Spurious Valleys in Two-layer Neural Network Optimization Landscapes

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Abstract

Neural networks provide a rich class of high-dimensional, non-convex optimization problems. Despite their non-convexity, gradient-descent methods often successfully optimize these models. This has motivated a recent spur in research attempting to characterize properties of their loss surface that may explain such success.

In this paper, we address this phenomenon by studying a key topological property of the loss: the presence or absence of spurious valleys, defined as connected components of sub-level sets that do not include a global minimum. Focusing on a class of two-layer neural networks defined by smooth (but generally non-linear) activation functions, we identify a notion of intrinsic dimension and show that it provides necessary and sufficient conditions for the absence of spurious valleys. More concretely, finite intrinsic dimension guarantees that for sufficiently overparametrised models no spurious valleys exist, independently of the data distribution. Conversely, infinite intrinsic dimension implies that spurious valleys do exist for certain data distributions, independently of model overparametrisation. Besides these positive and negative results, we show that, although spurious valleys may exist in general, they are confined to low risk levels and avoided with high probability on overparametrised models.

1 Introduction

Modern machine learning applications involve datasets of increasing dimensionality, complexity and size, which in turn motivate the use of high-dimensional, non-linear models, as illustrated in many deep learning algorithms across computer vision, speech and natural language understanding. The prevalent strategy for learning is to rely on Stochastic Gradient Descent (SGD) methods, that typically operate on non-convex objectives. In this context, an

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outstanding goal is to provide a theoretical framework that explains under what conditions – relating input data distribution, choice of architecture and choice of optimization scheme – this setup will be successful.

More precisely, let \( \Phi_\theta : \mathbb{R}^n \rightarrow \mathbb{R}^m \) denote a model class parametrized by \( \theta \in \Theta \subseteq \mathbb{R}^D \), which in the case of Neural Networks (NNs) contains the aggregated weights across all layers. In a supervised learning setting, this model is deployed on some data \((X, Y)\) random variable taking values in \(\mathbb{R}^n \times \mathbb{R}^m\), to predict targets \(Y\) given features \(X\), and its risk for a given \(\theta\) is

\[
L(\theta) = \mathbb{E}_{(X,Y) \sim P}[\ell(\Phi_\theta(X), Y)]
\]

where \(\ell\) is a convex loss, such as a square loss or a logistic regression loss. In the following we refer to (1) as the risk, the energy or the loss interchangeably. The aim is to find

\[
\theta^* \in \arg \min_{\theta \in \Theta} L(\theta)
\]

and this is attempted in practice by running SGD iteration on the parameter

\[
\theta_{k+1} = \theta_k - \alpha_k \nabla_{\theta=\theta_k} L(\theta)
\]

where \(\{(x_j, y_j)\}_{j=1}^M\) are (i.i.d.) drawn from \(P\). Under some technical conditions, the expected gradient \(\mathbb{E}[\nabla_{\theta=\theta_k} L(\theta)]\) is known to converge to 0 [7]. Understanding the nature of such stationary points - and therefore the landscape of the loss function - is a task of fundamental importance to understand performance of SGD.

Whereas there is a growing literature in analyzing the behavior of SGD on non-convex objectives [43, 28, 25, 44], we focus here on properties of the optimization problem above that are algorithm independent. Many authors in the literature have attempted to characterize the landscape of the loss function (1) by studying its critical points. Global optimality results have been obtained for NN architectures with linear activations [26, 29, 46], quadratic activations [41, 18] and some more general non-linear activations, under appropriate regularity assumptions [42, 34, 20]. Some other insights have been obtained by leveraging tools for complexity analysis of spin glasses [11] and random matrix theory [35]. Other analysis involved studying goodness of the initialization of the parameter values \(\theta_0\) [15, 37, 19] or other topological properties of the loss (1), such as connectivity of sub-level sets [17, 21]. A common factor shared in the above cited works (and in common practice) is that over-parametrisation of the model class (i.e. \(D \gg 1\)) often leads to improved performance, despite the potential increase in generalization error.

Each model defines a functional space \(\text{span}(\{f = \Phi_\theta : \theta \in \Theta\})\), whose complexity a priori increases with the dimensionality \(D\) of the parameter space \(\Theta\). Whereas several authors have studied these models from the lens of approximation theory [13, 12, 3] by focusing on specific aspects of the parameterisation (such as the depth of the network), in this work we explore another hypothesis, namely that over-parameterization remedies the complexity of that functional space, often leading to loss functions \(L(\theta)\) without poor local minima.

Our approach is inspired by Freeman and Bruna [21], and is related to recent work that also explores convexifications of neural networks [1, 47, 4]. Our analysis focuses mostly on the class of two-layer neural networks, with a hidden layer of size \(p\), and covers both empirical
and population risk landscapes. A given activation function $\rho$ determines a functional space $V_\rho = \text{span}(\{x \mapsto \rho(\langle x, w \rangle) : w \in \mathbb{R}^n\})$. In essence, our work identifies notions of intrinsic dimension of this functional space, and establishes the following facts:

1. If the hidden layer size $p$ is at least equal to the upper intrinsic dimension, then the resulting loss landscape is free of poor local minima, independently of the data distribution;

2. If $p$ is smaller than the lower intrinsic dimension, then there exist data distributions yielding arbitrarily poor local minima.

We articulate the notion of poor local minima via what we call spurious valleys, defined as connected components of the sublevel sets that do not contain a global minima. Upper and lower intrinsic dimensions define only two scenarios: either (i) they are both finite, enabling positive results; or (ii) they are both infinite, implying the negative results. Moreover, case (i) only occurs for polynomial activation functions or when the data distribution is discrete, corresponding to generic empirical risk minimization. The negative result covers many classes of activation functions with infinite intrinsic dimension. In particular, they generalize previously known negative results (such as leaky ReLUs) \cite{10, 38} to a far wider class of activations. While in general the upper and lower intrinsic dimension may not match, we show that in some cases (linear and quadratic networks) the gap between the positive and negative results can be closed by improving on the former.

The negative results are worst-case in nature, and leave open the question of how complex is a ‘typical’ energy landscape corresponding to a generic data distribution. We answer this question by showing that, even if spurious valleys may appear in general, they are in practice easily avoided from random initializations, up to a low energy threshold, which approaches the global minimum at a rate inversely proportional to the hidden layer size up to log factors. This fact is shown for networks with homogeneous activations and generic data distributions and it is based on properties of random kernel quadrature rules \cite{2}.

Many other type of analysis of the convergence of NNs gradient-based optimization algorithms have been considered in the literature. For example, Ge et al. \cite{24} proved convergence of GD on a modified loss; Shamir \cite{40} compared optimization properties of residual networks with respect to linear models; in Dauphin et al. \cite{16} it is argued that the issues arising in the optimization of NN architectures are due to the presence of saddle points in the loss function rather than spurious local minima. Optimization landscapes have also been studied in other contexts than from NNs training, such as low rank \cite{22}, matrix completion \cite{23}, problems arising in semidefinite programming \cite{10, 23} and implicit generative modeling \cite{6}.

The rest of the paper is structured as follows. Section 2 formally introduces the notion of spurious valleys and explains why this is a relevant concept from the optimization point of view. It also defines the intrinsic dimensions of a network (Section 2.1). In Section 3 we state our main positive results (Theorem 7) and we discuss two settings where they bear fruit: polynomial activation functions and empirical risk minimization. For the case of linear and quadratic activations, we improve on our general result, by proving that, for the linear case, Theorem 7 holds without any assumptions on the distributions of the data or on the size/rank of any variables (which extends previous results on the optimization of linear NNs \cite{22, 40}), and by recovering, for the quadratic case, results which are in line with current literature \cite{41, 18}. Section 4 is dedicated to constructions of worst case scenarios for activation with
infinite lower intrinsic dimension. We then show, in Section 5, that, even if spurious valleys may exist, they tend to be confined to regimes of low risk. Some discussion is reported in Section 6.

1.1 Notation

We introduce notation we use throughout the rest of the paper. For any integers \( n \leq m \) we denote \([n, m] = \{n, n+1, \ldots, m\}\) and, if \( n > 0 \), \([n] = [1, n]\). We denote scalar valued variables as lowercase non-bold; vector valued variables as lowercase bold; matrix and tensor valued variables as uppercase bold. Given a vector \( \mathbf{v} \in \mathbb{R}^n \), we denote its components as \( v_i \); given a matrix \( \mathbf{W} \in \mathbb{R}^{n \times m} \), we denote its rows as \( \mathbf{w}_i \); given a tensor \( \mathbf{T} \in \mathbb{R}^{n_1 \times \cdots \times n_k} \), we denote its components as \( T_{i_1 \cdots i_k} \). Given some vectors \( \mathbf{v}_i \in \mathbb{R}^{n_i}, i \in [k] \), the tensor product \( \mathbf{v}_1 \otimes \cdots \otimes \mathbf{v}_k \) denotes the \( n_1 \times \cdots \times n_k \) dimensional tensor \( \mathbf{T} \) whose components are given by \( T_{i_1 \cdots i_k} = v_{i_1} \cdots v_{i_k} \); given a vector \( \mathbf{v} \), we denote \( \mathbf{v}^{\otimes k} = \otimes_{i=1}^k \mathbf{v} \). \( \mathbf{I} \) denotes the identity matrix and \( \mathbf{e}_1, \ldots, \mathbf{e}_n \) the standard basis in \( \mathbb{R}^n \). For any random variables (r.v.’s) \( \mathbf{X} \) and \( \mathbf{Y} \) with values in \( \mathbb{R}^n \) and \( \mathbb{R}^m \) respectively, we denote \( \Sigma_{\mathbf{X}} = \mathbb{E}[\mathbf{X}^T \mathbf{X}] \) and \( \Sigma_{\mathbf{XY}} = \mathbb{E}[\mathbf{X} \mathbf{Y}^T] \). For every integer \( n \geq 1 \), we denote by \( \text{GL}(n) \), \( O(n) \) and \( SO(n) \), respectively, the general linear group, the orthogonal group and the special orthogonal group of real \( n \times n \) matrices. We denote by \( S^k(\mathbb{R}^n) \) the space of order \( k \) symmetric tensors on \( \mathbb{R}^n \). For any \( \mathbf{T} \in S^k(\mathbb{R}^n) \), we define the symmetric rank \( \mathbf{r}_S(\mathbf{T}) = \min \{ p \geq 1 : \mathbf{T} = \sum_{i=1}^p \mathbf{u}_i \otimes \mathbf{w}_i^{\otimes k} \text{ for some } \mathbf{u} \in \mathbb{R}^p, \mathbf{w}_1, \ldots, \mathbf{w}_p \in \mathbb{R}^n \} \). We define \( \mathbf{r}_S(k, n) = \max \{ \mathbf{r}_S(\mathbf{T}) : \mathbf{T} \in S^k(\mathbb{R}^n) \} \). Finally, \( S^{n-1} \subset \mathbb{R}^n \) denotes the \((n-1)\)-dimensional sphere \( \{ \mathbf{x} \in \mathbb{R}^n : \| \mathbf{x} \| = 1 \} \).

