Stationary Points of Shallow Neural Networks with Quadratic Activation Function

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Abstract

We consider the problem of learning shallow neural networks with quadratic activation function and planted weights $W^* \in \mathbb{R}^{m \times d}$, where $m$ is the width of the hidden layer and $d \leq m$ is the data dimension. We establish that the landscape of the population risk $\mathcal{L}(W)$ admits an energy barrier separating rank-deficient solutions: if $W \in \mathbb{R}^{m \times d}$ with rank$(W) < d$, then $\mathcal{L}(W) \geq 2\sigma_{\text{min}}(W^*)^4$, where $\sigma_{\text{min}}(W^*)$ is the smallest singular value of $W^*$. We then establish that all full-rank stationary points of $\mathcal{L}(\cdot)$ are necessarily global optimum. These two results propose a simple explanation for the success of the gradient descent in training such networks, when properly initialized: gradient descent algorithm finds global optimum due to absence of spurious stationary points within the set of full-rank matrices.

We then show that if the planted weight matrix $W^* \in \mathbb{R}^{m \times d}$ is generated randomly (with iid Gaussian entries), and is sufficiently wide, that is $m > Cd^2$ for large enough $C$, then it is easy to construct a full rank matrix $W$ with population risk below the aforementioned energy barrier, starting from which gradient descent is guaranteed to converge to a global optimum.

Our final focus is on sample complexity: we identify a simple necessary and sufficient geometric condition on the training data under which any minimizer of the empirical loss has necessarily zero generalization error. We show that as soon as $n \geq n^* = d(d + 1)/2$, randomly generated data enjoys this geometric condition almost surely. At the same time we show that if $n < n^*$, then when the data has a Gaussian i.i.d. distribution, there always exists a matrix $W$ with empirical risk equal to zero, but with population risk bounded away from zero by the same amount as rank deficient matrices, namely by $2\sigma_{\text{min}}(W^*)^4$.

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1 Introduction

The main focus of many machine learning and statistics tasks is to extract information from a given collection of data, often by solving the following “canonical problem”: Let \((X_i, Y_i)_{i=1}^n\) be a data set, with \(X_i \in \mathbb{R}^d\) and \(Y_i \in \mathbb{R}\). The components \(Y_i\) are often called the labels. The problem, then, is to find a function \(f : \mathbb{R}^d \to \mathbb{R}\), which:

- Explains the unknown input-output relationship over the data set as accurately as possible, that is, if \(Y = (Y_1, Y_2, \ldots, Y_n)^T\) and \(f(X) = (f(X_1), \ldots, f(X_n))^T\), then it ensures that \(c(Y, X)\) is small, where \(c(\cdot, \cdot) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^+\) is some cost function. The resulting \(c(Y, X)\) is known as the “training error”.

- Has good prediction performance on the unseen data, that is, it generalizes well. In mathematical terms, if the training data \((X_i, Y_i)\) is generated from a distribution \(\mathcal{D}\) on \(\mathbb{R}^d \times \mathbb{R}\), then one demands that \(\mathbb{E}_{(X,Y) \sim \mathcal{D}}[c'(Y, f(X))]\) is small, where \(c'(\cdot, \cdot) : \mathbb{R} \times \mathbb{R} \to \mathbb{R}^+\) is some (perhaps different) cost function. Here the expectation is with respect to a fresh sample \((X, Y)\). The resulting \(\mathbb{E}_{(X,Y) \sim \mathcal{D}}[c'(Y, f(X))]\) is known as the “generalization error” or the “test error”.

One popular class of such functions \(f(\cdot)\) are neural networks, which attempt to explain the (unknown) input-output relationship with the following form:

\[
f(X) = a^T \sigma_L(W_{L-1} \sigma_{L-1}(W_{L-2} \cdots \sigma_2(W_2 \sigma_1(W_1 X)) \cdots)).
\]

Here, \(L\) is the ‘depth’ of the neural network, \(\sigma_1, \ldots, \sigma_L : \mathbb{R} \to \mathbb{R}\) are the non-linear functions called activations which act coordinate-wise, \(W_1, \ldots, W_{L-1}\) are the weight matrices of appropriate sizes; and \(a\) is a vector, carrying the output weights. The process of finding parameters \(W_1, \ldots, W_{L-1}\) and \(a\) which can interpolate the data set is called training.
Albeit being simple to state, neural networks turn out to be extremely powerful in tasks such as natural language processing [CW08], image recognition [HZRS16], image classification [KSH12], speech recognition [MDH11], and game playing [SSS+17]; and started becoming popular in other areas, such as applied mathematics [CRBD18, WHJ17], and clinical diagnosis [DFLRP+18], and so on.

1.1 Model

In this paper, we consider a shallow neural network model with one hidden layer ($L = 1$), consisting of $m$ neurons (that is, the “width” of the network is $m$), a (planted) weight matrix $W^* \in \mathbb{R}^{m \times d}$ (where for each $i \in [m]$, the $i^{th}$ row $W^*_i \in \mathbb{R}^d$ of this matrix is the weight vector associated to the $i^{th}$ neuron), and quadratic activation function $\sigma(x) = x^2$. This object, for every input vector $X \in \mathbb{R}^d$, computes the function:

$$f(W^*; X) = \sum_{j=1}^{m} (W^*_j, X)^2 = \|W^*X\|^2_2.$$

We note that, albeit being rarely used in practice, quadratic activations help us develop understanding for networks consisting of polynomials activations with higher degrees or sigmoid activations [LSSS14, SH18, VBB18].

The associated empirical risk minimization problem is then cast as follows: Let $X_1, \ldots, X_n \in \mathbb{R}^d$ be an iid sequence of input data. Generate the output labels $Y_i$ using a shallow neural network (the so-called teacher network) with the planted weight matrix $W^* \in \mathbb{R}^{m \times d}$, that is, $Y_i = f(W^*; X)$. This model is also known as the realizable model, as the labels $Y_i$ are generated according to a teacher network with planted weight matrix $W^* \in \mathbb{R}^{m \times d}$. Assume the learner has access to the training data $(X_i, Y_i)_{i=1}^n$. The empirical risk minimization problem (ERM) is the optimization problem

$$\min_{W \in \mathbb{R}^{m \times d}} \hat{L}(W)$$

where

$$\hat{L}(W) \triangleq \frac{1}{n} \sum_{i=1}^{n} (Y_i - f(W; X_i))^2,$$

of finding a weight matrix $W \in \mathbb{R}^{m \times d}$ that explains the input-output relationship for the training data set $(X_i, Y_i)_{i=1}^n$ in the best possible way. The focus is on tractable algorithms to solve this minimization problem and understanding its generalization ability, quantified by generalization error. The generalization error, also known as population risk associated with any solution candidate $W \in \mathbb{R}^{m \times d}$ (whether it is optimal with respect to (1) or not), is

$$\mathcal{L}(W) \triangleq \mathbb{E}[(f(W^*; X) - f(W; X))^2],$$

where the expectation is with respect to a "fresh" sample $X$, which has the same distribution as $X_i, 1 \leq i \leq n$, but is independent from the sample. This object provides information about how well $W$ generalizes, that is, how much error on average it makes on prediction for the yet
unseen data. Observe that due to the quadratic nature of the activation function, the ground truth matrix $W^*$, which is also an optimal solution to the empirical risk optimization problem $\min_W \hat{L}(W)$ (which has value zero) and population risk optimization problem $\min_W L(W)$ (which also has value zero), is invariant under rotation. Namely for every orthonormal $Q \in \mathbb{R}^{m \times m}$, $W = QW^*$ is also an optimal solution to both optimization problems.

The landscape of the loss function $\hat{L}(W)$ as a function of $W$ is highly non-convex, rendering the underlying optimization problem potentially difficult. Nevertheless, it has been empirically observed, and rigorously proven under certain assumptions (references below), that the gradient descent algorithm, despite being a simple first order procedure, is rather successful in training such neural networks: it appears to find a $W \in \mathbb{R}^{m \times d}$ with $\hat{L}(W) \approx 0$. This is a mystery yet to be understood.

1.2 Summary of the Main Results and Comparison with the Prior Work

We first study the landscape of the population risk function $L(W)$, and establish the following result under the Gaussianity assumption on the input data $X_i \in \mathbb{R}^d$, $1 \leq i \leq n$: If $W^* \in \mathbb{R}^{m \times d}$ is full-rank, then for any rank-deficient matrix $W \in \mathbb{R}^{m \times d}$, $L(W)$ is bounded away from zero, by an explicit constant controlled by the smallest singular value $\sigma_{\min}(W^*)$ of the planted weight matrix $W^*$. In particular, this result highlights the existence of an “energy barrier” separating full-rank points with ‘small cost’ from rank-deficient points, and shows that near the ground state $W^*$ one can only find full-rank points $W$. This is Theorem 2.1.

