R}_+^n \), we have \( A_{L-2,j} = ca_{L-2,j}^T \), where \( a_{L-1,j}^T = (a_{L-1,j}^T, w_{L-1,j})_+ \), \( a_{L-2,j} \in \mathbb{R}_{+}^{m_l} \), and \( \forall l \in [L-1], \forall j \in [m] \). Based on this observation, we have \( w_{L-1,j} = a_{L-2,j}/\|a_{L-2,j}\|_2 \), which reduces (46) to the following
\[
\arg\max_{\{\theta_i\}_{l=1}^{L-2} \in \Theta_{L-1}} |\lambda^T c \|a_{L-2,j}\|_2
\] (47)
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 \( \phi_{l,j} \in \mathbb{R}_{+}^{m_l} \), then we have the following formulation for the layer weights that solve (46)
\[
W_{l,j} = \frac{\phi_{l-1,j}}{\|\phi_{l-1,j}\|_2} \phi_{l,j}^T, \forall l \in [L-2], w_{L-1,j} = \frac{\phi_{L-2,j}}{\|\phi_{L-2}\|_2},
\] (48)
where \( \phi_{0,j} = a_0, \{\phi_{l,j}\}_{l=1}^{L-2} \) is a set of nonnegative vectors satisfying \( \|\phi_{l,j}\|_2 = t_{l,j}, \forall l \in [L-2] \). Therefore, the set of weights in (48) are optimal for (19). Moreover, as a direct consequence of Theorem [3.3] strong duality holds for this case as well.

**Theorem 4.2.** Let \( X \) be a matrix such that \( X = ca_0^T \), where \( c \in \mathbb{R}_+^n \) and \( a_0 \in \mathbb{R}^d \). Then, when \( L = 2 \), a set of optimal solutions to (19) is \( \{\{w_i, b_i\}\}_{i=1}^{m} \), where \( w_i = s_i \frac{a_0}{\|a_0\|_2}, b_i = -s_i c_i \|a_0\|_2 \) with \( s_i = \pm 1, \forall i \in [m] \).

**Proof of Theorem 4.2** Given \( X = ca_0^T \), all possible extreme points can be characterized as follows
\[
\arg\max_{b, w: \|w\|_2=1} |\lambda^T (Xw + b) \|_+ = \arg\max_{b, w: \|w\|_2=1} |\lambda^T (ca_0^T w + b) \|_+
\]
\[
= \arg\max_{b, w: \|w\|_2=1} \left| \sum_{i=1}^{n} \lambda_i (c_i a_0^T w + b) \right|_+
\]
which can be equivalently stated as
\[
\arg\max_{b, w: \|w\|_2=1} \left| \sum_{i \in S} \lambda_i c_i a_0^T w + \sum_{i \notin S} \lambda_i b \right| \text{ s.t. } \begin{cases} c_i a_0^T w + b \geq 0, \forall i \in S \\ c_j a_0^T w + b \leq 0, \forall j \in S^c \end{cases}
\]
which shows that \( w \) must be either positively or negatively aligned with \( a_0 \), i.e., \( w = s_i \frac{a_0}{\|a_0\|_2} \), where \( s_i = \pm 1 \). Thus, \( b \) must be in the range of \( [\max_{i \in S} (-s_i c_i \|a_0\|_2), \min_{k \in S^c} (-s_k c_k \|a_0\|_2)] \). Using these observations, extreme points can be formulated as follows
\[
w_\lambda = \begin{cases} \frac{a_0}{\|a_0\|_2} & \text{if } \sum_{i \in S} \lambda_i c_i \geq 0 \\ \frac{-a_0}{\|a_0\|_2} & \text{otherwise} \end{cases} \quad \text{and} \quad b_\lambda = \begin{cases} \min_{k \in S^c} (-s_k c_k \|a_0\|_2) & \text{if } \sum_{i \in S} \lambda_i \geq 0 \\ \max_{i \in S} (-s_i c_i \|a_0\|_2) & \text{otherwise} \end{cases}
\]
where \( s_\lambda = \text{sign}(\sum_{i \in S} \lambda_i c_i) \).