2 Problem setting

Let \((\mathbf{X}, \mathbf{Y})\) be two r.v.’s. These r.v.’s take values in \( \mathbb{R}^n \) and \( \mathbb{R}^m \) and represent the input and output data, respectively. We consider oracle square loss functions \( L : \Theta \rightarrow \mathbb{R} \) of the form

\[
L(\theta) = \mathbb{E}[\ell(\Phi(\mathbf{X}; \theta), \mathbf{Y})]
\]

where \( \ell : \mathbb{R}^m \times \mathbb{R}^m \rightarrow [0, \infty) \) is convex. For every \( \theta \in \Theta \), the function \( \Phi(\cdot; \theta) : \mathbb{R}^n \rightarrow \mathbb{R}^m \) models the dependence of the output on the input as \( \mathbf{Y} \simeq \Phi(\mathbf{X}; \theta) \). We focus on two-layers NN functions \( \Phi \), i.e. \( \Phi \) of the form

\[
\Phi(\mathbf{x}; \theta) = \mathbf{U}_\rho(\mathbf{Wx})
\]

where \( \theta = (\mathbf{U}, \mathbf{W}) \in \Theta = \mathbb{R}^{m \times p} \times \mathbb{R}^{p \times n} \). Here \( p \) represents the width of the hidden layer and \( \rho : \mathbb{R} \rightarrow \mathbb{R} \) is a continuous element-wise activation function.

The loss function \( L(\theta) \) is (in general) a non-convex object; it may present spurious (i.e. non global) local minima. In this work, we characterize \( L(\theta) \) by determining absence or presence of spurious valleys, as defined below.

**Definition 1.** For all \( c \in \mathbb{R} \) we define the sub-level set of \( L \) as \( \Omega_L(c) = \{ \theta \in \Theta : L(\theta) \leq c \} \). We define a spurious valley as a connected component of a sub-level set \( \Omega_L(c) \) which does not contain a global minimum of the loss \( L(\theta) \).
Since, in practice, the loss (2) is minimized with a gradient descent based algorithm, then absence of spurious valleys is a desirable property, if we wish the algorithm to converge to an optimal parameter. It is easy to see that $L(\theta)$ not having spurious valleys is equivalent to the following property:

P.1 Given any initial parameter $\tilde{\theta} \in \Theta$, there exists a continuous path $\theta : t \in [0, 1] \mapsto \theta_t \in \Theta$ such that:

(a) $\theta_0 = \tilde{\theta}$
(b) $\theta_1 \in \arg \min_{\theta \in \Theta} L(\theta)$
(c) The function $t \in [0, 1] \mapsto L(\theta_t)$ is non-increasing

As pointed out in Freeman and Bruna [21], this implies that $L$ has no strict spurious (i.e. non global) local minima. The absence of generic (i.e. non-strict) spurious local minima is guaranteed if the path $\theta_t$ is such that the function $L(\theta_t)$ is strictly decreasing. For many activation functions used in practice (such as the ReLU $\rho(z) = z_+$), the parameter $\theta$ determining the function $\Phi(\cdot; \theta)$ is determined up to the action of a symmetries group (e.g., in the case of the ReLU, $\rho$ is an positive homogeneous function). This prevents strict minima: for any value of the parameter $\theta \in \Theta$ there exists a (often large) manifold $U_\theta \subset \Theta$ intersecting $\theta$ along which the loss function is constant. Absence of spurious valleys for the loss (2) implies that it is always possible to move from any point in the parameter space to a global minima, without increasing the loss.

2.1 Intrinsic dimension of a network

The main result of this work is to exploit that the property of absence of spurious valleys is related to the complexity of the functional space $V_\rho = \{ f = \Phi(\cdot; \theta) : \theta \in \Theta \}$ defined by the network architecture. We therefore define two measures of such complexity which we will use to show, respectively, positive and negative results in this regard.

To simplify the discussion, we introduce some notation which we will use throughout the rest of the paper. Let $\rho : \mathbb{R} \to \mathbb{R}$ be a continuous activation function. For every $v \in \mathbb{R}^n$ we denote $\psi_{\rho, v}$ to be the function $\psi_{\rho, v} : x \in \mathbb{R}^n \mapsto \rho(\langle v, x \rangle) \in \mathbb{R}$. We refer to each $\psi_{\rho, v}$ as a filter function. If $X$ is a r.v. taking values in $\mathbb{R}^n$, we denote by $L_2^2(X)$ the space of square integrable function on $\mathbb{R}^n$ w.r.t. the probability measure induced by the r.v. $X$. We then define the two following functional spaces:

$$V_{\rho, p} = \{ f = \Phi(\cdot; \theta) : \theta = (u, W) \in \Theta = \mathbb{R}^p \times \mathbb{R}^{p \times n} \}$$

$$R_2(\rho, n) = \{ X \text{ r.v. taking values in } \mathbb{R}^n : \psi_{\rho, v} \in L_2^2(X) \text{ for every } v \in \mathbb{R}^n \}$$

$V_{\rho, p}$ represents the space of (one-dimensional output) functions modeled by the network architecture and $R_2(\rho, n)$ to be the space of (n-dimensional) input data distributions for which the filter functions have finite second moment. We finally define

$$V_\rho = \text{span}(\{ f : f \in V_{\rho, 1} \}) = \bigcup_{p=1}^{\infty} V_{\rho, p}$$

as the linear space spanned by the functions $\psi_{\rho, v}$ for $v \in \mathbb{R}^n$. 
Definition 2. Let \( \rho \) be a continuous activation function and \( X \in \mathcal{R}_2(\rho, n) \) a r.v. We define
\[
\dim^*(\rho, X) = \dim_{L^2_X}(V_{\rho})
\]
as the upper intrinsic dimension of the pair \((\rho, X)\). We define the level \( n \) upper intrinsic dimension of \( \rho \) as \( \dim^*(\rho, n) = \dim(V_{\rho}) = \sup\{\dim^*(\rho, X) : X \in \mathcal{R}_2(\rho, n)\} \).

The upper intrinsic dimension \( \dim^*(\rho, X) \) defined above is therefore the dimension of the functional space spanned by the filter functions \( \psi_{\rho,v} \in L^2_X \) or, equivalently, of the image of the map \( \Phi : \Theta \rightarrow \Phi(\cdot; \theta) \in L^2_X \). Notice that \( \dim^*(\rho, X) \leq \dim(L^2_X) \). In particular, if the distribution \( X \) is discrete, i.e. it is concentrated on a finite number of points \( \{x_1, \ldots, x_N\} \subset \mathbb{R}^n \), then \( \dim^*(\rho, X) \leq \dim(L^2_X) \leq N \). Otherwise, if the distribution \( X \) is not discrete, then \( \dim(L^2_X) = \infty \).

The \( n \) level upper intrinsic dimension \( \dim^*(\rho, n) \) is defined as the dimension of the functional linear space \( V_{\rho} \). We note that if \( X \in \mathcal{R}_2(\rho, n) \) is a r.v. with almost surely (a.s.) positive density w.r.t. the Lebesgue measure \( dx \), then \( \dim^*(\rho, n) = \dim^*(\rho, X) \).

The following lemma exhausts all the cases when the upper intrinsic dimension is not infinite.

Lemma 3. Let \( \rho \) be a continuous activation function and \( X \in \mathcal{R}_2(\rho, n) \) such that \( \dim(L^2_X) = \infty \). If \( \rho(z) = \sum_{k=0}^{d} a_k z^k \) is a polynomial, then
\[
\dim^*(\rho, X) \leq \sum_{i=1}^{d} \binom{n+i-1}{i} 1_{\{a_i \neq 0\}} = O(n^d)
\]
Otherwise (i.e. if \( \rho \) is not a polynomial) it holds \( \dim^*(\rho, X) = \infty \).

We then define the lower intrinsic dimension, which corresponds to the concept of ‘how many hidden neurons are needed to represent a generic function of \( V_{\rho} \).’

Definition 4. Let \( \rho \) be a continuous activation function and \( X \in \mathcal{R}_2(\rho, n) \) a r.v. We define
\[
\dim_*(\rho, X) = \max\left\{ p \geq 1 : V_{\rho,p-1} \subsetneq L^2_X \right\}
\]
as the lower dimension of the pair \((\rho, X)\). We define the level \( n \) lower dimension of \( \rho \) as \( \dim_*(\rho, n) = \max\{p \geq 1 : V_{\rho,p-1} \subsetneq V_{\rho,p}\} = \sup\{\dim_*(\rho, X) : X \in \mathcal{R}_2(\rho, n)\} \).