We then study the full-rank stationary points of $L(\cdot)$ by studying the corresponding analytical formula for the population gradient. We establish in Theorem 2.3 that again for Gaussian data, when $W^*$ is full rank, all full-rank stationary points $W \in \mathbb{R}^{m \times d}$ of $L(\cdot)$ are necessarily global optimum, and in particular, for any such $W$, there exists an orthonormal matrix $Q \in \mathbb{R}^{m \times m}$ such that $W = QW^*$. Combining with Theorem 2.1 discussed above, as a corollary we obtain the following interesting conclusion: if the gradient descent algorithm is initialized at a point $W$ which has a sufficiently small population risk, in particular if it is lower than smallest risk value achieved by rank deficient matrices $\hat{W}$, then the gradient descent converges to a global optimum of the population risk optimization problem $\min_W L(W)$.

We now briefly pause to make a comparison with some of the related prior work. Among these the most relevant to us is the work of Soltanolkotabi, Javanmard and Lee [SJL18]. Here the authors study the empirical loss landscape of a slightly more general version of our model: $Y_i = \sum_{j=1}^m v_j^* \sigma(\langle W_j^*, X_i \rangle)$, with the same quadratic activation function $\sigma(x) = x^2$, assuming $\sigma_{\min}(W^*) > 0$, and assuming all non-zero entries of $v^*$ have the same sign. Thus our model is the special case where all entries of $v^*$ equal unity. The authors establish that as long as $d \leq n \leq cd^2$ for some small fixed constant $c$, every local minima of the empirical risk function is also a global minima (namely, there exists no spurious local minima), and furthermore, every saddle point has a direction of negative curvature. As a result they show that gradient descent with an arbitrary initialization converges to a globally optimum solution of the empirical risk minimization problem. In particular, their result does not require the initialization point to be below some risk value, like in our case. Our result though shows that one needs not to worry about saddle points below some risk value as none exist per our first Theorem 2.1, when the population risk minimization problem is considered instead. We note also that the proof
technique [SJL18], more concretely, the proof of [SJL18, Theorem 3.2], which can be found in Section 6.2.1 therein, also appears to be a path to prove an empirical risk version of Theorem 2.3 with very minor modifications. Important, though, the regime \( n < c d^2 \) for small \( c \) is below the provable sample complexity value \( n^* \), as per our results discussed below. In particular, as we discuss below and prove in the main body of our paper, when \( n < n^* = d(d+1)/2 \), the empirical risk minimization problem admits global optimum solutions with zero empirical risk value, but with generalization error bounded away from zero. Thus, the regime \( n < n^* \) does not correspond to the regime where learning with guaranteed generalization error is possible.

Another work which is partially relevant to the present paper is the work by Du and Lee [DL18] who establish the following result: as long as \( m \geq d \), and \( \ell(\cdot, \cdot) \) is any smooth and convex loss, the landscape of the regularized loss function \( \frac{1}{n} \sum_{i=1}^{n} \ell(f(W; X_i), Y_i) + \frac{\lambda}{2} \|W\|_F^2 \) admits favorable geometric characteristics, that is, all local minima is global, and all saddle points are strict.

Next we study the question of proper initialization required by our analysis: is it possible to guarantee an initialization scheme under which one starts below the minimum loss value achieved by rank deficient matrices? We study this problem in the context of randomly generated weight matrices \( W^* \), and, in particular, when the weight matrix \( W^* \in \mathbb{R}^{m \times d} \) has iid Gaussian entries. We establish that as long as the network is wide enough, specifically \( m > C d^2 \) for some sufficiently large constant \( C \), the spectrum of the associated Wishart matrix \( (W^*)^T W^* \) is tightly concentrated, and as a result, it is possible to initialize \( W_0 \) so that with high probability the population loss \( \mathcal{L}(W_0) \) of \( W_0 \) is below the required threshold. This is the subject of our Theorem 2.5. The theorem relies on some results from the theory of random matrices regarding the concentration of the spectrum.

Our next focus is on the following question: in light of the fact that \( W^* \) (and any of its orthonormal equivalents) achieve zero generalization error for both the empirical and population risk, can we expect that an optimal solution to the problem of minimizing empirical loss function \( \min_W \hat{\mathcal{L}}(W) \) achieves the same? The answer turns out to be positive and we give necessary and sufficient conditions on the sample \( X_i, 1 \leq i \leq n \) to achieve this. We show that, if span(\( X_i X_i^T : i \in [n] \)) is the space of all \( d \times d \)-dimensional real-valued symmetric matrices, then any global minimum of the empirical loss is necessarily a global optimizer of the population loss, and thus, has zero generalization error. Note that, this condition is not retrospective in manner: this geometric condition can be checked ahead of the optimization task by computing span(\( X_i X_i^T : i \in [n] \)). Conversely, we show that if the span condition above is not met then there exists a global minimum \( W \) of the empirical risk function which induces a strictly positive generalization error. This is established in Theorem 2.6. To complement our analysis, we then ask the following question: what is the critical number \( n^* \) of the training samples, under which the (random) data \( X_i, 1 \leq i \leq n \) enjoys the aforementioned span condition? We prove the number to be \( n^* = d(d + 1)/2 \), under a very mild assumption that the coordinates of \( X_i \in \mathbb{R}^d \) are jointly continuous. This is shown in Theorem 2.8. Finally, in Theorem 2.9 we show that when \( n < n^* \) not only there exists \( W \) with zero empirical risk and strictly positive generalization error, but we bound this error from below by the same amount as the bound for all rank deficient matrices discussed in our first Theorem 2.1.

The rest of the paper is organized as follows. In Section 2.1 we present our main results on the landscape of the population risk, and in particular state our lower bound result for rank deficient matrices and our result about the absence of full-rank stationary points of a population risk function, except the globally optimum points. In Section 2.2, we present our results regarding
randomly generated weight matrices $W^*$ and sufficient conditions for good initializations. In Section 2.3, we study the critical number of training samples guaranteeing good generalization property. The proofs of all of our results are found Section 3.

**Notation**

We provide a set of notational convention that we follow throughout. The set of real numbers is denoted by $\mathbb{R}$, and the set of positive real numbers is denoted by $\mathbb{R}_+$. The set $\{1, 2, \ldots, k\}$ is denoted by $[k]$. Given any matrix $A$, $\sigma_{\min}(A)$ and $\sigma_{\max}(A)$ respectively denote the smallest and largest singular values of $A$; $\sigma(A)$ denotes the spectrum of $A$, that is, the set of all eigenvalues of $A$; and trace($A$) denotes the sum of the diagonal entries of $A$. Moreover, $\|A\|_2$ denotes the spectral norm of $A$, that is, the square root of the largest eigenvalue of $A^T A$. The objects with an asterisk denotes the planted objects, for instance, $W^* \in \mathbb{R}^{m \times d}$ denotes the planted weight matrix of the network. Given any vector $v \in \mathbb{R}^n$, $\|v\|_2$ denotes its Euclidean $\ell_2$ norm, that is, $\|v\|_2 = \sqrt{v_1^2 + \cdots + v_n^2}$. Given two vectors $x, y \in \mathbb{R}^n$, their Euclidean inner product $\sum_{i=1}^n x_i y_i$ is denoted by $\langle x, y \rangle$. Given a collection $Z_1, \ldots, Z_k$ of objects of the same kind (in particular, vectors or matrices), span($Z_i : i \in [k]$) is the set, $\left\{ \sum_{j=1}^k \alpha_j Z_j : \alpha_1, \ldots, \alpha_k \in \mathbb{R} \right\}$. $\Theta(\cdot), O(\cdot), o(\cdot)$ and $\Omega(\cdot)$ are standard (asymptotic) order notations for comparing the growth of two sequences. Finally, the population risk is denoted by $L(\cdot)$; and its empirical variant is denoted by $\hat{L}(\cdot)$.

## 2 Main Results

### 2.1 Landscape of Population Risk: Band-Gap and Optimality of Full-Rank Stationary Points

Our first result shows the appearance of a band gap structure in the landscape of the population risk $L(\cdot)$, below which rank-deficient $W$ matrices cease to exist. We recall that a random vector $X$ in $\mathbb{R}^d$ is defined to have jointly continuous distribution if there exists a measurable function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ such that for any $i \in [n]$ and Borel set $B \subseteq \mathbb{R}^d$,

$$ \mathbb{P}(X \in B) = \int_B f(x_1, \ldots, x_d) \, d\lambda(x_1, \ldots, x_d), $$

where $\lambda$ is the Lebesgue measure on $\mathbb{R}^d$.

**Theorem 2.1.** Let $W^* \in \mathbb{R}^{m \times d}$ be a matrix with rank($W^*$) = $d$, $f(W^*; X)$ be function computed by a one hidden layer neural network with weights $W^*$, and $f(W; X)$ be similarly the function computed by such a network with weights $W \in \mathbb{R}^{m \times d}$. Recall,

$$ L(W) = \mathbb{E}[(f(W^*; X) - f(W; X))^2], $$

where the expectation is with respect to the distribution of $X \in \mathbb{R}^d$.