**Proposition 4.1.** Theorem 4.1 still holds when we add a bias term to the last hidden layer, i.e., \( \sum_j (A_{L-2,j} w_{L-1,j} + b_j n) \), \( w_{L,j} = y \).

**Proof of Proposition 4.1.** Here, we add biases to the neurons in the last hidden layer of (19). For this case, all the equations in (41)-(43) hold except notational changes due to the bias term. Thus, (46) changes as
\[
\arg\max_{\{\theta_i\}_{l=1}^{L-2} \in \Theta_{L-1}, b} |\lambda^T (A_{L-2,j} w_{L-1,j} + b_j n) \|_+ = \arg\max_{\{\theta_i\}_{l=1}^{L-2} \in \Theta_{L-1}, b} |\lambda^T (ca_{L-2,j}^T w_{L-1,j} + b_j n) \|_+
\]
\[
= \arg\max_{\{\theta_i\}_{l=1}^{L-2} \in \Theta_{L-1}, b} \sum_{i=1}^{n} \lambda_i^* (c_i a_{L-2,j}^T w_{L-1,j} + b_j) \|_+
\] (49)
which can also be written as

$$\arg\max_{\{\theta_i\}_{i=1}^{L-1} \in \Theta_L -1} \sum_{j \in S} \lambda_i^* c_i a_{L-2,j}^T w_{L-1,j} + \sum_{j \in S} \lambda_i^* b_j \text{ s.t. } \begin{cases} c_i a_{L-2,j}^T w_{L-1} + b_j \geq 0, \forall i \in S \\ c_j a_{L-2,j}^T w_{L-1,j} + b_j \leq 0, \forall j \in S^c \end{cases}$$

where $S$ and $S^c$ are the indices for which ReLU is active and inactive, respectively. This shows that $w_{L-1,j}$ must be $w_{L-1,j} = \pm \frac{a_{L-2,j}}{\|a_{L-2,j}\|_2}$ and $b_j \in [\max_{i \in S}(-c_i\|a_{L-2,j}\|_2), \min_{k \in S^c}(-c_k\|a_{L-2,j}\|_2)]$. Then, we obtain the following

$$w^*_{L-1,j} = \begin{cases} \frac{a_{L-2,j}}{\|a_{L-2,j}\|_2} & \text{if } \sum_{i \in S} \lambda_i^* c_i \geq 0 \\ \frac{-a_{L-2,j}}{\|a_{L-2,j}\|_2} & \text{otherwise} \end{cases} \quad \text{and } b^* = \begin{cases} \min_{k \in S^c}(-s_{\lambda^*} c_k\|a_{L-2,j}\|_2) & \text{if } \sum_{i \in S} \lambda_i^* \geq 0 \\ \max_{i \in S}(-s_{\lambda^*} c_i\|a_{L-2,j}\|_2) & \text{otherwise} \end{cases}$$

(50)

where $s_{\lambda^*} = \text{sign}\left(\sum_{i \in S} \lambda_i^* c_i\right)$. This result reduces (49) to the following problem

$$\arg\max_{\{\theta_i\}_{i=1}^{L-2} \in \Theta_L -1} \|C(\lambda^*, c)\|_2$$

where $C(\lambda^*, c)$ is constant scalar independent of $\{W_{l,j}\}_{l=1}^{L-2}$. Hence, this problem and its solutions are the same with (47) and (48), respectively.

\[\square\]

**Corollary 4.1.** As a result of Theorem 4.2 when we have one dimensional data, i.e., $x \in \mathbb{R}^n$, an optimal solution to (19) can be formulated as $\{(w_i, b_i)\}_{i=1}^m$, where $w_i = s_i, b_i = -s_i x_i$ with $s_i = \pm 1, \forall i \in [m]$. Therefore, the optimal network output has kinks only at the input data points, i.e., the output function is in the following form: $f_{\theta,1}(x) = \sum_i (\hat{x} - x_i)_+$. Hence, the network output becomes a linear spline interpolation.