If \( \dim_*(\rho, X) \) is finite, then it corresponds to the minimum number of hidden neurons which are needed to represent any function of \( V_{\rho} \) with the NN architecture.[3] Clearly, this implies that
\[
\dim_*(\rho, X) \leq \dim^*(\rho, X)
\]
for every continuous activation function \( \rho \) and any \( X \in \mathcal{R}_2(\rho, n) \). As with the upper intrinsic dimension, we note that if \( X \in \mathcal{R}_2(\rho, n) \) is a r.v. with a.s. positive density w.r.t. the Lebesgue measure \( dx \), then \( \dim_*(\rho, n) = \dim_*(\rho, X) \).

In the case of homogenous polynomial activations \( \rho(z) = z^k \) with \( k \geq 1 \) integer, the level \( n \) lower dimension of \( \rho \) coincides with the notion of (maximal) symmetric tensor rank.

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1For any linear subspace \( V \subseteq L^2_X \), \( \dim_{L^2_X}(V) \) denotes the dimension of \( V \) as a subspace of \( L^2_X \).

2For any subsets \( V, W \subseteq L^2_X \), we say that \( V \subseteq L^2_X W \) if \( V \subseteq W \) as subsets of \( L^2_X \) (and similar with other inclusions or equalities).

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Lemma 5. Let $\rho(z) = z^k$, with $k$ positive integer. Then
$$\dim_*(\rho, n) = \text{rk}_S(k, n)$$

Finally, the next lemma implies that for most non-polynomial activation functions practical interest, the lower intrinsic dimension $\dim_*(\rho, n)$ is infinite.

Lemma 6. Let $\rho$ be a continuous activation function such that $\rho \in L^2(\mathbb{R}, e^{-x^2/2} \, dx)$ and $n > 1$. Then $\dim_*(\rho, n) = \infty$ if and only if $\rho$ is not a polynomial.

3 Finite network dimension and absence of spurious valleys

In this section we provide our positive results. Essentially they state that if the width of the network matches the dimension of the functional space $V_\rho$ spanned by its filter functions, then no spurious valleys exist. We first provide the main result (Theorem 7) in a general form, which allows a straight-forward derivation of two cases of interest: empirical risk minimization (Corollary 8) and polynomial activations (Corollary 9).

Theorem 7. For any continuous activation function $\rho$ and r.v. $X \in \mathcal{R}_2(\rho, n)$ with finite upper intrinsic dimension $\dim^*(\rho, X) < \infty$, the loss function
$$L(\theta) = E[\ell(\Phi(X; \theta), Y)]$$

for two-layers NNs $\Phi(x; \theta) = U\rho(Wx)$ admits no spurious valleys in the over-parametrized regime $p \geq \dim^*(\rho, X)$.

The above result can be re-phrased as follows: if the network is such that any of its output units $\Phi_i$ can be chosen from the whole linear space spanned by its filter functions $V_\rho$, then the associated optimization problem is such that there always exists a descent path to an optimal solution, for any initialization of the parameters.

Applying the observations in Section 2.1 describing the cases of finite intrinsic dimension, we immediately get the following corollaries.

Corollary 8 (ERM). Consider $N$ data points $\{(x_i, y_i)\}_{i=1}^N \subset \mathbb{R}^{n \times m}$. For two-layers NNs $\Phi(x; \theta) = U\rho(Wx)$, where $\rho$ is any continuous activation function, the empirical loss function
$$L(\theta) = \frac{1}{N} \sum_{i=1}^N \ell(\Phi(x_i; \theta), y_i)$$

admits no spurious valleys in the over-parametrized regime $p \geq N$.

This result is in line with previous works that considered the landscape of empirical risk minimization for half-rectified deep networks [42, 45, 31, 34]. However, its proof illustrates the danger of studying empirical risk minimization landscapes in over-parametrized regimes, since it bypasses all the geometric and algebraic properties needed in the population risk setting - which may be more relevant to understand the generalization properties of the model.
Corollary 9 (Polynomial activations). For two-layers NNs $\Phi(x; \theta) = U \rho(Wx)$ with polynomial activation function $\rho(z) = a_0 + a_1 z + \cdots + a_d z^d$, the loss function $L(\theta) = \mathbb{E}[\ell(\Phi(X; \theta), Y)]$ admits no spurious valleys in the over-parametrized regime

$$p \geq \sum_{i=1}^{d} \binom{n + i - 1}{i} 1_{\{a_i \neq 0\}} = O(n^d)$$

Under the hypothesis of Corollary 9 with $p = O(n^d)$, a generic function of $V_\rho$, $\Phi(x; \theta) = u^T \rho(Wx)$, can be also represented, for some $\gamma = \gamma(\theta)$, in the generalized linear form

$$\Phi(x; \theta) = \langle \gamma, \varphi(x) \rangle$$

with $\varphi(x) = (x_{k_1} \cdots x_{k_j})_{1 \leq k_1 \leq \cdots \leq k_j \leq n, j \in J}$. The parameters $\theta$ and $\gamma$ differ for their dimensions:

$$\dim(\gamma) = O(n^d) < \dim(\theta) = (n + 1) \cdot O(n^d) = O(n^{d+1})$$

One would therefore like Corollary 9 to hold also (at least) for $p = O(n^d)$. In the next section we address this problem for the linear activation $\rho(z) = z$ and the quadratic activation $\rho(z) = z^2$.

### 3.1 Improved over-parametrization bounds for homogeneous polynomial activations

The over-parametrization bounds obtained in Corollary 9 are quite non-desirable in practical applications. We show that they can indeed be improved, for the case of linear and quadratic networks.

#### 3.1.1 Linear networks case

Linear networks have been considered as a first order approximation of feed-forward multi-layers networks [29]. It was shown, in several works [29, 21, 46], that, for linear networks of any depth

$$\Phi(x; \theta) = W_{K+1} \cdots W_1 x$$

with $\theta = (W_{K+1}, W_K, \ldots, W_2, W_1) \in \mathbb{R}^{n \times p_{K+1}} \times \mathbb{R}^{p_{K+1} \times p_K} \times \cdots \times \mathbb{R}^{p_2 \times p_1} \times \mathbb{R}^{p_1 \times n}$, the loss function [2] has no spurious local minima, if $\min_{i \in [K+1]} p_i \geq \min\{n, m\}$. This corresponds exactly with over-parametrization regime in Corollary 9 for the case of two-layers networks. The following theorem improves on Corollary 9 for the case of multi-layers linear networks, showing that no over-parametrization is required in this case to avoid spurious valleys, for square loss functions.

**Theorem 10 (Linear networks).** For linear NNs (4) of any depth $K \geq 1$ and of any layer widths $p_k \geq 1$, $k \in [K + 1]$, and any input-output dimensions $n, m \geq 1$, the square loss function $L(\theta) = \mathbb{E}[\|\Phi(X; \theta) - Y\|^2]$ admits no spurious valleys.
3.1.2 Quadratic networks case

Quadratic activations have been considered in the literature [31, 13, 41] as second order approximation of general non-linear activations. In particular, for two-layers networks with one dimensional output and square loss functions evaluated on \( N \) samples, it was shown in Du and Lee [13] that, if \( p \geq \sqrt{2N} \), the loss has no spurious local minima. Corollary 9 requires an over-parametrization bound \( p \geq n(n+1)/2 \) for the case of quadratic activations. In the following theorem we show that \( p > 2n \) is sufficient for the statement to hold, in the case of square loss functions and one dimensional output \( (m = 1) \).

**Theorem 11** (Quadratic networks). For two-layers NNs \( \Phi(x; \theta) = u^T \rho(Wx) \) with quadratic activation function \( \rho(z) = z^2 \) and one-dimensional output \( (m = 1) \), the square loss function \( L(\theta) = \mathbb{E}[(\Phi(X; \theta) - Y)^2] \) admits no spurious valleys in the over-parametrized regime \( p \geq 2n + 1 = O(n) \).

This result is in line with the one from Soltanolkotabi et al. [41], where the authors proved absence of spurious local minima when \( p \geq 2n \), but for fixed second layer weights. The proof (reported in Section A) consists in constructing a path satisfying (P.1) and improves upon the proof of Theorem 7 by leveraging the special linearized structure of the network for quadratic activation. For every parameter \( \theta = (u,W) \in \mathbb{R}^p \times \mathbb{R}^{p \times n} \), we can write

\[
\Phi(x; \theta) = \sum_{i=1}^{p} u_i \langle w_i, x \rangle^2 = \left\langle \sum_{i=1}^{p} u_i w_i w_i^T, xx^T \right\rangle_F.
\]

We notice that \( \Phi(\cdot; \theta) \) can also be represented by a NN \( \Phi(\cdot; \hat{\theta}) \) with \( n \) layers; indeed, if \( \sum_{i=1}^{n} \sigma_i v_i v_i^T \) is the SVD of \( \sum_{i=1}^{p} u_i w_i w_i^T \), then \( \Phi(x; \theta) = \left\langle \sum_{i=1}^{n} \sigma_i v_i v_i^T, xx^T \right\rangle_F \). Therefore \( p \geq n \) is sufficient to describe any element in \( V_p \). The factor 2 in the statement is due to some technicalities in the proof, but a more involved proof should be able to extend the result to the regime \( p \geq n \). The extension of such mechanism for higher order tensors (appearing as a result of multiple layers or high-order polynomial activations) using tensor decomposition also seems possible and is left for future work.

3.1.3 Lower to upper intrinsic dimension gap

As observed in Lemma 3 \( \dim_\ast(\rho(z) = z, n) = 1 \) and \( \dim_\ast(\rho(z) = z^2, n) = n \) for all integer \( n \geq 1 \). Therefore, Theorem 10 and Theorem 11 say that, for \( \rho(z) = z^k \), \( k \in [2] \), and \( m = 1 \), the square loss function \( L(\theta) = \mathbb{E}[\Phi(X; \theta) - Y]^2 \) admits no spurious valleys in the over-parametrized regime \( p \geq O(\dim_\ast(\rho, n)) \). We conjecture that this hold for any (sufficiently regular) activation function with finite intrinsic lower dimension.