(a) Suppose the distribution of $X$ is jointly continuous. Then $L(W) = 0$, that is, $f(W^*; X) = f(W; X)$ almost surely with respect to $X$, if and only if $W = Q W^*$ for some orthonormal matrix $Q \in \mathbb{R}^{m \times m}$.  


(b) Suppose $X_i, 1 \leq i \leq n$ are i.i.d. with standard normal independent coordinate distribution $\mathcal{N}(0, I_d)$. Then
\[
\min_{W \in \mathbb{R}^{m \times d}, \text{rank}(W) < d} \mathcal{L}(W) \geq 2\sigma_{\min}(W^*)^4.
\]

(c) Under assumption (b) there exists $W \in \mathbb{R}^{m \times d}$ such that $\text{rank}(W) \leq d - 1$, and $\mathcal{L}(W) = 3(\sigma_{\min}(W^*)^4)$.

The proof of Theorem 2.1 is deferred to Section 3.1.

This theorem indicates that there is a threshold $\eta = \Theta(\sigma_{\min}(W^*)^4)$, such that for any $W$ with $\mathcal{L}(W) < \eta$, it is the case that $W$ is full rank. This value of $\eta$ is the aforementioned energy value below which any rank-deficient $W$ ceases to exist. Part (c) of Theorem 2.1 implies that our lower bound on the value is tight up to a multiplicative constant.

Note that, the characterization of the “optimal orbit” per part (a) is not surprising: any matrix $W$ with the property $W = QW^*$ where $Q \in \mathbb{R}^{m \times m}$ is an orthonormal matrix, that is, $Q^TQ = I_m$ has the property that $f(W; X) = \|WX\|_2^2 = X^TW^TWX = f(W^*; X)$ for any data $X \in \mathbb{R}^d$. Part (a) then says the the reverse is true as well, provided that the distribution of $X$ is jointly continuous.

As a corollary to Theorem 2.1, we obtain that the landscape of the population risk still admits an energy barrier, even if we consider the same network architecture with planted weight matrix $W^* \in \mathbb{R}^{m \times d}$, and quadratic activation function having lower order terms, that is, the activation $\sigma(x) = \alpha x^2 + \beta x + \gamma$, with $\alpha \neq 0$. This barrier is quantified by $\sigma_{\min}(W^*)$ and $\alpha$.

**Corollary 2.2.** For any $W \in \mathbb{R}^{m \times d}$, define $\tilde{f}(W; X) = \sum_{j=1}^m \tilde{\sigma}(W_j, X)$, where $\tilde{\sigma}(x) = \alpha x^2 + \beta x + \gamma$ with $\alpha, \beta, \gamma \in \mathbb{R}$ arbitrary. Let
\[
\tilde{\mathcal{L}}(W) = \mathbb{E}[(\tilde{f}(W; X) - \tilde{f}(W^*; X))^2],
\]
where $X \overset{d}{=} \mathcal{N}(0, I_d)$. Then,
\[
\min_{W \in \mathbb{R}^{m \times d}, \text{rank}(W) < d} \tilde{\mathcal{L}}(W) \geq 2\alpha^2\sigma_{\min}(W^*)^4.
\]

The proof of this corollary is deferred to Section 3.2.

Our next result establishes that any full-rank stationary point (of the population risk) is necessarily a global minimum.

**Theorem 2.3.** Suppose $W^* \in \mathbb{R}^{m \times d}$ with $\text{rank}(W^*) = d$. Suppose $X \in \mathbb{R}^d$ has $\mathcal{N}(0, I_d)$ distribution. Let $W \in \mathbb{R}^{m \times d}$ be a stationary point of the population risk with full-rank, that is, $\nabla \mathcal{L}(W) = \mathbb{E}[\nabla(f(W^*; X) - f(W; X))^2] = 0$, and $\text{rank}(W) = d$. Then, $W = QW^*$ for some orthogonal matrix $Q$, and $\mathcal{L}(W) = 0$.

The proof of Theorem 2.3 is deferred to Section 3.3. Note that an implication of Theorem 2.3 is that the population loss admits no rank-deficient saddle points.

Combining Theorem 2.3 with Theorem 2.1 discussed above, as a corollary we obtain the following interesting conclusion: if the gradient descent algorithm is initialized at a point $W$ which has a sufficiently small population risk, in particular if it is lower than smallest risk value achieved by rank deficient matrices $\hat{W}$, then the gradient descent converges to a global optimum.
of the population risk optimization problem min_W \mathcal{L}(W). Indeed, for any differentiable loss, gradient descent algorithm is known to generate a sequence (W_k)_{k \geq 0} of iterates (with W_0 being initialization) such that \mathcal{L}(W_k) \geq \mathcal{L}(W_{k+1}) for any k \geq 0 (namely, the cost is non-increasing), and W_k \to W^\infty where W^\infty is a stationary point of the loss function. Now, suppose that the initialization is nice enough, that is, \mathcal{L}(W_0) < \eta. Then, W_0 is full-rank; and that, it remains within the aforementioned energy band. Since the cost is non-increasing along the trajectory of the gradient descent, we then deduce that the gradient descent converges to a W^\infty, which is full-rank, and moreover, a stationary point of the loss. Thus, per Theorem 2.3, we deduce it is a global optimum.

In the next section, we complement our result by giving an initialization guarantee when the (planted) weights are generated randomly.

### 2.2 On Initialization: Randomly Generated Planted Weights

As noted in the previous section, our Theorems 2.1 and 2.3 offer an alternative conceptual explanation for the success of training gradient descent in learning aforementioned neural network architectures from the landscape perspective; provided that the algorithm is initialized properly.

In this section, we provide a way to properly initialize such networks, in the case the weight matrix W^* \in \mathbb{R}^{m \times d} consists of iid standard normal entries, and the network is overparametrized, in the sense that m > Cd^2 for some large constant C (note that, in this case W^* is a tall matrix).

The rationale behind this approach relies on the following observations:

(a) If \lambda_1, \ldots, \lambda_d are the eigenvalues of W^TW - (W^*)^TW^*, then an inspection of the proof of Theorem 2.1 reveals that, \mathcal{L}(W) = 2 \sum_{i=1}^d \lambda_i^2 + \left(\sum_{i=1}^d \lambda_i\right)^2. Namely, the spectrum of W^TW - (W^*)^TW^* completely determines the population loss.

(b) Suppose that, the spectrum of (W^*)^TW^* is tightly concentrated around a value \kappa, that is, for some sufficiently small \epsilon > 0, \sigma((W^*)^TW^*) \subset [\kappa - \epsilon, \kappa + \epsilon]. Now, assume the initialization W_0 \in \mathbb{R}^{m \times d} is such that W_0^TW_0 = \kappa I_d, and thus, \sigma(W_0^TW_0 - (W^*)^TW^*) \subset [-\epsilon, \epsilon]. Then, the population loss per equation above can be made small enough (in particular, smaller than the energy barrier stated in the previous section), provided \epsilon > 0 is small enough.

We start with the following auxiliary result from the theory of random matrices, stating that the spectrum of tall random matrices are essentially concentrated:

**Theorem 2.4.** Let A be an m \times d matrix with independent standard normal entries. For every t \geq 0, with probability at least 1 - 2 \exp(-t^2/2), we have:

\[ \sqrt{m} - \sqrt{d} - t \leq \sigma_{\min}(A) \leq \sigma_{\max}(A) \leq \sqrt{m} + \sqrt{d} + t. \]

Namely, sufficiently tall random matrices are approximately isometric embeddings of \mathbb{R}^d into \mathbb{R}^m. Interested reader is referred to [Ver10, Corollary 5.35] (and references therein) for further details.

With Theorem 2.4 at our disposal, we provide the following result, a high probability guarantee for the cost of a particular choice of initialization:
Theorem 2.5. Let $W^* \in \mathbb{R}^{m \times d}$ be a random matrix with iid standard normal entries, and let the initial weight matrix $W_0 \in \mathbb{R}^{m \times d}$ be such that, $(W_0)_{i,i} = \sqrt{m + 4d}$ for $1 \leq i \leq d$, and $(W_0)_{i,j} = 0$ otherwise (hence, $W_0^T W_0 = \gamma I_d$ with $\gamma = m + 4d$). Recall that,

$$\mathcal{L}(W) = \mathbb{E}[(f(W; X) - f(W^*; X))^2],$$

where the expectation is taken with respect to the randomness in the fresh sample $X \sim \mathcal{N}(0, I_d)$. Then, provided $m > Cd^2$ for some absolute constant $C > 0$,

$$\mathcal{L}(W_0) < \min_{W \in \mathbb{R}^{m \times d}} \mathcal{L}(W), \quad \text{rank}(W) \leq d-1$$

with probability at least $1 - \exp(-\Omega(d))$, where the probability is with respect to the draw of $W^*$.

The proof of this theorem is provided in Section 3.4. With this, we now turn our attention to the number of training samples required to learn such models.