**Corollary 4.2.** As a result of Theorem 4.2 and Proposition 4.1, for one dimensional data, i.e., $x \in \mathbb{R}^n$, the optimal network output has kinks only at the input data points, i.e., the output function is in the following form: $f_{\theta,L}(x) = \sum_i (\hat{x} - x_i)_+$. Therefore, the optimal network output is a linear spline interpolation.

**Proof of Corollary 4.1 and 4.2** Let us particularly consider the input sample $a_0$. Then, the activations of the network defined by (48) and (50) are

$$a_{1,j}^T = \left(a_0^T W_1\right)_+ = \left(a_0^T \frac{a_0}{\|a_0\|_2} \phi_1^T\right)_+ = \|a_0\|_2 \phi_{1,j}^T$$

$$a_{2,j}^T = \left(a_{1,j}^T W_2\right)_+ = \left(a_{1,j}^T \frac{a_{1,j}}{\|a_{1,j}\|_2} \phi_{2,j}^T\right)_+ = \|a_0\|_2 \|a_{1,j}\|_2 \phi_{2,j}^T$$

$$\vdots$$

$$a_{L-2,j}^T = \left(a_{L-3,j}^T W_{L-2,j}\right)_+ = \left(a_{L-3,j}^T \frac{a_{L-3,j}}{\|a_{L-3,j}\|_2} \phi_{L-2,j}^T\right)_+ = \|a_0\|_2 \|a_{L-3,j}\|_2 \phi_{L-2,j}^T$$

Thus, if we feed $c_i a_0$ to the network, we get $a_{L-1,j} = (c_i a_{L-2,j} - c_i b_{L-2,j})_+ = (c_i a_{L-2,j} - b_{L-2,j})_+ = 0$, where we use the fact that optimal biases are in the form of $b_j = -c_i a_{L-2,j}$ as proved in (50). This analysis proves that the kink of each ReLU activation occurs exactly at one of the data points.

\[\square\]

**Proposition 4.2.** Theorem 4.7 extends to deep ReLU networks with vector outputs, therefore, the optimal layer weights can be formulated as in Theorem 4.7

**Proof of Proposition 4.2** For vector outputs, we have the following training problem

$$\min_{\{\theta_i\}_{i=1}^{L}} \frac{1}{2} \left\|f_{\theta,L}(X) - Y\right\|_F^2 + \frac{\beta}{2} \sum_{j=1}^{m} \sum_{l=1}^{L} \|W_{l,j}\|_F^2.$$
After a suitable rescaling as in the previous case, the above problem has the following dual

\[
P^* \geq D^* = \max_{\lambda} -\frac{1}{2} \left\langle \lambda, A - Y \right\rangle_F + \frac{1}{2} \left\| Y \right\|_F^2 \ \text{s.t.} \ \left\langle A^T (A_{L-2,j} w_{L-1,j})_+ \right\|_2 \leq \beta, \ \forall \theta_l \in \Theta_{L-1}, \ \forall l \in [L-1], \ \forall j \in [m].
\]

Using (51), we can characterize the optimal layer weights as the extreme points that solve

\[
\arg\max_{\{\theta_l\}_{l=1}^{L-1} \in \Theta_{L-1}} \left\| \Lambda^* \right\|_2, \ (A_{L-2,j} w_{L-1,j})_+, \ (L-1)
\]

where \( \Lambda^* \) is the optimal dual parameter. Since we assume that \( X = ca_i^T \) with \( c \in \mathbb{R}_+^n \), we have \( A_{L-2,j} = ca_i^T \), where \( a_i^T = (a_{L-1,j}^T W_{l,j})_+ \), \( a_{l,j} \in \mathbb{R}_+^m \) and \( \forall l \in [L-1] \). Based on this observation, we have \( w_{L-1,j} = a_{L-2,j}/a_{L-2,j} \), which reduces (52) to the following

\[
\arg\max_{\{\theta_l\}_{l=1}^{L-1} \in \Theta_{L-1}} \left\| \Lambda^* \right\|_2, \ (a_{L-2,j})_+.
\]