4 Infinite intrinsic dimension and presence of spurious valleys

This section is devoted to the construction of worst-case scenarios for non-over parametrized networks. The main result (Theorem 12) essentially states that, for networks with width smaller than the lower intrinsic dimension defined above, spurious valleys can be created by choosing adversarial data distributions. We then show how this implies negative results for under-parametrized polynomial architectures and a large variety of architectures used in practice.
Theorem 12. Consider the square loss function \( L(\theta) = \mathbb{E}\|\Phi(x; \theta) - y\|^2 \) for two-layers NNs \( \Phi(x; \theta) = U\rho(Wx) \) with non-negative activation function \( \rho \geq 0 \) such that \( \rho \in L^2(\mathbb{R}, e^{-x^2} \, dx) \). If \( p \leq \frac{1}{2} \text{dim}_s(\rho, n - 1) \), then there exists a r.v. \( (X, Y) \) such that the square loss function \( L \) admits spurious valleys. In particular, for any given \( M > 0 \), the r.v. \( Y \) can be chosen in such a way that there are two disjoint open subsets \( \Omega_1, \Omega_2 \subset \Theta \) such that

\[
\min_{\theta \in \Omega_2} L(\theta) \geq \min_{\theta \in \Omega_1} L(\theta) + M
\]  

and any path \( \theta : [0, 1] \to \Theta \) such that \( \theta_0 \in \Omega_2 \) and \( \theta_1 \) is a global minima verifies

\[
\max_{t \in [0, 1]} L(\theta_t) \geq \min_{\theta \in \Omega_2} L(\theta) + M
\]

Equation (5) in Theorem 12 says that any local descent algorithm, if initialized with a parameter value belonging to a spurious valleys, at its best it will only be able to produce a final parameter value which is at least \( M \) far from optimality. Equation (6) implies that there exists an open subset of the spurious valleys such that any path starting in a parameter belonging to such subset must ‘up-climb’ at least \( M \) in the loss value. In the following we refer to such property, as stated in Theorem 12, by saying that the loss function has arbitrarily bad spurious valleys. Note that this result ensures that spurious valleys have positive Lebesgue measure (given by \( \mu(\Omega_2) \)), so there is a positive probability that gradient descent methods initialized with a measure that is absolutely continuous with respect to Lebesgue will get stuck in a bad local minima.

Applying the observations describing the values of the lower intrinsic dimension for different activation functions, we get the following corollaries.

Corollary 13 (Homogeneous even degree polynomial activations). Assume that \( \rho(z) = z^{2k} \) with \( k \geq 1 \) integer. For two-layers NNs \( \Phi(x; \theta) = U\rho(Wx) \), if \( n \geq 2 \) and the hidden-layer width satisfies

\[
p \leq \begin{cases} 
  n - 1 & \text{if } k = 1 \\
  \frac{1}{2} \text{rk}_S(2k, n - 1) & \text{if } k > 1 
\end{cases}
\]

then there exists a r.v. \( (X, Y) \) such that the square loss function \( L(\theta) = \mathbb{E}\|\Phi(x; \theta) - y\|^2 \) has arbitrarily bad spurious valleys.

This follows by Theorem 12 and Corollary 3, since \( \text{dim}_s(\rho(z) = z^{2k}, n) = \text{rk}_S(2k, n) \). For the well known case \( k = 2 \) (symmetric matrices) it holds \( \text{rk}_S(2, n) = n \); therefore Corollary 13 implies that the bound provided in Corollary 3 is almost (up to a factor 2) tight. Still, this is in line with recent works which explored quadratic architectures [41, 18].

Corollary 14 (Spurious valleys exist in generic architectures). If \( n \geq 2 \), for two-layers NNs \( \Phi(x; \theta) = U\rho(Wx) \) with any hidden-layer width \( p \geq 1 \) and continuous non-negative non-polynomial activation function \( \rho \in L^2(\mathbb{R}, e^{-x^2/2}) \), then there exists a r.v. \( (X, Y) \) such that the square loss function \( L(\theta) = \mathbb{E}\|\Phi(x; \theta) - y\|^2 \) has arbitrarily bad spurious valleys. This setting includes the following activation functions:

- The ReLU activation function \( \rho(z) = z_+ \) and some relaxations of it, such as softplus activation functions \( \rho(z) = \beta^{-1} \log(1 + e^{\beta z}) \), with \( \beta > 0 \);
• The sigmoid activation function \( \rho(z) = (1 + e^{-z})^{-1} \) and the approximating erf function \( \rho(z) = \frac{2}{\pi} \int_0^z e^{-u} du \), which represents an approximation to the sigmoid function.

This follows by Theorem 12 by observing that \( \dim_\ast(\rho, n) = \infty \) if \( \rho \) is one of the above activation functions. Corollary 14 generalizes on some recent negative results \([38, 46]\) for practical activations. We remark that while in these works the authors proved existence of spurious local minima, we prove that, in fact, arbitrarily bad spurious valleys can exist, which is a stronger negative characterization.

The results of this section can be interpreted as worst-case scenarios for the problem of optimizing (2). We showed that, even for simple two-layers neural network architectures with non-linear activation functions used in practice (such as ReLU), global optimality results can not hold, unless we make some assumptions on the data distributions.

5 Typical Spurious Valleys and Low-Energy Barriers

In the previous section it was shown that whenever the number of hidden units \( p \) is below the lower intrinsic dimension, then one can show worst-case data distributions that yield a landscape with arbitrarily bad spurious valleys.

In this section, we study the energy landscape under generic data distributions in case of homogeneous activation, and show that, although spurious valleys may appear, they tend do so below a certain energy level, controlled by the decay of the spectral decomposition of the kernel defined by the activation function and by the amount of parametrisation \( p \).

This phenomena is consistent with the empirical success of gradient-descent algorithms in conditions where \( p \) is indeed below the intrinsic dimension.

We consider oracle square loss functions of the form

\[
L(\theta) = E|\Phi(X; \theta) - Y|^2
\]

for one-dimensional output two-layers NNs \( \Phi(x; \theta) = u^T \rho(Wx + b) \), with \( \theta = (u, b, W) \in \mathbb{R}^p \times \mathbb{R}^p \times \mathbb{R}^{p \times n} \), \( \rho \) a positively homogeneous function, and \( X, Y \) square integrable r.v. \((E\|X\|^2, EY^2 < \infty)\). Notice that we can write

\[
L(\theta) = E|\Phi(X; \theta) - f^*(X)|^2 + E|Y - f^*(X)|^2
\]

for some measurable \( f^* : \mathbb{R}^n \to \mathbb{R} \) such that \( f^*(X) = E[Y | X] \). In particular this implies that

\[
\min_{\theta \in \Theta} L(\theta) \geq \mathcal{R}(X, Y) = E|Y - f^*(X)|^2
\]

As \( p \to \infty \), the optimization problem (7) becomes convex, a fact that is exploited in several recent works \([32, 36, 10]\). As observed by Bach in \([2]\), the effect of having only a finite number of hidden neurons can be recast as obtaining a quadrature rule for the reproducing kernel associated to the activation function. The following theorem is a direct application of Proposition 1 from \([2]\), and relates the quadrature error with the ability to avoid large loss barriers with high probability.

**Theorem 15.** Let \( d\tau \) be the uniform distribution over the unit sphere \( S^n \) and consider an initial parameter \( \theta = (\hat{u}, \hat{b}, \hat{W}) \) with \((\hat{w}_i, \hat{b}_i) \sim d\tau \) sampled i.i.d. Then the following hold:
1. There exists a path \( t \in [0, 1] \mapsto \theta_t \) such that \( \theta_0 = \tilde{\theta} \), the function \( t \in [0, 1] \mapsto L(\theta_t) \) is non-increasing, and

\[
L(\theta_1) \leq R(X, Y) + \lambda \quad \text{if} \quad p \geq O(-\lambda^{-1} \log(\lambda \delta))
\]

with probability greater or equal then \( 1 - \delta \), for every \( \lambda, \delta \in (0, 1) \).

2. If \( f^* \) is sufficiently regular\(^3\), there exists a path \( t \in [0, 1] \mapsto \theta_t \) such that \( \theta_0 = \tilde{\theta} \), the function \( t \in [0, 1] \mapsto L(\theta_t) \) is non-increasing, and

\[
L(\theta_1) \leq R(X, Y) + O(p^{-1+\delta})
\]

with probability greater or equal then \( 1 - e^{-O(p^{\delta})} \) for every \( \delta \in (0, 1) \).

The above result implies that convex optimization over the second layer is sufficient to reach a model whose error relative to the best possible one is inversely proportional to the hidden-layer size (up to logarithm factors). Nevertheless, in practice, this approach will generally perform worse than standard gradient-descent training, which may require less over-parametrization to give satisfying results (see for example the numerical experiments in [10], Section 4). This shows the importance of understanding gradient descent dynamics on the first layer, amenable to analysis in the limit \( p \to \infty \) using mean-field techniques [36, 32] as well as optimal transport on Wasserstein metrics [10]. Precisely quantifying how much is gained by optimizing jointly in the non-asymptotic case remains an important open question [10] left for future work.

6 Future directions

We considered the problem of characterizing the loss surface of neural networks from the perspective of optimization, with the goal of deriving weak certificates that enable - or prevent - the existence of descent paths towards global minima.

The topological properties studied in this paper, however, do not yet capture fundamental aspects that are necessary to explain the empirical success of deep learning methods. We identify a number of different directions that deserve further attention.