2.3 Critical Number of Training Samples

Our next focus is on the number of training samples required for controlling the generalization error. In particular we focus on the following question: is there a necessary and sufficient condition on the training data under which any minimizer of the empirical loss (which, in the case of planted weights, necessarily interpolates the data) has zero generalization error? A natural follow-up question is: what is the smallest number $n^*$ of training samples, such that (randomly generated) training data $X_1, \ldots, X_n$ satisfies the aforementioned condition, if there is any such, so long as $n \geq n^*$?

Our first result provides an affirmative answer to the first question, and provides a geometric condition on the training data under which any minimizer of the empirical risk is necessarily a minimizer of the population risk.

Theorem 2.6. Let $X_1, \ldots, X_n \in \mathbb{R}^d$ be a set of data.

(a) Suppose

$$\text{span}\{X_i X_i^T : 1 \leq i \leq n\} = \mathcal{S},$$

where $\mathcal{S}$ is the set of all $d \times d$ symmetric real-valued matrices. Then for any $W \in \mathbb{R}^{m \times d}$ interpolating the data, that is $f(W^*; X_i) = f(W; X_i)$ for every $i \in [n]$, it holds that $W = Q W^*$ for some orthonormal matrix $Q \in \mathbb{R}^{m \times m}$.

(b) Suppose,

$$\text{span}\{X_i X_i^T : 1 \leq i \leq n\},$$

is a strict subset of $\mathcal{S}$. Then, for any $W^* \in \mathbb{R}^{m \times d}$ with $\text{rank}(W^*) = d$, there exists a $W \in \mathbb{R}^{m \times d}$ such that $W^T W \neq (W^*)^T W^*$, while $W$ interpolates the data, that is, $f(W^*; X_i) = f(W; X_i)$ for all $i \in [n]$. In particular, for this $W \in \mathbb{R}^{m \times d}$, $\mathcal{L}(W) > 0$, where $\mathcal{L}$ is defined with respect to any jointly continuous distribution on $\mathbb{R}^d$. 
The proof of Theorem 2.6 is deferred to Section 3.5.

Note that, there is no randomness in the setting of Theorem 2.6, and it provides a purely geometric necessary and sufficient condition for the following: As long as \( \text{span}(X_iX_i^T : i \in [n]) = \mathcal{S} \) is the space of all symmetric matrices (in \( \mathbb{R}^{d \times d} \)) we have that any (global) minimizer of the empirical risk has zero generalization error. Conversely, in the absence of this geometric condition, there are optimizers \( W \in \mathbb{R}^{m \times d} \) of the empirical risk \( \mathcal{L}() \) such that while \( \mathcal{L}(W) = 0 \), the generalization error of \( W \) is bounded away from zero, that is, \( W^TW \neq (W^*)^TW^* \). Soon in Theorem 2.9, we give a more refined version of this result, with a concrete lower bound on \( \mathcal{L}(W) \), in the more realistic setting, where the training data is generated randomly.

We note that Theorem 2.6 still remains valid under a slightly more general setup, where each node \( j \in [m] \) has an associated positive but otherwise arbitrary output weight \( a_j^* \in \mathbb{R}_+ \).

**Corollary 2.7.** Let \( W \in \mathbb{R}^{m \times d}, a \in \mathbb{R}_+^m \), and \( \hat{f}(a,W,X) \) be the function computed by the neural network with input \( X \in \mathbb{R}^d \), quadratic activation function, planted weights \( W \in \mathbb{R}^{m \times d} \), and output weights \( a \in \mathbb{R}_+^m \), that is, \( \hat{f}(a,W,X) = \sum_{j=1}^{m} a_j(W_j,X)^2 \). Let \( X_1, \ldots, X_n \in \mathbb{R}^d \) be a set of data.

(a) Suppose,
\[
\text{span}\{X_iX_i^T : 1 \leq i \leq n \} = \mathcal{S}.
\]
Then for any \( (a,W) \in \mathbb{R}_+^m \times \mathbb{R}^{m \times d} \) interpolating the data, that is \( \hat{f}(a^*,W^*,X_i) = \hat{f}(a,W,X_i) \) for every \( i \in [n] \), it holds that \( \hat{f}(a,W,X) = \hat{f}(a^*,W^*,X) \) for every \( X \in \mathbb{R}^d \). In particular, \( (a,W) \) achieves zero generalization error.

(b) Suppose
\[
\text{span}\{X_iX_i^T : 1 \leq i \leq n \}
\]
is a strict subset of \( \mathcal{S} \). Then, for any \( (a^*,W^*) \in \mathbb{R}_+^m \times \mathbb{R}^{m \times d} \), there is a pair \( (a,W) \in \mathbb{R}_+^m \times \mathbb{R}^{m \times d} \), such that while \( (a,W) \) interpolates the data, that is, \( \hat{f}(a,W,X_i) = \hat{f}(a^*,W^*,X_i) \) for every \( i \in [n] \), \( (a,W) \) has strictly positive generalization error, with respect to any jointly continuous distribution on \( \mathbb{R}^d \).

The proof of this corollary is deferred to Section 3.6.

The next result establishes sufficient conditions under which (randomized) data enjoys the geometric condition of Theorem 2.6, thereby answering the second question in the opening.

**Theorem 2.8.** Let \( n^* = d(d + 1)/2 \), and \( X_1, \ldots, X_n \in \mathbb{R}^d \) be iid random vectors with jointly continuous distribution. Then,

(a) If \( n \geq n^* \), then \( \mathbb{P}(\text{span}(X_iX_i^T : i \in [n]) = \mathcal{S}) = 1 \).

(b) If \( n < n^* \), then for arbitrary \( Z_1, \ldots, Z_n \in \mathbb{R}^d \), \( \text{span}(Z_iZ_i^T : i \in [n]) \subsetneq \mathcal{S} \).

The proof of Theorem 2.8 is deferred to Section 3.7.

The critical number \( n^* \) is obtained to be \( d(d + 1)/2 \) since \( \text{dim}(\mathcal{S}) = \binom{d}{2} + d = d(d + 1)/2 \). Note also that, with this observation, part (b) of Theorem 2.8 is trivial, since we do not have enough number of matrices to span the space \( \mathcal{S} \).

In particular, combining Theorems 2.6 and 2.8, we will obtain the following result:
Theorem 2.9. Let \( X_i, 1 \leq i \leq n \) be i.i.d. with jointly continuous distribution on \( \mathbb{R}^d \). Let the corresponding outputs \( (Y_i)_{i=1}^n \) be generated via \( Y_i = f(W^*; X_i) \), with \( W^* \in \mathbb{R}^{m \times d} \) with \( \text{rank}(W^*) = d \). Then,

(a) Suppose \( n \geq n^* \). Then with probability one over the training data \( X_1, \ldots, X_n \), if \( W \in \mathbb{R}^{m \times d} \) is such that \( f(W; X_i) = Y_i \) for every \( i \in [n] \), then \( f(W; X) = f(W^*; X) \) for every \( X \in \mathbb{R}^d \).

(b) Suppose \( X_i, 1 \leq i \leq n \) are i.i.d. with \( \mathcal{N}(0, I_d) \) distribution. If \( n < n^* \), then there exists a \( W \in \mathbb{R}^{m \times d} \) such that \( f(W; X_i) = Y_i \) for every \( i \in [n] \), yet the generalization error satisfies

\[
\mathcal{L}(W) \geq 2 \sigma_{\min}(W^*)^4.
\]

Theorems 2.6 and 2.8 together provide the necessary and sufficient number of data points for training a shallow neural network with quadratic activation function so as to guarantee good generalization property.

3 Proofs

In this section, we present the proofs of the main results of this paper. Some of our results use the following auxiliary results:

Theorem 3.1. [CT05] Let \( \ell \) be an arbitrary positive integer; and \( P : \mathbb{R}^\ell \to \mathbb{R} \) be a polynomial. Then, either \( P \) is identically 0, or \( \{ x \in \mathbb{R}^\ell : P(x) = 0 \} \) has zero Lebesgue measure, namely, \( P(x) \) is non-zero almost everywhere.

Theorem 3.2. [HJ12, Theorem 7.3.11] For two matrices \( A, B \in \mathbb{R}^{m \times d} \), \( A^T A = B^T B \) if and only if \( A = Q B \) for some orthonormal matrix \( Q \in \mathbb{R}^{m \times m} \).

3.1 Proof of Theorem 2.1

First, we have

\[
f(W; X) - f(W^*; X) = X^T ((W^*)^T W^* - W^T W) X \triangleq X^T A X,
\]

where \( A = (W^*)^T W^* - W^T W \in \mathbb{R}^{d \times d} \) is a symmetric matrix. In particular, \( A \) admits a diagonalization \( A = Q \Lambda Q^T \) with \( Q \in \mathbb{R}^{d \times d} \) an orthonormal matrix, and \( \Lambda \in \mathbb{R}^{d \times d} \) is a diagonal matrix.