Then, the rest of steps directly follow Theorem 4.1 yielding the following weight matrices

\[
W_{l,j} = \frac{\phi_{l-1,j}}{\left\| \phi_{l-1,j} \right\|_2} \phi_{l,j}, \ \forall l \in [L-2], \ w_{L-1,j} = \frac{\phi_{L-2,j}}{\left\| \phi_{L-2,j} \right\|_2},
\]

where \( \phi_{0,j} = a_0, \ (\phi_{l,j})_{l=1}^{L-2} \) is a set of nonnegative vectors satisfying \( \left\| \phi_{l,j} \right\|_2 = t_j^*, \ \forall l \in [L-2], \ \forall j \in [m] \).

**Theorem 4.3.** Let \( \{X, Y\} \) be a dataset such that \( XX^T = I_n \) and \( Y \) is one-hot encoded, then a set of optimal solutions for the following regularized training problem

\[
\min_{\theta \in \Theta} \frac{1}{2} f_{\theta,L}(X) - Y^2 + \frac{\beta}{2} \sum_{j=1}^{m} \sum_{l=1}^{L} \|W_{l,j}\|_2^2
\]

(20)
can be formulated as follows

\[
W_{l,j} = \begin{cases} \frac{\phi_{l-1,j}}{\left\| \phi_{l-1,j} \right\|_2} \phi_{l,j}, & \text{if } l \in [L-1] \\ \left(\left\| \phi_{0,j} \right\|_2 - \beta\right)_+ \phi_{l-1,j} e_r^T, & \text{if } l = L \end{cases}
\]

where \( \phi_{0,j} = X^T y_j, \ (\phi_{l,j})_{l=1}^{L-2} \) are vectors such that \( \phi_{l,j} \in \mathbb{R}_+^n, \ \left\| \phi_{l,j} \right\|_2 = t_j^*, \ \text{and} \ \phi_{l,T} \phi_{l,j} = 0, \ \forall i \neq j \). Moreover, \( \phi_{L-1,j} = e_j \) is the \( j \)-th ordinary basis vector.

**Proof of Theorem 4.3.** For vector outputs, we have the following training problem

\[
P^* = \min_{\theta \in \Theta} \frac{1}{2} f_{\theta,L}(X) - Y^2 + \frac{\beta}{2} \sum_{j=1}^{m} \sum_{l=1}^{L} \|W_{l,j}\|_2^2
\]

(53)

After a suitable rescaling as in the previous case, the above problem has the following dual

\[
P^* \geq D^* = \max_{\lambda} -\frac{1}{2} \left\langle \lambda, A - Y \right\rangle_F + \frac{1}{2} \left\| Y \right\|_F^2 \ \text{s.t.} \ \left\langle A^T (A_{L-2,j} w_{L-1,j})_+ \right\|_2 \leq \beta, \ \forall \theta_l \in \Theta_{L-1}, \ \forall l \in [L-1], \ \forall j \in [m].
\]

Using (54), we can characterize the optimal layer weights as the extreme points that solve

\[
\arg\max_{\{\theta_l\}_{l=1}^{L-1} \in \Theta_{L-1}} \left\| \Lambda^* \right\|_2, \ (A_{L-2,j} w_{L-1,j})_+.
\]