The positive results presented above rely on being able to reduce the network to the case when (convex) optimization over the second layer is sufficient to reach optimal weight values. A better understanding of first layer dynamics needs to be carried out. Moreover, in such positive results we only proved non-existence of (high) energy barriers. While this is an interesting property from the optimization point of view, it is also not sufficient to guarantee convergence of local descent algorithms. Another informative property of the loss function that should be addressed in future works is the existence of local descents in non optimal points: for every \( \theta_0 \in \Theta \) non optimal and any neighborhood \( U \subseteq \Theta \) of \( \theta_0 \), there exists \( \theta \in U \) such that \( L(\theta) < L(\theta_0) \). More generally, our present work is not informative on the performance of gradient descent in the regimes with no spurious valley.

The other very important point to be addressed in future is how to extend the above results to architectures of more practical interest. Depth and the specific linear structure

\[^3\text{More precisely, if the function } f^* \text{ can be written as } f^*(x) = \int_W g^*(w)\psi_w(x)\,d\tau(w) \text{ for some } g^* \in L^\infty_{d\tau}. \]
of Convolutional Neural Networks, critical to explain the excellent empirical performance of deep learning in computer vision, text or speech, need to be exploited, as well as specific design choices such as Residual connections and several normalization strategies – as done recently in [40] and [39] respectively. This also requires making specific assumptions on the data distribution, and is left for future work.

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A Proofs of Section 3

A.1 Proof of Theorem 7

We note that, under the assumptions of Theorem 7, the same optimal NN functions \( \Phi_i(\cdot; \theta) \) could also be obtained using a generalized linear model, where the representation function has the linear form

\[
\Phi_i(x; \theta) = \langle \theta_i, \varphi(x) \rangle
\]

for some parameter independent function \( \varphi : \mathbb{R}^n \rightarrow \mathbb{R}^{\text{dim}\rho(X)} \). The main difference between the two models is that the former requires the choice of a non-linear activation function \( \rho \), while the latter implies the choice of a kernel functions. This is the content of the following lemma.

Lemma 16. Let \( \rho : \mathbb{R} \rightarrow \mathbb{R} \) be a continuous function and \( X \in \mathcal{R}_2(\rho, n) \) a r.v. Assume that the linear space

\[
V_{\rho,X} = \text{span}\{f : f \in V_{\rho,1}\} \subseteq L^2_X
\]

is finite dimensional. Then there exists a scalar product \( \langle \cdot, \cdot \rangle \) on \( V_{\rho,X} \) and a map \( x \in \mathbb{R}^n \mapsto \varphi(x) \in V_{\rho,X} \) such that

\[
\langle \psi_{\rho,w}, \varphi(x) \rangle = \psi_{\rho,w}(x) = \rho(\langle w, x \rangle)
\]

for all \( w \in \mathbb{R}^n \). Moreover, the function \( w \in \mathbb{R}^n \mapsto \psi_{\rho,w} \in V_{\rho,X} \) is continuous.

Proof. For sake of simplicity, in the following we write \( \psi_w \) for \( \psi_{\rho,w} \) and \( V \) for \( V_{\rho,X} \). Let \( \psi_{w_1}, \ldots, \psi_{w_q} \) be a basis of \( V \). If \( \psi_w = \sum_{i=1}^q \alpha_i \psi_{w_i} \) and \( \psi_V = \sum_{j=1}^q \beta_j \psi_{w_j} \), then we can define a scalar product on \( V \) as

\[
\langle \psi_w, \psi_V \rangle \doteq \sum_{i=1}^q \alpha_i \beta_i
\]
If we define the map \( x \in \mathbb{R}^n \mapsto \varphi(x) \in V \) as
\[
\varphi(x) = \sum_{i=1}^{q} \psi_{w_i}(x) \psi_{w_i},
\]
then property [3] follows directly by the definition of the function \( \psi_{w_i} \). Moreover, we can choose \( x_1, \ldots, x_q \) such that \( \varphi(x_1), \ldots, \varphi(x_q) \) is a basis of \( V \). Now we need to show that, for \( i \in [q] \), the map \( w \mapsto \langle \psi_{w_i}, \psi_{w_i} \rangle \) is continuous. Let \( M \) be the matrix \( M = \langle \psi_{w_i}(x_i) \rangle_{i,j} \in \mathbb{R}^{q \times q} \) and \( z(w) \) be the vector \( z(w) = \langle \psi_{w}(x_i) \rangle_{i} \in \mathbb{R}^q \). Then \( \langle \psi_{w}, \psi_{w_i} \rangle = (M^{-1} z(w))_i \), which is continuous in \( w \). This shows that the map \( w \in \mathbb{R}^n \mapsto \psi_{w} \in V \) is continuous. \( \square \)

The non-trivial fact captured by Theorem [7] is the following: when the capacity of network is large enough to match a generalized linear model, but still finite, then the problem of optimizing the loss function [2], which is in general a highly non-convex object, satisfies an interesting optimization property in view of the local descent algorithms which are used in practice to solve it.

**Proof of Theorem [7]** Thanks to Lemma [16] there exist two continuous maps \( \varphi, \psi : \mathbb{R}^n \to \mathbb{R}^q \cong V_{\rho, X}, \) with \( q = \dim^*(\rho, X) \), such that \( \rho((w, x)) = \langle \psi(w), \varphi(x) \rangle \) for every \( w, x \in \mathbb{R}^n \). Therefore, every two-layers NN \( \Phi(x; \theta) = U \rho(W x) \) can be written as \( \Phi(x; \theta) = U \psi(W) \varphi(x) \), where, if \( W \in \mathbb{R}^{P \times n} \), then \( \psi(W) \in \mathbb{R}^{P \times q} \) (that is \( \psi \) is applied row-wise).

The proof of the Theorem consists in exploiting the above linearized representation of \( \Phi \) to show that property [4.1] holds (remind that this is equivalent to saying that the loss function has no spurious valleys). Given an initial parameter \( \theta = (U, W) \), we want to construct a continuous path \( t \in [0, 1] \mapsto \theta_t = (U_t, W_t) \), such that the function \( t \in [0, 1] \mapsto L(\theta_t) \) is non-increasing and such that \( \theta_0 = \tilde{\theta}, \theta_1 \in \arg \min_{\theta} L(\theta), \) where \( L(\theta) = \mathbb{E}[\ell(\Phi(X; \theta), Y)] \).

The construction of such a path can be articulated in two main steps:

**Step 1.** The first part of the path consists showing that we can assume that \( \text{rk}(\psi(W)) = q \) w.l.o.g.

Let \( w_1^1, \ldots, w_q^1 \in \mathbb{R}^n \) be the rows of \( W \); suppose that \( \text{rk}(\psi(W)) = r < q \) (otherwise there is nothing to show) and that \( \psi(w_1), \ldots, \psi(w_r) \) are linearly independent. Denote \( I = \{i_1, \ldots, i_r\}, J = [1, p] \setminus I = \{j_1, \ldots, j_{p-r}\} \) and \( u_1, \ldots, u_p \) the columns of \( U \). For \( j \in J \), we can write
\[
\psi(w_j) = \sum_{k=1}^{r} a_j^k \psi(w_{i_k}) \quad \text{for some } a_j^k \in \mathbb{R} \tag{9}
\]

If we define \( U_1 \) such that (denoting \( u_{1,i} \) the \( i \)-th row of \( U_1 \))
\[
u_{1,i} = u_i + \sum_{k=1}^{n-r} a_{i}^{k} u_{j_k} \quad \text{for } i \in I, \quad u_{1,j} = 0 \quad \text{for } j \in J
\]
then \( U_1 W = \tilde{U} W \). The path \( t \in [0, 1/2] \mapsto \theta_t = (2t U_1 + (1-2t) \tilde{U}, \tilde{W}) \) leaves the network unchanged, i.e. \( \Phi(\cdot; \theta_t) = \Phi(\cdot; \theta_t) \) for \( t \in [0, 1/2] \). At this point, we can select \( w_1^1, \ldots, w_{1,j_{p-r}} \in \mathbb{R}^n \) such that the matrix \( W_1 \) with rows \( w_{1,i} = w_i \) for \( i \in I \) and \( w_{1,j} \) for \( j \in J \), verifies \( \text{rk}(\psi(W_1)) = q \). Notice that the existence of such vectors \( w_{1,j}, k \in [p-r], \) is guaranteed by the definition of \( q = \dim^*(\rho, X) \). The path \( t \in [1/2, 1] \mapsto \theta_t = (U_1, (2t - 1)W_1 + (2 - 2t)\tilde{W}) \) leaves the network unchanged, i.e. \( \Phi(\cdot; \theta_0) = \Phi(\cdot; \theta_t) \) for \( t \in [1/2, 1] \). The new parameter value \( \theta_1 = (U_1, W_1) \) satisfies \( \text{rk}(\psi(W_1)) = q \).
Step 2. By step 1, we can assume that $\text{rk}(\tilde{W}) = q$. Since the network has the form $\Phi(x; \theta) = U\psi(W)\varphi(x)$ and since the function $\ell$ is convex, there exists $U^* \in \mathbb{R}^{m \times p}$ such that $\theta = (U^*, \tilde{W}) \in \arg\min_{\theta} L(\theta)$. The proof is therefore concluded by selecting the path $t \in [0, 1] \mapsto \theta_t = (tU^* + (1-t)\tilde{U}, W)$.

This shows that property $\mathcal{P}_1$ holds and therefore it proves the theorem.