(a) Recall Theorem 3.1. In particular, if \( \mathcal{L}(W) = 0 \), then we have \( P(X) = X^T A X = 0 \) almost surely. Since \( P(\cdot) : \mathbb{R}^d \to \mathbb{R} \) a polynomial, it then follows that \( P(X) = 0 \) identically. Now, since \( A \) is symmetric, it has real eigenvalues, called \( \lambda_1, \ldots, \lambda_d \) with corresponding (real) eigenvectors \( \xi_1, \ldots, \xi_d \). Now, taking \( X = \xi_i \), we have \( X^T A X = \xi_i^T A \xi_i = \lambda_i \langle \xi_i, \xi_i \rangle = 0 \). Since \( \xi_i \neq 0 \), we get \( \lambda_i = 0 \) for any \( i \). Finally, since \( A = Q \Lambda Q^T \), it must necessarily be the case that \( A = 0 \). Hence, \( W^T W = (W^*)^T W^* \), which imply \( W = Q W^* \) for some \( Q \in \mathbb{R}^{m \times m} \) orthonormal, per Theorem 3.2.
(b) Recall the diagonalization: \( A = Q\Lambda Q^T \), where \( Q \in \mathbb{R}^{d \times d} \) is an orthonormal matrix. Then, \( Y \triangleq QX \triangleq N(0, I_d) \). Hence,
\[
f(W; X) - f(W^*; X) = X^TQ\Lambda Q^TX = Y^T\Lambda Y = \sum_{i=1}^{d} \lambda_i Y_i^2,
\]
where \( \lambda_1, \ldots, \lambda_d \) are the eigenvalues of the matrix \( A = (W^*)^TW^* - W^TW \). Thus,
\[
\mathbb{E}[(Y^T\Lambda Y)^2] = \mathbb{E} \left[ \sum_{i=1}^{d} \lambda_i^2 Y_i^4 + 2 \sum_{1 \leq i < j \leq d} \lambda_i \lambda_j Y_i^2 Y_j^2 \right] = 2 \sum_{i=1}^{d} \lambda_i^2 + \left( \sum_{i=1}^{d} \lambda_i \right)^2,
\]
using the fact that, \( Y_1, \ldots, Y_d \) are iid standard normal.

Now, fix any \( W \in \mathbb{R}^{m \times d} \) with \( \text{rank}(W) < d \). Let \( a_1 \geq \cdots \geq a_d \) be the eigenvalues of \( (W^*)^TW^* \); \( b_1 \geq \cdots \geq b_d \) be the eigenvalues \( -W^TW \); and \( \lambda_1 \geq \cdots \geq \lambda_d \) be the eigenvalues of \( (W^*)^T W^* - W^TW \). Since \( W \) is rank-deficient, we have \( b_1 = 0 \). Furthermore, \( a_d = \sigma_{\text{min}}(W^*)^2 \), since the eigenvalues of \( (W^*)^TW^* \) are precisely the squares of the singular values of \( W^* \). Now, recall the (Courant-Fischer) variational characterization of the eigenvalues [HJ12]. If \( M \) is a \( d \times d \) matrix with eigenvalues \( c_1 \geq \cdots \geq c_d \), then:

\[
c_1 = \max_{x: \|x\|_2 = 1} x^TMx \quad \text{and} \quad c_d = \min_{x: \|x\|_2 = 1} x^TMx.
\]

With this, fix an \( x \in \mathbb{R}^d \) with \( \|x\|_2 = 1 \). Then,
\[
x^T((W^*)^TW^* - W^TW)x \geq \min_{x: \|x\|_2 = 1} x^T(W^*)^TW^*x + x^T(-W^TW)x = a_d + x^T(-W^TW)x.
\]

Since this inequality holds for every \( x \) with \( \|x\|_2 = 1 \), we can take the max over all \( x \), and arrive at,
\[
\lambda_1 = \max_{x: \|x\|_2 = 1} x^T((W^*)^TW^* - W^TW)x \geq a_d + b_1 = a_d \geq \sigma_{\text{min}}(W^*)^2.
\]

Therefore,
\[
\varphi(W) = 2 \sum_{i=1}^{d} \lambda_i^2 + \left( \sum_{i=1}^{d} \lambda_i \right)^2 \geq 2\lambda_1^2 \geq 2\sigma_{\text{min}}(W^*)^4,
\]
as claimed.

(c) Let the eigenvalues of \( (W^*)^TW^* \) be denoted by \( \lambda_1^*, \ldots, \lambda_d^* \), with the corresponding orthogonal eigenvectors \( q_1^*, \ldots, q_d^* \). Namely, diagonalize \( (W^*)^TW^* \) as \( Q^* \Lambda^*(Q^*)^T \) where the columns of \( Q^* \in \mathbb{R}^{d \times d} \) are \( q_1^*, \ldots, q_d^* \), and \( \Lambda^* \in \mathbb{R}^{d \times d} \) is a diagonal matrix with \( (\Lambda^*)_{i,i} = \lambda_i^* \) for every \( 1 \leq i \leq d \). Let
\[
W = \sum_{j=1}^{d-1} \sqrt{\lambda_j^*} q_j^*(q_j^*)^T \in \mathbb{R}^{d \times d}.
\]

Observe that, \( W^TW = Q^*\Lambda Q^* \), where \( \Lambda \in \mathbb{R}^{d \times d} \) is a diagonal matrix with \( (\Lambda)_{i,i} = (\Lambda^*)_{i,i} \) for every \( 1 \leq i \leq d-1 \), and \( (\Lambda)_{d,d} = 0 \); and that, \( \text{rank}(W) = d - 1 \). Now, let \( W_1, \ldots, W_d \in \mathbb{R}^d \) be the rows of \( W \), and fix a \( j \in [d] \) such that \( W_j \neq 0 \).
Having constructed a $W \in \mathbb{R}^{d \times d}$, we now prescribe $W \in \mathbb{R}^{m \times d}$ as follows. For $1 \leq i \leq d$, $i \neq j$, let $W_i = W_{i,i}$, where $W_i$ is the $i$th row of $W$. Then set $W_j = \frac{1}{2}W_j$, and for every $d + 1 \leq i \leq m$, set $W_i = \frac{\sqrt{3}}{2\sqrt{m-d}}W_j$. For this matrix, we now claim

$$W^T W = \overline{W}^T \overline{W}.$$ 

To see this, fix an $X \in \mathbb{R}^d$, and recall that $X^T W^T W X - X^T \overline{W}^T \overline{W} X = \|WX\|^2_2 - \|\overline{W}X\|^2_2$. We now compute this quantity more explicitly:

$$\|WX\|^2_2 - \|\overline{W}X\|^2_2 = \sum_{k=1}^d \langle W_k, X \rangle^2 - \sum_{k=1}^m \langle \overline{W}_k, X \rangle^2$$

$$= \sum_{k=1, k \neq j}^d \langle W_k, X \rangle^2 + \langle W_j, X \rangle^2 - \sum_{k=1, k \neq j}^d \langle W_k, X \rangle^2 - \left( \frac{1}{2} \right) \langle W_j, X \rangle^2 - \sum_{k=d+1}^m \langle \frac{\sqrt{3}}{2\sqrt{m-d}}W_j, X \rangle^2$$

$$= \langle W_j, X \rangle^2 - \frac{1}{4} \langle W_j, X \rangle^2 - \frac{3}{4(m-d)} (m-d) \langle W_j, X \rangle^2 = 0.$$ 

Hence, for every $X \in \mathbb{R}^d$, we have:

$$X^T W^T W X = X^T \overline{W}^T \overline{W} X.$$ 

Now let $\Xi = W^T W - \overline{W}^T \overline{W}$. Note that $\Xi \in \mathbb{R}^{d \times d}$ is symmetric, and $X^T \Xi X = 0$ for every $X \in \mathbb{R}^d$. Now, taking $X$ to be $e_i$, that is, the $i$th element of the standard basis for the Euclidean space $\mathbb{R}^d$, we deduce $\Xi_{i,i} = 0$ for every $i \in [d]$. For the off-diagonal entries, let $X = e_i + e_j$. Then, $X^T \Xi X = \Xi_{i,j} + \Xi_{j,i} + \Xi_{j,j} + \Xi_{i,i} = 0$, which, together with the fact that the diagonal entries of $\Xi$ are zero, imply $\Xi_{i,j} = -\Xi_{j,i}$; namely $\Xi$ is skew-symmetric.

Finally, since $\Xi$ is also symmetric we have $\Xi_{i,j} = \Xi_{j,i}$, which then implies for every $i, j \in [d]$, $\Xi_{i,j} = 0$, that is, $\Xi = 0$, and thus, $W^T W = \overline{W}^T \overline{W}$.