(55)
where $\Lambda^*$ is the optimal dual parameter. We first note that since $X$ is whitened such that $XX^T = I_n$ and labels are one-hot encoded, the dual problem has a closed-form solution as follows

$$
\lambda_k^* = \begin{cases} 
\frac{\beta t_j^{2-L} y_k}{\|y_k\|_2} & \text{if } \beta \leq \|y_k\|_2, \\
\text{otherwise} & \forall k \in [K]. 
\end{cases} \tag{56}
$$

We now note that since $Y$ has orthogonal one-hot encoded columns, the dual constraint can be decomposed into $k$ maximization problems each of which can be maximized independently to find a set of extreme points. In particular, the $j^{th}$ problem can be formulated as follows

$$
\arg\max_{(\theta_i)_{i=1}^L} \left| Y_k^T (A_{L-2,j} W_{L-1,j}) + | \leq \max \left\{ \| (y_k)_+ \|_2, \| (-y_k)_+ \|_2 \right\} .
$$

Then, noting the whitened data assumption, the rest of steps directly follow Theorem 4.1 yielding the following weight matrices

$$
W_{l,j} = \frac{\phi_{l-1,j}}{\|\phi_{l-1,j}\|_2} \phi_{l,j}^T, \forall l \in [L - 2], \ W_{L-1,j} = \frac{\phi_{L-2,j}}{\|\phi_{L-2,j}\|_2}, \tag{57}
$$

where $\phi_{0,j} = X^T y_k$ and $\{\phi_{l,j}\}_{l=1}^{L-2}$ is a set of nonnegative vectors satisfying $\|\phi_{l,j}\|_2 = t_j^*$, $\forall l$ and $\phi_{l,i}^T \phi_{l,j} = 0 \forall i \neq j$.

We now note that given the hidden layer weight in (57), the primal problem in (53) is convex and differentiable with respect to the output layer weight $W_L$. Thus, we can find the optimal output layer weights by simply taking derivative and equating it to zero. Applying these steps yields the following output layer weights

$$
W_{L-1} = \left[ \frac{\phi_{L-2,1}}{\|\phi_{L-2,1}\|_2} \cdots \frac{\phi_{L-2,K}}{\|\phi_{L-2,K}\|_2} \right] = \sum_{r=1}^K \frac{\phi_{L-2,r}}{\|\phi_{L-2,r}\|_2} \phi_{L-1,r}^T, \tag{58}
$$

where $\phi_{L-1,r} = e_r$ is the $r^{th}$ ordinary basis vector.

Let us now assume that $t_j^* = 1$ for notational simplicity and then show that strong duality holds, i.e., $P^* = D^*$. We first denote the set of indices that yield an extreme point as $E = \{ j : \beta \leq \|y_j\|_2, j \in [o] \}$. Then we compute the objective values for the dual problem (54) using (56)

$$
D = -\frac{1}{2} \| \Lambda^* - Y \|_F^2 + \frac{1}{2} \| Y \|_F^2 \\
= -\frac{1}{2} \sum_{j \in E} (\beta - \|y_j\|_2)^2 + \frac{1}{2} \sum_{j=1}^o \|y_j\|_2^2 \\
= -\frac{1}{2} \beta^2 |E| + \beta \sum_{j \in E} \|y_j\|_2 + \frac{1}{2} \sum_{j \notin E} \|y_j\|_2^2. \tag{59}
$$

We next compute the objective value for the primal problem (53) (after applying the rescaling in Lemma A.4) using the weights in (57) and (58) as follows