A.2 Proof of Theorem 10

The first step for proving Theorem 10 consists in extending the result of Theorem 7 to the case of two-layers linear NNs $\Phi(x; \theta) = UWx$ with $U \in \mathbb{R}^{m \times p}$, $W \in \mathbb{R}^{p \times n}$ with $p < n$ and square loss functions $L(\theta) = \mathbb{E}\|\Phi(X; \theta) - Y\|^2$. We start by pointing out a symmetry property of this type of networks: for every $G \in GL(p)$ it holds that

$$\Phi(x; (U, W)) = UWx = (UG^{-1})(GW)x = \Phi(x; (UG^{-1}, GW))$$

This means that the map $\theta \mapsto \Phi(\cdot; \theta)$ is defined up to an action of the group $GL(p)$ over the parameter space $\Theta = \mathbb{R}^{m \times p} \times \mathbb{R}^{p \times n}$; the same remark holds for the loss function $L(\theta)$. We can therefore think about the loss function as defined over the topological quotient $\Theta/GL(p)$. We denote the orbit of an element $\theta = (U, W) \in \Theta$ as

$$[\theta] = [U, W] = \{G \cdot \theta = (UG^{-1}, GW) : G \in GL(p)\}$$

If $g$ is a real-valued function defined on $\Theta$ such that $g(G \cdot \theta) = g(\theta)$ for all $G \in GL(p)$ and $\theta \in \Theta$, then one can equivalently consider $g$ as defined on $\Theta/GL(p)$ as $g([\theta]) = g(\theta)$; for simplicity we denote $g(\{\theta\}) = g([\theta])$. This is exactly the case for the loss function $L(\theta)$. In the proof of Theorem 7 we describe how to construct a path from an initial parameter value $\tilde{\theta} = (\tilde{U}, \tilde{W})$ to a parameter value $\theta_1 = (q(W_1), W_1)$, with $\text{rk}(W_1) = p$ and $q : \mathbb{R}^{p \times n} \rightarrow \mathbb{R}^{m \times p}$ the function defined by

$$q(W) = \Sigma_{XX} W^T (WS_X W^T)^\dagger \in \arg\min_U L(\theta)|_{\theta = (U, W)}$$

(see Lemma 23). Therefore, let $\hat{\theta} = (q(\tilde{W}), \tilde{W})$ with $\text{rk}(\tilde{W}) = p$, be an initial parameter. Since an optimal parameter is given by $\theta = (q(W), W)$ for some $W$, we seek for a path in the form $\theta_t = (q(W_t), W_t)$ with $\text{rk}(W_t) = p$ for all $t \in [0, 1]$. This path must be such that $t \mapsto L(\theta_t)$ is non-increasing. If we assume that $\Sigma_X = I$, it holds

$$L(\theta_t) = \text{tr}(\Sigma_Y) - \text{tr}(\Sigma_P W_t)$$

where $M$ is a PSD matrix and, for every matrix $W$, $P_W$ denotes the orthogonal projection on the rows of $W$, that is $P_W = W^T W$ (see Lemma 23). Therefore it is equivalent for the path $\theta_t = (q(W_t), W_t)$ to be such that the function

$$t \in [0, 1] \mapsto f(W_t) = \text{tr}(MP_{W_t})$$

is non-decreasing. In particular, the function $f$ is defined up to the action of the group $GL(p)$ on $\Theta$. Since we look for $W_t$ of rank $p$, we can consider $f$ as defined on $G(p, n)$, the Grassmanian of $p$ dimensional linear subspaces of $\mathbb{R}^n$. The proof below for the linear two-layers
We then show that such a path can be \textit{lifted} to a corresponding path \( W_t \in \mathbb{R}^{p \times n} \) (Lemma 18). Finally, we show that we can drop the assumption \( \Sigma_X = I \) and the result still holds (Lemma 19).

**Lemma 17.** Let \( \tilde{W} \in G(p,n) \) and assume \( \Sigma_X = I \). Then there exists a continuous path \( t \in [0,1] \mapsto [W_t] \in G(p,n) \) such that \( [W_0] = [\tilde{W}] \), \( [W_1] \) maximizes \( f \) and such that the function \( t \in [0,1] \mapsto f[W_t] \) is non-decreasing.

**Proof.** While it is geometrically intuitive that the results should hold, we derive a constructive proof. We start by noticing that if \( [W] \in G(p,n) \) and \( w_1, \ldots, w_p \) is an orthonormal basis of \( [W] \), then

\[
  f[W] = \sum_{i=1}^{p} w_i^T M w_i
\]

Moreover, if \( M = \sum_{j=1}^{n} \sigma_j v_j v_j^T \) is the SVD of \( M \), where \( \sigma_1 \geq \cdots \geq \sigma_n \geq 0 \), then (11) can be written as

\[
  f[W] = \sum_{j=1}^{n} \sigma_j \sum_{i=1}^{p} \langle v_j, w_i \rangle^2
\]

In particular the maximum of \( f \) is obtained for \( [W] = [V] \equiv [v_1, \ldots, v_p] \) (with some abuse of notation, we identify a subspace with one of its basis). To prove the result is therefore sufficient to show a path \( [W_t] \) from any \( [W_0] = [\tilde{W}] \) to \( [W_1] = [V] \), such that the function \( t \in [0,1] \mapsto f[W_t] \) is non-decreasing. To do this we construct a finite sequence of paths

\[
  [W_t^i] \quad \text{such that} \quad [W_0^i] = [W^{i-1}] \quad \text{and} \quad [W_1^i] = [W^i]
\]

for \( i \in [p] \), with \( [W^0] = [\tilde{W}] \), \( [W^p] = [V] \) and

\[
  W^i = [v_1, \ldots, v_i, w_{i+1}^{i-1}, \ldots, w_p^{i-1}] \quad \text{for} \quad i \in [p]
\]

where \( w_1^j = v_1, \ldots, w_j^j = v_j, w_{j+1}^j, \ldots, w_p^j \) is an orthonormal basis of \( [W^j] \), for \( j \in [0,p] \). Moreover, the paths \( [W_t^i] \) are such that the functions \( t \in [0,1] \mapsto f[W_t^i] \) are non-decreasing. Such paths are defined as follows. Let \( i \in [0, p-1] \) and consider

\[
  [W^i] = [w_1^i = v_1, \ldots, w_i^i = v_i, w_{i+1}^i, \ldots, w_p^i]
\]

We define

\[
  u_{i+1}^i = \begin{cases} \frac{P_{W^i} v_{i+1}}{\|P_{W^i} v_{i+1}\|} & \text{if} \ P_{W^i} v_{i+1} \neq 0 \\ 0 & \text{o.w.} \end{cases}
\]

Then we complete \( v_1, \ldots, v_i, u_{i+1}^i \) to an orthonormal basis of \( [W^i] \):

\[
  v_1, \ldots, v_i, u_{i+1}^i, \ldots, u_p^i
\]

We call \( w_j^{i+1} = u_j^i \) for \( j \in [i+2,p] \) and we define

\[
  [W^{i+1}] = [v_1, \ldots, v_i, w_{i+1}^{i+1} = v_{i+1}, w_{i+2}^{i+1}, \ldots, w_p^{i+1}]
\]
Therefore the path \([\mathbf{W}_t^i]\) is then obtained by moving \(\mathbf{u}_{i+1}^t\) to \(\mathbf{v}_{i+1}\) on a geodesic on the unit sphere \(S^{n-1} \subset \mathbb{R}^n\), i.e.

\[
[\mathbf{W}_t^{i+1}] = [\mathbf{v}_1, \ldots, \mathbf{v}_i, \mathbf{u}_{i+1}^t(t), \mathbf{u}_{i+2}^t, \ldots, \mathbf{u}_p^t]
\]

where we defined

\[
\mathbf{u}_{i+1}^t(t) = (1 - (1 - \mu_{i+1}t))\mathbf{u}_{i+1}^t + \sqrt{1 - (1 - (1 - \mu_{i+1}t)^2)} \cdot \frac{\mathbf{v}_{i+1} - \mathbf{u}_{i+1}^t}{\sqrt{1 - \mu_{i+1}^2}}
\]

for \(\mu_{i+1} = \langle \mathbf{u}_{i+1}^t, \mathbf{v}_{i+1}\rangle\). The fact that the function \(t \in [0, 1] \mapsto f[\mathbf{W}_t^{i+1}]\) is non-decreasing can be proved by noticing that

\[
f[\mathbf{W}_t^{i+1}] - f[\mathbf{W}_t^i] = \sum_{j=i+1}^{n} \sigma_j \langle \mathbf{u}_{i+1}^t(t), \mathbf{v}_j \rangle^2
\]

and by showing that the derivative of the RHS is greater or equal than 0. This concludes the proof of the lemma.

**Lemma 18.** Let \(\mathbf{W} \in \mathbb{R}^{p \times n}\) and assume \(\Sigma_X = \mathbf{I}\). Then there exists a continuous path \(t \in [0, 1] \mapsto \mathbf{W}_t \in \mathbb{R}^{p \times n}\) such that \(\mathbf{W}_0 = \mathbf{W}\), \(\mathbf{W}_1\) maximizes \(f\) and such that the function \(t \in [0, 1] \mapsto f(\mathbf{W}_t)\) is non-decreasing.