Hence, we have for $W \in \mathbb{R}^{m \times d}$ with rank($W$) = $d - 1$,

$$W^T W - (W^*)^T W^* = Q^* \Lambda' (Q^*)^T,$$

with $(\Lambda')_{i,i} = 0$ for every $1 \leq i \leq d - 1$; and $(\Lambda')_{d,d} = -\lambda'_d$. Using part $(b)$ of the theorem, we then have:

$$\mathcal{L}(W) = 2 \sum_{i=1}^d (\Lambda')_{i,i}^2 + \left( \sum_{i=1}^d (\Lambda)_{i,i} \right)^2 = 3(\lambda'_d)^2 = 3\sigma_{\min}(W^*)^4.$$ 

Therefore, the lower bound is tight, up to a multiplicative constant.
3.2 Proof of Corollary 2.2

Let $W \in \mathbb{R}^{n \times d}$, and $\tilde{f}(W; X) = \sum_{j=1}^{m} \tilde{a}(W_j, X)$ where \( \tilde{a}(x) = \alpha x^2 + \beta x + \gamma \). Now, note the decomposition: $\tilde{f}(W; X) = \alpha f(W; X) + \beta g(W; X) + \gamma m$, where $f(W; X) = \sum_{j=1}^{m} W_j^2$ and $g(W; X) = \sum_{j=1}^{m} (W_j, X_j)$. In particular, defining:

$$
\Delta_f = f(W; X) - f(W^*; X) \quad \text{and} \quad \Delta_g = g(W; X) - g(W^*; X),
$$

we have $(\tilde{f}(W; X) - \tilde{f}(W^*; X))^2 = (\alpha \Delta_f + \beta \Delta_g)^2 \geq \alpha^2 \Delta_f^2 + 2\alpha \beta \Delta_f \Delta_g$. Taking expectations on both sides with respect to $X \sim \mathcal{N}(0, I_d)$, we then have:

$$
\bar{\mathcal{L}}(W) \geq \alpha^2 \mathcal{L}(W) + 2\alpha \beta \mathbb{E}[\Delta_f \Delta_g] = \alpha^2 \mathcal{L}(W) + 2\alpha \beta \sum_{1 \leq i, j, k \leq d} \mathbb{E}[X_i X_j X_k] A_{ij} \theta_k = \alpha^2 \mathcal{L}(W), \quad (2)
$$

where $\mathcal{L}(W)$ is the quantity defined in Theorem 2.1, $A = W^T W - (W^*)^T W^*$, and $\theta_k = \sum_{j=1}^{m} W_{j,k} - W_{j,k}^*$. Taking the minimum over all rank deficient matrices in Equation (2), we arrive at:

$$
\min_{W \in \mathbb{R}^{n \times d}: \text{rank}(W) < d} \bar{\mathcal{L}}(W) \geq \min_{W \in \mathbb{R}^{n \times d}: \text{rank}(W) < d} \mathcal{L}(W) \geq 2\alpha^2 \sigma_{\text{min}}(W^*)^4,
$$

where the second inequality is due to Theorem 2.1 (b).

3.3 Proof of Theorem 2.3

3.3.1 Step 1: Computing the Gradient Explicitly

Fix a $k_0 \in [m]$ and $\ell_0 \in [d]$. Note that, $\nabla_{k_0, \ell_0} \mathcal{L}(W) = \mathbb{E}[\nabla_{k_0, \ell_0} (f(W^*; X) - f(W; X))^2]$, using dominated convergence theorem. Call $(f(W^*; X) - f(W; X))^2 = \phi(W)$. Next, $\mathbb{E}[\nabla_{k_0, \ell_0} \phi(W)] = 0$ implies that, for every $k_0 \in [m]$ and $\ell_0 \in [d]$:

$$
\sum_{j=1}^{m} \mathbb{E}[(W_j^*, X)^2 \langle W_{k_0}, X \rangle X_{\ell_0}] = \sum_{j=1}^{m} \mathbb{E}[(W_j, X)^2 \langle W_{k_0}, X \rangle X_{\ell_0}] .
$$

Now, recall that, if $Z \sim \mathcal{N}(0, 1)$, then $\mathbb{E}[Z^4] = 3$, and if $Z' \sim \mathcal{N}(0, 1)$ independent of $Z$, then $\mathbb{E}[Z^2 Z'^2] = 1$. Next, note that, $\sum_{j=1}^{m} \mathbb{E}[(W_j^*, X)^2 \langle W_{k_0}, X \rangle X_{\ell_0}]$ computes as,

$$
3 \sum_{j=1}^{m} (W_j^*)^2 W_{k_0, \ell_0} + \sum_{j=1}^{m} \sum_{1 \leq \ell \leq d, \ell \neq \ell_0} W_{k_0, \ell_0} (W_j^*)^2 + 2 \sum_{j=1}^{m} \sum_{1 \leq \ell \leq d, \ell \neq \ell_0} W_{k_0, \ell} W_{j, \ell}^* W_{j, \ell}^* .
$$

We now put this object into a more convenient form. Notice that the expression above is

$$
\sum_{j=1}^{m} \sum_{\ell=1}^{d} W_{k_0, \ell_0} (W_j^*)^2 + 2 \sum_{j=1}^{m} \sum_{\ell=1}^{d} W_{k_0, \ell} W_{j, \ell_0} W_{j, \ell}^* = W_{k_0, \ell_0} ||W^*||_F^2 + 2 \sum_{j=1}^{m} \sum_{\ell=1}^{d} W_{k_0, \ell} W_{j, \ell_0} W_{j, \ell}^* .
$$

We now study the second object. Recall that $W_i^*$ is the $i$th row $W^*$. Observe that, $\sum_{j=1}^{m} W_{j, \ell_0} W_{j, \ell}^* = ((W^*)^T W^*)_{\ell_0, \ell}$. Hence,

$$
\sum_{j=1}^{m} \sum_{\ell=1}^{d} W_{k_0, \ell} W_{j, \ell_0} W_{j, \ell}^* = \sum_{\ell=1}^{d} W_{k_0, \ell} W_{j, \ell_0} W_{j, \ell}^* = \sum_{\ell=1}^{d} W_{k_0, \ell} ((W^*)^T W^*)_{\ell_0, \ell} = (W((W^*)^T W^*))_{k_0, \ell_0} .
$$
Hence, we have, for every \(k_0 \in [m]\) and \(\ell_0 \in [d]\):
\[
\sum_{j=1}^{m} \mathbb{E}[\langle W_j^*, X \rangle^2 \langle W_{k_0}, X \rangle X_{\ell_0}] = W_{k_0, \ell_0} \|W^*\|_F^2 + 2(W((W^*)^T W^*))_{k_0, \ell_0}.
\]

In particular, stationarity yields:
\[
W\|W^*\|_F^2 + 2W((W^*)^T W^*) = W\|W\|_F^2 + 2W(W^T W),
\tag{3}
\]
where an entrywise equality is converted into equality of two matrices, by varying \(k_0 \in [m]\) and \(\ell_0 \in [d]\).

### 3.3.2 Step 2: Study of the Stationarity Equation

Now, let \(W \in \mathbb{R}^{m \times d}\) be a stationary point with \(\text{rank}(W) = d\). We first establish \(\|W\|_F = \|W^*\|_F\).

Since \(W \in \mathbb{R}^{m \times d}\) is a stationary point, it holds that for every \((k_0, \ell_0) \in [m] \times [d]\), \(\nabla_{k_0, \ell_0} \mathcal{L}(W) = 0\).

In particular, Equation (3) holds, which then yields:
\[
W_{k_0, \ell_0}(\|W^*\|_F^2 - \|W\|_F^2) = 2(W(W^T W - (W^*)^T W^*))_{k_0, \ell_0} \quad \forall k_0 \in [m], \ell_0 \in [d].
\tag{4}
\]

Let \(\gamma = \frac{\|W^*\|_F^2 - \|W\|_F^2}{2} \in \mathbb{R}\). We claim \(\gamma = 0\). Note that, as a consequence of (4), we have:
\[-\gamma W = W((W^*)^T W^* - W^T W) \iff W(-\gamma I_d) = W((W^*)^T W^* - W^T W),
\]
where \(I_d \in \mathbb{R}^{d \times d}\) is identity matrix of dimension \(d\). Since \(W\) is full rank, it follows from the rank-nullity theorem that \(\ker(W)\) is trivial, that is, \(\ker(W) = \{0\}\). Hence, for matrices \(M_1, M_2\) (with matching dimensions), whenever \(WM_1 = WM_2\) holds, we deduce \(M_1 = M_2\), since each column of \(M_1 - M_2\) is contained in \(\ker(W)\). Thus, it follows that,
\[-\gamma I_d = (W^*)^T W^* - W^T W.
\]

Now, taking the traces of both sides, together with the fact that \(\text{trace}(W^T W) = \|W\|_F^2\) for any matrix \(W\), and \(\text{trace}(-\gamma I_d) = -d \gamma\), we have:
\[-d \gamma = \text{trace}((W^*)^T W^* - W^T W) = \text{trace}((W^*)^T W^*) - \text{trace}(W^T W) = \|W^*\|_F^2 - \|W\|_F^2 = 2 \gamma,
\]

namely, \(\gamma = 0\). In particular, using the hypothesis \(\nabla_{k_0, \ell_0} \mathcal{L}(W) = 0\) for every \(k_0 \in [m], \ell_0 \in [d]\), we conclude that \(W((W^*)^T W^*) = W(W^T W)\). Now, since \(\text{rank}(W) = d\) and thus \(\ker(W)\) is trivial (namely, \{0\}), the matrix \((W^*)^T W^* - W^T W\) is a zero matrix. Hence, \(W = QW^*\) for some orthonormal \(Q \in \mathbb{R}^{m \times m}\) per Theorem 3.2, and \(\mathcal{L}(W) = 0\).