$$
P = \frac{1}{2} \| f_{\theta,L}(X) - Y \|_F^2 + \frac{\beta}{2} \sum_{j=1}^m \| W_{L,j} \|_2 \\
= \frac{1}{2} \left( \sum_{j \in E} (\|y_j\|_2 - \beta) \frac{y_j}{|y_j|_2} e_j^T - Y \right)_F^2 + \beta \sum_{j \notin E} (\|y_j\|_2 - \beta) \\
= \frac{1}{2} \sum_{j \in E} \beta \frac{y_j}{|y_j|_2} e_j^T |E| + \frac{1}{2} \sum_{j \notin E} \|y_j\|_2 \|e_j\|_F^2 + \beta \sum_{j \in E} \|y_j\|_2 - \beta^2 |E| \\
= -\frac{1}{2} \beta^2 |E| + \frac{1}{2} \sum_{j \notin E} \|y_j\|_2^2 + \beta \sum_{j \in E} \|y_j\|_2,
which has the same value with (59). Therefore, strong duality holds, i.e., \( P^* = D^* \), and the set of weights proposed in (57) and (58) is optimal.

**Theorem 4.4.** Suppose \( \mathbf{Y} \) is one hot encoded and the network is overparameterized such that the range of \( \mathbf{A}_{L-2,j} \) is \( \mathbb{R}^n \), then an optimal solution to the following problem\(^{10}\)

\[
\min_{\theta \in \Theta} \frac{1}{2} \sum_{j=1}^{m} \left( \text{BN}_{1,\alpha} \left( \mathbf{A}_{L-2,j} \mathbf{w}_{L-1,j} \right) \right)_+ \mathbf{w}_{L,j}^T - \mathbf{Y} \right\|_F^2 \\
+ \beta \sum_{j=1}^{m} \left( \gamma_j^{(L-1)^2} + \alpha_j^{(L-1)^2} \right),
\]

is optimal.

\( \gamma_j^{(L-1)^2} + \alpha_j^{(L-1)^2} \) can be formulated in closed-form as follows

\[
\mathbf{w}_{L-1,j}^*, \mathbf{w}_{L,j}^* = \left( \mathbf{A}_{L-2,j}^T \mathbf{Y}_j, (\|\mathbf{y}_j\|_2 - \beta) \mathbf{e}_j \right)
\]

\( \forall j \in [K], \) where \( \mathbf{e}_j \) is the \( j \)th ordinary basis vector.

**Proof of Theorem 4.4.** We first state the primal problem after applying the scaling between \( \mathbf{w}_L \) and \( \left( \gamma^{(L-1)}, \alpha^{(L-1)} \right) \) as in Lemma A.4

\[
P^* = \min_{\theta \in \Theta} \frac{1}{2} \sum_{j=1}^{m} \left( \text{BN}_{1,\alpha} \left( \mathbf{A}_{L-2,j} \mathbf{w}_{L-1,j} \right) \right)_+ \mathbf{w}_{L,j}^T - \mathbf{Y} \right\|_F^2 \\
+ \beta \sum_{j=1}^{m} \|\mathbf{w}_{L,j}\|_2, \tag{60}
\]

where \( \Theta = \{ \theta \in \Theta : \gamma_j^{(L-1)^2} + \alpha_j^{(L-1)^2} = 1, \forall j \in [m] \} \) and the corresponding dual is

\[
P^* \geq D^* = \max_{\mathbf{A}} \frac{1}{2} \|\mathbf{A} - \mathbf{Y}\|_F^2 + \frac{1}{2} \|\mathbf{Y}\|_F^2 \text{ s.t. } \max_{\theta \in \Theta} \left| \mathbf{A}^T \left( \text{BN}_{1,\alpha} \left( \mathbf{A}_{L-2,j} \mathbf{w}_{L-1,j} \right) \right)_+ \right| \leq \beta. \tag{61}
\]

We now show that the following set of solutions for the primal and dual problem achieves strong duality, i.e., \( P^* = D^* \), therefore, optimal.