**Proof.** The only thing we need to prove in this case is that we can lift the paths \([\mathbf{W}_t^i] \in G(p, n)\) from the proof of Lemma 17 to continuous paths \(\mathbf{W}_t^i \in \mathbb{R}^{n \times p}\). We first notice that if the basis \(\{\mathbf{w}_1, \ldots, \mathbf{w}_p\}\) and \(\{\mathbf{w}_1, \ldots, \mathbf{w}_i, \mathbf{u}_{i+1}^t, \ldots, \mathbf{u}_p^t\}\) are defined as above, then we can assume (up to changing some signs) that they have all the same orientation, for all \(i \in [0, p]\). Therefore we can define the matrices \(\mathbf{W}_i \in \mathbb{R}^{p \times n}\) with rows \(\mathbf{w}_1, \ldots, \mathbf{w}_i\) and the matrices \(\mathbf{U}_i \in \mathbb{R}^{p \times n}\) with rows \(\mathbf{w}_1, \ldots, \mathbf{w}_i, \mathbf{u}_{i+1}^t, \ldots, \mathbf{u}_p^t\), for \(i \in [0, p]\). The paths \(\mathbf{W}_t^{i+1}\) are defined in the same way as in the proof of Lemma 17. Notice that such paths go from \(\mathbf{W}_0^{i+1} = \mathbf{U}_i\) to \(\mathbf{W}_1^{i+1} = \mathbf{W}^{i+1}\). It remains to construct paths from \(\mathbf{W}_i\) to \(\mathbf{U}_i\). Consider the matrix

\[
\mathbf{O}_i = \mathbf{W}_i^T \mathbf{U}_i \in SO(n)
\]

Notice that \(\mathbf{W}_i^T \mathbf{U}_i = \mathbf{U}_i\). In particular there exist \(\mathbf{A}_i\) real skew-symmetric such that \(\mathbf{O}_i = e^{\mathbf{A}_i}\). Therefore the paths \(t \in [0, 1] \mapsto \mathbf{U}_t^i = \mathbf{W}_i^T e^{t \mathbf{A}_i}\) go from \(\mathbf{U}_0^i = \mathbf{W}_i^i\) to \(\mathbf{U}_t^i = \mathbf{U}_i\). Moreover \(f(\mathbf{U}_t^i)\) is constant in \(t\) (since the underlying linear subspace does not change). The only thing that remains to prove is that, given the matrix \(\mathbf{W} \in \mathbb{R}^{n \times p}\) with columns \(\mathbf{w}_1, \ldots, \mathbf{w}_p\), there is a path from \(\mathbf{W}\) to \(\mathbf{W}^0\). Now, \(\mathbf{W}^0\) was chosen as a matrix with orthonormal columns such that \([\mathbf{W}] = [\mathbf{W}^0]\). Therefore if \(\mathbf{W} = \mathbf{O} \mathbf{A} \mathbf{U}\) is the SVD of \(\mathbf{W}\) with \(\mathbf{U} = \mathbf{W}^0\), \(\mathbf{A} = \text{diag}(\sigma_1, \ldots, \sigma_p) \in \mathbb{R}^{p \times p}\) (with \(\sigma_i > 0\), \(i \in [p]\)) and \(\mathbf{O} \in SO(p)\), there exists \(\mathbf{A}\) real skew-symmetric such that \(\mathbf{O} = e^{\mathbf{A}}\). Thus the path \(t \in [0, 1] \mapsto \mathbf{W}_t = e^{(1-t)\mathbf{A}} \mathbf{A}^{1-t} \mathbf{W}^0\) is a path between \(\mathbf{W}_0 = \mathbf{W}\) and \(\mathbf{W}_1 = \mathbf{W}^0\). This concludes the proof of the lemma.

**Lemma 19.** Lemma 18 holds even if we drop the assumption \(\Sigma_X = \mathbf{I}\).

**Proof.** For sake of simplicity we distinguish two cases.

**Case 1:** \(\text{rk}(\Sigma_X) = n\). Let \(\mathbf{K} = (\Sigma_X)^{1/2}\). Then \(\mathbf{X} = \mathbf{K}^{-1} \mathbf{X}\) is such that \(\Sigma_X = \mathbf{I}\). Therefore, if \(t \in [0, 1] \mapsto \mathbf{\theta}_t = (\mathbf{U}_t, \mathbf{W}_t)\) is the path given by Lemma 18 for the case \(\mathbf{X} = \mathbf{X}\), the sought
path (for $X = X$) is given by $t \in [0, 1] \mapsto (U_t, W_tK^{-1})$.

Case 2: $r_k(\Sigma_X) < n$. In this case, if $r = r_k(\Sigma_X)$, $X$ belongs to a $r$-dimensional subspace of $\mathbb{R}^n$ (a.s.), call it $V$. If $O \in \mathbb{R}^{n \times r}$ is a matrix with an orthonormal basis of $V$ as columns, then $O\Theta = X$ (a.s.), and, if $\tilde{X} = O^T X$ then $\tilde{X} \in \mathbb{R}^r$ and $r_k(\Sigma_{\tilde{X}}) = r$. Therefore, if $t \in [0, 1] \mapsto \theta_t = (U_t, W_t)$ is the path given by case 1 for $X = \tilde{X}$, the sought path (for $X = X$) is given by $t \in [0, 1] \mapsto (U_t, W_tO^T)$. \hfill \Box

This concludes the proof of non-existence of spurious valleys for the square loss function of linear two-layers NNs $\Phi(x; \theta) = UWx$. The fact that such proof does not require any assumptions on the dimensions of the layers $n, p, m$ neither on the rank of the initial layers, allows us to prove non-existence of spurious valleys for the square loss function of linear NNs of any depth $K \geq 1$:

$$\Phi(x; \theta) = W_{K+1} \cdots W_1x$$ (12)

We start by proving a simple lemma.

**Lemma 20.** Let $\tilde{U} = M_1 \cdots M_n$, where $\tilde{U} \in \mathbb{R}^{r_0 \times r_n}$ and $M_i \in \mathbb{R}^{r_{i-1} \times r_i}$. Suppose that $t \in [0, 1] \mapsto U_t$ is a given continuous path between $U_0 = \tilde{U}$ and another matrix $U_1 \in \mathbb{R}^{r_0 \times r_n}$. If $r_i \geq \min \{r_0, r_n\}$ for all $i$, then there exist continuous paths $M_i^t$ such that $M_0 = \tilde{M}$ and such that $U_t = M_1^t \cdots M_n^t$.

**Proof.** The statement can be proved by induction. If $n = 1$ there is nothing to prove. Assume now (by induction) that it holds for all decompositions of $U_0$ with size less than $n$. Let $r = r_h = \min_{i \in [n-1]} r_i$ and assume (w.l.o.g.) that $r_n = \min \{r_0, r_n\}$. We want to describe two paths $t \in [0, 1] \mapsto V_t \in \mathbb{R}^{r_0 \times r}$, $t \in [0, 1] \mapsto W_t \in \mathbb{R}^{r \times r_n}$ such that $U_t = V_tW_t$ and $V_0 = \tilde{M}_1 \cdots \tilde{M}_n$, $W_0 = M^h \cdots M^n$. By operating as in step 1 in the proof of Theorem 7, we can assume $r(V_0) = r_n$. Moreover (up to adding a linear path in $V_t$) we can assume that $V_0 = U_0W_0$. We then define $V_t = U_tW_0$ and $W_t = W_0$ for $t \in (0, 1]$. We thus factorized $U_t$ as $U_t = V_tW_t$. By induction, we can assume that we can factorize $V_t = M_1^t \cdots M_n^t$ and $W_t = M_1^{h+1} \cdots M_h^n$. This concludes the proof. \hfill \Box

We can now conclude the proof of Theorem [10].

**Proof of Theorem [10]** Consider a linear network $\Phi(x; \theta)$ as in (12), where

$$W_k \in \mathbb{R}^{p_k \times p_{k-1}} \quad \text{for} \quad k \in [K+1]$$

We select $p_s = \min_{i \in [K]} p_k$. Then the network can be written as

$$\Phi(x; \theta) = \tilde{W}^2\tilde{W}^1x \quad \text{where} \quad \tilde{W}^2 = W^{K+1} \cdots W^{s+1}, \quad \tilde{W}^1 = W^s \cdots W^1$$ (13)

Now we want to prove property that given an initial parameter $\hat{\theta} = (\tilde{W}^{K+1}, \ldots, \tilde{W}^1)$, there exists a continuous path $\theta_t = (W_t^{K+1}, \ldots, W_t^1)$ such that $L(\theta_t)$ is non-increasing and such that $\theta_0 = \hat{\theta}$ and $L(\theta_1) = \min_\theta L(\theta)$. If we call $\tilde{W}^i$, $i = 1, 2$, the matrices defined in (13) for $\theta = \hat{\theta}$, then by Lemma [19] there exists a path $(\tilde{W}_t^2, \tilde{W}_t^1)$ satisfying the above. Thanks to Lemma 20, we can decompose

$$\tilde{W}_t^2 = W_t^{K+1} \cdots W_t^{s+1}, \quad \tilde{W}_t^1 = W_t^s \cdots W_t^1$$ (14)
in a continuous way. Since \( p_s \) was to chosen as the minimum, it also holds that

\[
\min_{\theta=(\mathbf{W}_2^*, \mathbf{W}_1^*)} L(\theta) = \min_{\theta=(\mathbf{W}_{k+1}^*, ..., \mathbf{W}_1^*)} L(\theta)
\]

Therefore this is a suitable path and this concludes the proof of the theorem. \( \square \)

A.3 Proof of Theorem 11

Proof of Theorem 11. Let \( \tilde{\theta} = (\tilde{u}, \tilde{W}) \) be a starting parameter value. We aim to construct a continuous path \( t \in [0,1] \mapsto \theta_t \in \Theta \) starting in \( \theta_0 = \theta \) and such that \( L(\theta_1) = \min_{\theta} L(\theta) \) and such that the function \( t \in [0,1] \mapsto L(\theta_t) \) is non-increasing. Such a path can be constructed in two steps.

Step 1. Let \( \mathbf{A} = \sum_{k=1}^{p} \tilde{u}_k \tilde{w}_k \tilde{w}_k^T \) and \( \sum_{k=1}^{p} u_k^* w_k^*(w_k^*)^T \) be the SVD of \( \mathbf{A} \). We define the parameters value \( \theta^* = (u^*, W^*) \) where \( u^* = (u_1^*, ..., u_n^*, 0, ..., 0) \) and \( W^* \) is the \( p \times n \) matrix with rows \( w_i^* \) for \( i \in [n] \) and 0 for \( i \in [n+1, p] \). The first step consists in continuously mapping \( \tilde{\theta} = (\tilde{u}, \tilde{W}) \) to \( \theta^* = (u^*, W^*) \) with a path \( \theta_t \) such that \( L(\theta_t) \) is constant; the construction of such a path is detailed in Lemma 21.