### 3.4 Proof of Theorem 2.5

Let \(t = \sqrt{d}\). Then, using Theorem 2.4, it holds that with probability \(1 - 2 \exp(-d/2)\):
\[
\sqrt{m} - 2\sqrt{d} \leq \sigma_{\min}(W^*) \leq \sigma_{\max}(W^*) \leq \sqrt{m} + 2\sqrt{d}
\]
\[
\Rightarrow m + 4d - 4\sqrt{md} \leq \lambda_{\min}((W^*)^T W^*) \leq \lambda_{\max}((W^*)^T W^*) \leq m + 4d + 4\sqrt{md}.
\]

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Recall that $\sigma(A)$ denotes the spectrum of $A$, i.e., $\sigma(A) = \{\lambda : \lambda$ is an eigenvalue of $A\}$. We claim then the spectrum of $\gamma I - A$ is $\gamma - \sigma(A)$. To see this, simply note the following line of reasoning:

\[ \gamma - \lambda \in \sigma(\gamma I - A) \iff \det((\gamma - \lambda)I - (\gamma I - A)) = 0 \iff \det(\lambda I - A) = 0 \iff \lambda \in \sigma(A). \]

Now, let $W_0 \in \mathbb{R}^{m \times d}$ be such that $W_0^T W_0 = \gamma I$ with $\gamma = m + 4d$. In particular, if $\lambda_1 \leq \cdots \leq \lambda_d$ are the eigenvalues of $\gamma I - (W^*)^TW^*$ with $\gamma = m + 4d$; then, it holds that:

\[ -4\sqrt{md} \leq \lambda_1 \leq \cdots \leq \lambda_d \leq 4\sqrt{md}. \]

Now, recall by the proof of Theorem 2.1 that,

\[ \mathcal{L}(W_0) = 2 \sum_{i=1}^{d} \lambda_i^2 + \left( \sum_{i=1}^{d} \lambda_i \right)^2, \quad \text{where} \quad \sigma(W_0^T W_0 - (W^*)^TW^*) = \{\lambda_1, \ldots, \lambda_d\}. \]

We immediately have, $2 \sum_{i=1}^{d} \lambda_i^2 \leq 32md^2$. For the second term, note first that, if $\lambda'_1 \leq \cdots \leq \lambda'_d$ are the eigenvalues of $(W^*)^TW^*$, then

\[ \sum_{k=1}^{d} \lambda'_k = \text{trace}((W^*)^TW^*) = \sum_{i=1}^{m} \sum_{j=1}^{d} (W^*_{ij})^2 \Rightarrow \sum_{k=1}^{d} (\lambda'_k - m) = \sum_{i=1}^{m} \sum_{j=1}^{d} ((W^*_{ij})^2 - 1), \]

where $W^*_{ij} \equiv \mathcal{N}(0,1)$ iid. Note also that, $(W^*_{ij})^2 - 1$ is a centered random variable, and has sub-exponential tail, see [Ver10, Lemma 5.14]. Now, letting $Z_{ij} = (W^*_{ij})^2 - 1$, and applying the Bernstein-type inequality [Ver10, Proposition 5.16], we have that for some absolute constants $K, c > 0$, it holds:

\[ \mathbb{P}\left( \left| \sum_{i=1}^{m} \sum_{j=1}^{d} Z_{ij} \right| > d\sqrt{m} \right) \leq 2 \exp\left( -c \min\left( \frac{d}{K^2}, \frac{d\sqrt{m}}{K} \right) \right) \leq 2 \exp(-cd/K^2) = \exp(-\Omega(d)), \]

for $m$ sufficiently large. In particular, with probability at least $1 - \exp(-\Omega(d))$, it therefore holds that,

\[ \left| \sum_{k=1}^{d} (\lambda'_k - m) \right| \leq d\sqrt{m}. \]

Finally, using triangle inequality,

\[ \left| \sum_{k=1}^{d} \lambda_k \right| = \left| \sum_{k=1}^{d} (\lambda'_k - (m + 4d)) \right| \leq \left| \sum_{k=1}^{d} (\lambda'_k - m) \right| + 4d^2 \leq d\sqrt{m} + 4d^2, \]

with probability $1 - \exp(-\Omega(d))$. After squaring, we obtain a bound $16d^4 + 8d^3\sqrt{m} + d^2m$, and using $m > C'd^2$, this term is at most:

\[ \frac{16}{C^2}m^2 + \frac{8}{C^{3/2}}m^2 + \frac{1}{C}m^2 = C'm^2, \]
for some constant $C'$, which converges to 0 as $C \to +\infty$. Next, observe that, $\sqrt{m} - 2\sqrt{d} \geq \frac{1}{2}\sqrt{m}$ for $m$ large (in the regime $m > Cd^2$, with $C$ large enough). Thus, using what we have established in Theorem 2.1, we arrive at:

$$\min_{W \in \mathbb{R}^{m \times d}} \mathcal{L}(W) > 2\sigma_{\min}(W^*)^4 \geq (\sqrt{m} - 2\sqrt{d})^4 \geq \frac{1}{16}m^2.$$  

Provided, 

$$\frac{1}{2} > C'(C) = \frac{16}{C^2} + \frac{8}{C^{3/2}} + \frac{1}{C},$$

that is, provided $C$ is sufficiently large, we have the claim.

### 3.5 Proof of Theorem 2.6

(a) Let $\text{span}(X_i^T : i \in [n]) = \mathcal{S}$, the set of all $d \times d$ symmetric matrices, and let $M \in \mathcal{S}$ be such that for any $i$, $X_i^T MX_i = 0$. We will establish $M = 0$. Let $1 \leq k, \ell \leq d$ be two fixed indices. To that end, let $\theta^{(k,\ell)}_i \in \mathbb{R}$ be such that, $\sum_{i=1}^n \theta^{(k,\ell)}_i X_i^T X_i = e^T_k e^T_\ell + e^T_\ell e^T_k$, where the column vectors $e_k, e_\ell \in \mathbb{R}^d$ are respectively the $k^{th}$ and $\ell^{th}$ elements of the standard basis for $\mathbb{R}^d$. Such $\theta^{(k,\ell)}_i$ indeed exist, due to the spanning property. Observe that $2M_{k,\ell} = e^T_k M e_\ell + e^T_\ell M e_\ell = \text{tr}(e^T_k M e_\ell + e^T_\ell M e_\ell)$. Now, using the fact that $\text{tr}(BCA) = \text{tr}(CAB)$ for every matrices $A, B, C$ (with matching dimensions), we have:

$$2M_{k,\ell} = \text{tr}(M e_\ell e^T_k + M e_k e^T_\ell) = \text{tr} \left( \sum_{i=1}^n \theta^{(k,\ell)}_i MX_i X_i^T \right) = \sum_{i=1}^n \theta^{(k,\ell)}_i \text{tr}(X_i^T MX_i) = 0,$$

for every $k, \ell \in [d]$. Finally, if $W$ is such that $\hat{\mathcal{L}}(W) = 0$, then $X_i^T MX_i = 0$ for any $i$, where $M = (W^*)^T W^* - W^T W$. Hence, provided that the geometric condition holds, we have $M = 0$, that is, $W^T W = (W^*)^T W^*$, and thus, $W = QW^*$ for some $Q \in \mathbb{R}^{m \times m}$ orthonormal per Theorem 3.2, and that, it has zero generalization error, i.e. $\mathcal{L}(W) = 0$.