\[
\mathbf{w}_{L-1,j}^*, \mathbf{w}_{L,j}^* = \begin{cases} 
\left( \mathbf{A}_{L-2,j}^T \mathbf{Y}_j, (\|\mathbf{y}_j\|_2 - \beta) \mathbf{e}_j \right) & \text{if } \beta \leq \|\mathbf{y}_j\|_2 \\
\text{otherwise} & \end{cases}
\]

\[
\frac{\gamma_j^{(L-1)^2} \alpha_j^{(L-1)^2}}{\|\mathbf{y}_j\|_2} = \frac{1}{\|\mathbf{y}_j\|_2} \left[ \|\mathbf{y}_j - \frac{1}{\sqrt{n}} \mathbf{1}_n \mathbf{y}_j\|_2 \right], \quad \forall j \in [K].
\]

\[
\mathbf{\lambda}_j^* = \begin{cases} 
\beta \frac{\mathbf{y}_j}{\|\mathbf{y}_j\|_2} & \text{if } \beta \leq \|\mathbf{y}_j\|_2 \\
\text{otherwise} & \end{cases}
\]

Now let us first denote the set of indices that achieves the extreme point of the dual constraint as \( \mathcal{E} = \{ j : \beta \leq \|\mathbf{y}_j\|_2, j \in [K] \} \). Then the dual objective in (61) using the optimal dual parameter above

\[
D^*_L = \frac{1}{2} \|\mathbf{\lambda}^* - \mathbf{Y}\|_F^2 + \frac{1}{2} \|\mathbf{Y}\|_F^2 \\
= \frac{1}{2} \sum_{j \in \mathcal{E}} (\beta - \|\mathbf{y}_j\|_2)^2 + \frac{1}{2} \sum_{j=1}^{K} \|\mathbf{y}_j\|_2^2 \\
= \frac{1}{2} \beta^2 |\mathcal{E}| + \beta \sum_{j \in \mathcal{E}} \|\mathbf{y}_j\|_2 + \frac{1}{2} \sum_{j \notin \mathcal{E}} \|\mathbf{y}_j\|_2^2. \tag{62}
\]

\(^{10}\)Notice here we only regularize the last layer’s parameters, however, regularizing all the parameters does not change the analysis and conclusion as proven in Appendix A.4
We next restate the scaled primal problem

\[ P_L^* = \frac{1}{2} \left( \sqrt{\frac{n}{K}} \left( I_n - \frac{1}{n} 1_n 1_n^T \right) A_{L-1} L_{-1,j} \right) \left( w_{L-1,j}^* \gamma^{(L-1)*} + \frac{1}{\sqrt{n}} \alpha_j^{(1)*} \right) + \beta \sum_{j=1}^{K} \| w_{L,j} \|^2 \]

\[ = \frac{1}{2} \left( \beta \sum_{j \in E} \| y_j \|_2^2 - \beta \| y_j \|_2 \| e_j \|_2^T \right)^2 + \beta \sum_{j \in E} (\| y_j \|_2 - \beta) \sum_{j \in E} \| y_j \|_2 - \beta^2 |E| \]

\[ = \frac{1}{2} \beta^2 |E| + \beta \sum_{j \in E} \| y_j \|_2^2 + \beta \sum_{j \in E} \| y_j \|_2 \]

(63)

which is the same with (62). Therefore, strong duality holds, i.e., \( P^* = D^* \), and the proposed set of weights is optimal for the primal problem (60).

\[ \square \]

**Corollary 4.3.** Computing the last hidden layer activations after BN, i.e., \( A_{L-1} \in \mathbb{R}^{n \times K} \), using the optimal layer weight in Theorem 4.4 and then subtracting their global mean as in \( \text{Papyan et al.} \) 2020 yields

\[ \left( I_n - \frac{1}{n} 1_n 1_n^T \right) A_{L-1} = \sqrt{\frac{n}{K}} \left( I_K \otimes 1_K^T - \frac{1}{K} 1_n 1_n^T \right), \]

where we assume that samples are ordered, i.e., the first \( n/K \) samples belong to class 1, next \( n/K \) samples belong to class 2 and so on. Therefore, all the activations for a certain class \( k \) are the same and their mean is given by \( \sqrt{\frac{n}{K}} (e_k - 1_K/K) \), which is the \( k \)th column of a general simplex ETF with \( \alpha = \sqrt{(K-1)/n} \) and \( U = I_K \).