(b) Our goal is to construct a $W \in \mathbb{R}^{m \times d}$ with $f(W^*; X_i) = f(W; X_i)$, for every $i \in [n]$, whereas $W^T W \neq (W^*)^T W^*$. Consider the inner product $\langle A, B \rangle = \text{trace}(AB)$, in the space of all symmetric $d \times d$ matrices. Find $0 \neq M \in \mathbb{R}^{d \times d}$ a symmetric matrix, such that, $M \in \text{span}(X_i^T X_i^T : i \in [n])$, that is, $X_i^T MX_i = 0$ for every $i \in [n]$. We can find such $M$ satisfying $\|M\|_2 = 1$. Consider the linear matrix function $M(\delta) = (W^*)^T W^* + \delta M$. Note that, $M(\delta)$ is symmetric for every $\delta$. We claim that under the hypothesis of the theorem, there exists a $\delta_0 > 0$ such that $M(\delta)$ is positive semidefinite for every $\delta \in [0, \delta_0]$, and that there exists $W_\delta \in \mathbb{R}^{m \times d}$ with $W_\delta^T W_\delta = M(\delta)$, for all $\delta \in [0, \delta_0]$. Observe that, since $\text{rank}(W^*) = d$, then $(W^*)^T W^* \in \mathbb{R}^{d \times d}$ with rank($(W^*)^T W^*) = d$. Therefore, the eigenvalues $\lambda_1^*, \ldots, \lambda_d^*$ of $(W^*)^T W^*$ are all positive. In particular, $\{\lambda_i^* : i \in [d]\} \subset [\delta_1, \infty)$, with $\delta_1 = \sigma_{\min}(W^*)^2$. Now, let $\mu_1(\delta), \ldots, \mu_d(\delta)$ be the eigenvalues of $M(\delta)$. Using Weyl’s inequality [HJ12], we have $|\mu_i(\delta) - \lambda_i^*| \leq \delta \|M\|_2 = \delta$, for every $i$. In particular, taking $\delta \leq \delta_1$, we deduce for every $i \in [d]$, it holds that $\mu_i(\delta) \geq \lambda_i^* - \delta_1 \geq 0$, that is, $\{\mu_i(\delta) : i \in [d]\} \subset [0, \infty)$. In particular, we also have $M(\delta)$ is symmetric, and thus, it is PSD. Thus, there exists a $\overline{W}_\delta \in \mathbb{R}^{d \times d}$ such that $\overline{W}_\delta^T \overline{W}_\delta = M(\delta)$. Now, using the same idea as
in the proof of Theorem 2.1 part (c), we then deduce there exists a matrix $W_δ ∈ \mathbb{R}^{m×d}$ such that $W_δ^TW_δ = W_δ^T W_δ = M(δ)$. In particular, for this $W_δ$, if $f(W_δ, X)$ is the function computed by the neural network with weight matrix $W_δ ∈ \mathbb{R}^{m×d}$, then on the training data $(X_i : i ∈ [n])$, $f(W_δ; X_i) = X_i^T W_δ^T W_δ X_i = X_i^T (W^*)^T W^* X_i = f(W^*; X_i)$, since $X_i^T M X_i = 0$ for all $i ∈ [n]$. At the same time $W_δ^T W_δ - (W^*)^T W^* = δM ≠ 0$, since $δ ≠ 0$ and $M ≠ 0$, and therefore $W_δ^T W_δ ≠ (W^*)^T W^*$.

Finally, to show $\mathcal{L}(W_δ) > 0$, we argue as follows. Suppose $\mathcal{L}(W_δ) = 0$. Then, by Theorem 3.1, it follows that $ψ(X) = X^TA X = 0$ identically, where $A = W_δ^T W_δ - (W^*)^T W^*$. Now, letting $ξ_1, …, ξ_d$ be the eigenvectors of $A$ (with corresponding eigenvalues $λ_1, …, λ_d$), we obtain $ξ_i^TAξ_i = λ_i|ξ_i|^2 = 0$, we namely obtain $λ_i = 0$ for every $i ∈ [d]$. Finally, since $A$ is symmetric, and hence admits a diagonalization of form $A = QΛQ$ with diagonal entries of $Λ$ being zero, we deduce $A$ is identically zero, which contradicts with the fact that $A = δM$, which is a non-zero matrix.

3.6 Proof of Corollary 2.7

The proof relies on the following observation: given any pair $(a^*, W^*) ∈ \mathbb{R}_+^m × \mathbb{R}^{m×d}$, construct a matrix $W^* ∈ \mathbb{R}^{m×d}$ whose $j$th row is $W_j^* = \sqrt{α_j}W_j ∈ \mathbb{R}^d$. Define $W ∈ \mathbb{R}^{m×d}$ similarly as the matrix whose $j$th row is $W_j = \sqrt{α_j}W_j ∈ \mathbb{R}^d$. Now, let $e = (1,1,…,1)^T ∈ \mathbb{R}^m$ be the vector of all ones. Then note that,

$$f(a^*, W^*, X) = \hat{f}(e, W^*, X) = f(W^*, X) \quad \text{and} \quad f(a, W, X) = \hat{f}(e, W^*, X) = f(W, X),$$

where $f(W; X)$ is the same quantity as in Theorem 2.6. Applying Theorem 2.6 then establishes both parts.

3.7 Proof of Theorem 2.8

Recall that, $\mathcal{S} = \{ M ∈ \mathbb{R}^{d×d} : M^T = M \}$. Note that, this space has dimension $d^2 + 1$: for any $1 ≤ k ≤ ℓ ≤ d$, it is easy to see that the matrices $e_k e_k^T + e_1 e_1^T$ are linearly independent; and there are precisely $d^2 + 1$ such matrices. With this in mind, the statement of part (b) is immediate.

We now prove the part (a) of the theorem. For any $X_i$, let $X_i(j)$ be the $j$th coordinate of $X_i$, with $j ∈ [d]$; and let $\mathcal{Y}_i$ be a $d(d+1)/2$-dimensional vector, obtained by retaining $X_i(1)^2,…,X_i(d)^2$; and the products, $X_i(k)X_i(ℓ)$ with $1 ≤ k < ℓ ≤ d$. Now, let $\mathcal{X}$ be an $n × d(d+1)/2$ matrix, whose rows are $\mathcal{Y}_1,…,\mathcal{Y}_n$. Our goal is to establish,

$$\mathbb{P}[\text{det}(\mathcal{X}) = 0] = 0,$$

when $n = d(d+1)/2$, where the probability is taken with respect to the randomness in $X_1,…,X_n$ (in particular, this yields for $n ≥ d(d+1)/2$, $\mathbb{P}(\text{rank}(\mathcal{X}) = d(d+1)/2)$, almost surely). Now, recalling Theorem 3.1, it then suffices to show that $\text{det}(\mathcal{X})$ is not identically zero, when viewed as a polynomial in $X_i(j)$ with $i ∈ [n], j ∈ [d]$.

We now prove part (b) by providing a deterministic construction (of the matrix $\mathcal{X}$) under which $\text{det}(\mathcal{X}) ≠ 0$. Let $p_1 < … < p_d$ be distinct prime numbers. For every $1 ≤ t ≤ n$, set:

$$X_t = (p_t^{l-1},…,p_d^{l-1})^T ∈ \mathbb{R}^d.$$
In particular, $X_1 = (1, 1, \ldots, 1)^T \in \mathbb{R}^d$, which then implies $Y_1$ is a vector of all ones. Now, we study $Y_2$. The entries of $Y_2$, called $z_1, \ldots, z_{d(d+1)/2}$, are of form $p_i^2$ with $i \in [d]$; or $p_ip_j$, where $1 \leq i < j \leq d$. By the fundamental theorem of arithmetic, we have $p_ip_j = p_kp_\ell \Rightarrow \{p_i, p_j\} = \{p_k, p_\ell\}$; and therefore, $z_1, \ldots, z_{d(d+1)/2}$ are pairwise distinct. With this construction, the matrix $X$ is a Vandermonde matrix with determinant:

$$
\prod_{1 \leq k < \ell \leq d(d+1)/2} (z_k - z_\ell).
$$

Since $z_k \neq z_\ell$ for every $k \neq \ell$ (from the construction on $Y_2$, which, in turn, is constructed from $X_2$), this determinant is non-zero, proving the claim.

3.8 Proof of Theorem 2.9

(a) Note that, if $n \geq n^*$, then combining parts (a) of Theorems 2.6 and 2.8, we have that with probability one, $\text{span}(X_iX_i^T : i \in [n]) = S$, which, together with $\hat{L}(W) = 0$, imply that,

$$
\mathbb{P}(E \neq \emptyset) = 0,
$$

where $E = \{W \in \mathbb{R}^{m \times d} : W^TW \neq (W^*)^TW^*; \hat{L}(W) = 0\}$, from which the desired conclusion follows.

(b) Assume $W$ is taken as in proof of Theorem 2.6 (b), that is,

$$(W^*)^TW^* - W^TW = \delta M \quad \text{where} \quad \delta = \sigma_{\text{min}}(W^*)^2 \quad \text{and} \quad \|M\| = 1,$$

with $M^T = M$. Now, running the exact same argument, as in proof of Theorem 2.1, we obtain:

$$
\mathcal{L}(W) = 2 \sum_{i=1}^{d} \lambda_i^2 + \left(\sum_{i=1}^{d} \lambda_i\right)^2,
$$

where $\{\lambda_1, \ldots, \lambda_d\}$ is the spectrum of $\delta M$ with $\delta = \sigma_{\text{min}}(W^*)^2$, and $\|M\| = 1$. From here, we get that,

$$
\mathcal{L}(W) \geq 2\lambda_{\text{max}}(\delta M)^2 = 2\sigma_{\text{min}}(W^*)^4.
$$

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