**Proof of Corollary 4.3.** We first restate a crucial assumptions in \( \text{Papyan et al.} \) 2020.

**Assumption 1.** The training dataset has balanced class distribution. Therefore, if we denote the number of data samples as \( n \), then we have \( n/K \) samples for each class \( j \in [K] \).

Due to Assumption 1 and one-hot encoded labels, we have \( \| y_1 \|_2 = \| y_2 \|_2 = \ldots = \| y_K \|_2 = \sqrt{n/K} \). Now, we assume that \( \sqrt{n/K} > \beta \) since otherwise none of the neurons will be optimal as proven in Theorem 4.4. We also remark that \( \sqrt{n/K} > 1 \gg \beta \) in practice so that this assumption is trivially satisfied for practical scenarios considered in \( \text{Papyan et al.} \) 2020. Therefore, the weights in Theorem 4.4 imply that

\[ A_{(L-1),j} = \frac{(I_n - \frac{1}{n} 1_n 1_n^T) A_{L-2,j} w_{(L-2),j}^*}{\| (I_n - \frac{1}{n} 1_n 1_n^T) A_{L-2,j} w_{(L-2),j}^* \|_2} \gamma^{(L-1)*} + \frac{1}{\sqrt{n}} \alpha_j^{(L-1)*} \]

\[ = \left( \frac{y_j}{\| y_j \|_2} + \frac{1_n 1_n^T y_j}{n \| y_j \|_2} \right) + \frac{\sqrt{K} y_j}{\sqrt{n}}, \]

where \( A_{(L-1),j} \) denotes the \( j \)th column of the last hidden layer activations after BN and the last equality follows from...
Assumptions: We then subtract mean from $A_{L-1}$ as follows

$$
\left(I_n - \frac{1}{n} \mathbf{1}_{n \times n}\right) A_{L-1} = \left(I_n - \frac{1}{n} \mathbf{1}_{n \times n}\right) \frac{\sqrt{K}}{\sqrt{n}} \mathbf{Y} = \frac{\sqrt{K}}{\sqrt{n}} \begin{bmatrix}
1 - \frac{1}{K} & \frac{1}{K} & \frac{1}{K} & \cdots & \frac{1}{K} \\
\frac{1}{K} & 1 - \frac{1}{K} & \frac{1}{K} & \cdots & \frac{1}{K} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
-\frac{1}{K} & \frac{1}{K} & -\frac{1}{K} & \cdots & -\frac{1}{K} \\
-\frac{1}{K} & \frac{1}{K} & -\frac{1}{K} & \cdots & -\frac{1}{K} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
\end{bmatrix}
$$

$$
= \frac{\sqrt{K}}{\sqrt{n}} \left(I_K \otimes \mathbf{1}_{n \times K} - \frac{1}{K} \mathbf{1}_{n \times K}\right),
$$

where we assume that samples are ordered, i.e., the first $n/K$ samples belong to class 1, next $n/K$ samples belong to class 2 and so on. Therefore, all the activations for a certain class $k$ are the same and their mean is given by

$$
\frac{\sqrt{K}}{\sqrt{n}} \left[e_k \mathbf{1}_K - \frac{1}{K} \mathbf{1}_K \right],
$$

which is the $k^{th}$ column of a general simplex ETF with $\alpha = \sqrt{(K-1)/n}$ and $U = I_K$ in Definition 2. Hence, our analysis in Theory 4.4 completely explains why the patterns claimed in (Papyan et al., 2020) emerge throughout the training of the state-of-the-art architectures. We also remark that even though we use squared loss for the derivations, this analysis directly applies to the other convex loss functions including cross entropy and hinge loss as proven in Appendix A.1.