Step 2. As noticed above, the network can be written as \( \Phi(x; \theta) = \mathbf{u}^T \rho(\mathbf{W}x) = \langle \mathbf{A}, \mathbf{M} \rangle_F \), where \( \mathbf{A} = \sum_{k=1}^{p} u_k w_k w_k^T \) and \( \mathbf{M} = xx^T \). The square loss \( L(\theta) \) is convex in the parameter \( \mathbf{A} \). Be \( \hat{\mathbf{A}} \) a mimima of \( L \) as function of \( \mathbf{A} \) and \( \sum_{i=1}^{n} \tilde{u}_k \tilde{w}_k \tilde{w}_k^T \) be the SVD of \( \hat{\mathbf{A}} \); also let \( \tilde{\mathbf{u}} = (0, ..., 0, \tilde{u}_1, ..., \tilde{u}_n) \) and \( \tilde{\mathbf{W}} \) be the \( p \times n \) matrix with rows 0 for \( i \in [p-n] \) and \( \tilde{w}_i \) for \( i \in [n+1, p] \). By the previous step we can assume that the initial parameter \( \theta = (\tilde{\mathbf{u}}, \tilde{\mathbf{W}}) \) is such that \( \tilde{u}_i = 0 \) and \( \tilde{w}_i = 0 \) for \( i \in [n+1, p] \). Then the path \( \theta_t = (1-t)(\mathbf{u}, \mathbf{W}) + t(\tilde{\mathbf{u}}, \tilde{\mathbf{W}}) \) verifies property [P.1]. This indeed follows from the fact that \( \Phi(x; \theta_t) = (1-t)\langle \mathbf{A}, \mathbf{M} \rangle_F + t\langle \hat{\mathbf{A}}, \mathbf{M} \rangle_F \) and from the convexity of the loss \( L \) as function of \( \mathbf{A} \).

This shows that property [P.1] holds and so it concludes the proof of Theorem 11. \( \square \)

To conclude the proof we just need to prove the following lemmas.

Lemma 21. Let \( \theta = (\mathbf{u}, \mathbf{W}) \) be an initial parameter and \( \theta^* = (u^*, W^*) \) be as in step 1 of the proof of Theorem 11. Then there exists a continuous path \( \theta_t \) from \( \theta \) to \( \theta^* \) such that the loss \( L(\theta_t) \) is constant (as a function of \( t \)).

Proof. Notice that we can assume \( \mathbf{u} \in \{-1, 0, 1\}^p \). This can be done simply scaling (continuously) each row \( \mathbf{w}_k \) of \( \mathbf{W} \) by \( \sqrt{|u_k|} \). Assume first that \( \mathbf{u} \in \{\pm 1\}^p \). The general case \( u_k = 0 \) for some \( k \) is addressed in Remark 1. The sought path \( \theta_t \) can be constructed by iterating two steps (a finite amount of times). First we select a row \( \mathbf{w}_k \) and construct a continuous path that maps this row to one of the \( \mathbf{w}_i^* \); then we orthogonalize (w.r.t. such \( \mathbf{w}_i^* \)) the rest of rows \( \mathbf{w}_j, j \neq k \). These two steps are constructed so that \( \mathbf{A} \) never changes and therefore the loss is constant. The first step is described in Lemma 22 while the second is detailed in Lemma 23. At this point the parameter \( \theta = (\mathbf{u}, \mathbf{W}) \) verifies \( u_i = u_i^* \), \( \mathbf{w}_i = \mathbf{w}_i^* \) and \( \mathbf{w}_j \in \{\mathbf{w}_i^*\}^\perp \) for \( j \neq k \). In particular it holds

\[
\sum_{j=1 \; j \neq i}^{n} u_j^* w_j^*(w_j^*)^T = \sum_{j=1 \; j \neq k}^{p} u_k w_k w_k^T
\]
Therefore, an induction step applied on the reduced parameter values

\[ u_{-k} = (u_1, \ldots, \hat{u}_k, \ldots, u_p) \]

and \( W_{-k} = [w_1, \ldots, \hat{w}_k, \ldots, w_p]^T \), where \( P \leq \sum_{j=1, j\neq i}^n w_j^* e_j^T \in \mathbb{R}^{n \times (n-1)} \), concludes the proof. The fact that the non-zero components of \( u \) and \( W \) coincide with the first \( n \) is not necessary, but we can clearly assume it to hold w.l.o.g.

Lemma 22. The first step described in the Proof of Lemma 21 can be performed when \( p > 2n \).

Proof. Let \( E_+ = \{ k \in [p] : u_k = 1 \} \), \( E_- = \{ k \in [p] : u_k = -1 \} \) and \( p_+ = |E_+|, p_- = |E_-| \). Accordingly we define

\[ W_+ = ([w_k]_{k \in E_+})^T \in \mathbb{R}^{p_+ \times n} \quad \text{and} \quad W_- = ([w_k]_{k \in E_-})^T \in \mathbb{R}^{p_- \times n} \]

Notice that then we can write

\[ A = W_+^T W_+ - W_-^T W_- \]

The main step of the proof is to observe that \( A \) (and therefore the loss) is invariant to the action of orthogonal matrices \( Q_+ \in SO(p_+) \) and \( Q_- \in SO(p_-) \). So, if \( Q_+(t) \) (resp. \( Q_-(t) \)) is a continuous paths in \( SO(p_+) \) (resp. in \( SO(p_-) \)) starting at the identity, acting on \( W \) as

\[ W_+(t) \triangleq Q_+(t)W_+, \quad W_-(t) \triangleq Q_-(t)W_- \]

we have that

\[ A = W_+(t)^T W_+(t) - W_-(t)^T W_-(t) \]

is constant for all \( t \). Now, since \( p = p_+ + p_- > 2n \), it follows that either \( p_+ > n \) or \( p_- > n \). Assume w.l.o.g. that \( p_+ > n \). Since \( p_+ > n \), we can rotate the subspace generated by the columns of \( W_+ \) so that its first row is \( \mathbf{0} \). That is, there exist \( h \in \mathbb{R}^{p_+} \) non-zero such that \( h^T W_+ = 0 \) and \( ||h|| = 1 \). It suffices to choose a path \( Q(t) \) in \( SO(p_+) \) whose first row equals \( h \) at \( t = 1 \). It follows that \( Q(1)W_+ \) has a first row equal to \( \mathbf{0} \). We then set the corresponding \( u_1 = 0 \), which does not change the loss, and finally set \( w_1 \) to the desired eigenvector \( w_1^* \).

Lemma 23. Assume that after the step in Lemma 22 the first row of \( W_+ \) (resp. \( W_- \)) is given by \( w_1^* \). Then we can map all the other rows of \( W \) to be orthogonal to \( w_1^* \), while keeping \( A \) constant.

Proof. To simplify the notation we assume (w.l.o.g.) that \( w_1^* = w_1^* \) and that

\[ W = [w_1^*, w_2, \ldots, w_p]^T \]

Now we want to construct a path

\[ u_t = (u_{1,t}, u_2, \ldots, u_p) \]
\[ W_t = [w_{1,t}^*, w_{2,t}, \ldots, w_{p,t}]^T \]

such that \( w_{2,1}, \ldots, w_{p,1} \in \langle \{w_1^*\} \rangle^\perp \). To do this we simply take

\[ w_{k,t} = w_k - t(w_1^*, w_k)w_1^* \]
If \( A_t = \sum_{k=1}^{p} u_{k,t} w_{k,t} w_{k,t}^T \), we can show that there exists a choice of \( u_{1,t} \) such that \( A_t = A \) for all \( t \in [0,1] \). It holds that

\[
A_t = u_{1,t} w_1^*(w_1^*)^T + \sum_{k=2}^{p} u_k [(1-t)^2(w_k^1)^2 w_1^*(w_1^*)^T + (1-t) w_k^1(w_k^* w_1^* + w_k^* w_k^T) + \bar{w}_k \bar{w}_k^T]
\]

where \( w_k^1 = \langle w_k, w_1^* \rangle \) and \( \bar{w}_k = w_k - w_k^1 w_1^* \). In particular

\[
A_t = V^* \begin{bmatrix} a_t \\ b_t \end{bmatrix} A_{2,2,2}^T (V^*)^T
\]

where \( V^* = [w_1^*, \cdots, w_n^*] \in O(n) \). Since \( \sum_{k=2}^p u_k w_k = 0 \), it follows

\[
b_t = (1-t) \sum_{k=2}^p u_k w_k^1 \bar{w}_k = 0 \quad \text{for all } t \in [0,1]
\]

If we take

\[
u_{1,t} = \lambda_1 - (1-t)^2 \sum_{k=2}^p u_k (w_k^1)^2
\]

it holds that

\[
a_t = u_{1,t} + (1-t)^2 \sum_{k=2}^p u_k (w_k^1)^2 = \lambda_1 \quad \text{for all } t \in [0,1]
\]

Therefore, \( A_t = A \) constant. This concludes the proof of the lemma.

**Remark 1.** In the proof of Lemma 21 we assumed that (after rescaling) \( u \in \{\pm 1\}^p \). In general, it could be that \( u_k = 0 \) for some \( k \). In this case we can first map the corresponding vectors \( w_k \) to \( \mathbf{0} \) and the map such \( u_k \) to 1, without affecting the loss.

## B Proofs of Section 4

**Proof of Theorem 22.** We consider here the case \( m = 1 \), but the same proof can be extended to the case \( m > 1 \). We start by properly choosing a r.v. \( (X, Y) \). Be \( \bar{X} \in \mathcal{R}_2(\rho, n-1) \) a \((n-1)\) dimensional r.v. and \( \tilde{X} \in \mathcal{R}_2(\rho, 1) \) a one dimensional r.v. We consider \( \bar{X} = Z \bar{X}, \) \( \bar{X}_n = (1-Z)\tilde{X}_n \) and \( X = (\bar{X}, \tilde{X}_n) \), where \( Z \sim \text{Ber}(1/2) \) and \( \bar{X}, \tilde{X}_n, Z \) are independent. By hypothesis, \( p \leq 2^{-\dim(\rho, \bar{X})} \). The proof is based on the fact that (for a proper choice of \( \bar{X} \)) this implies that \( V_{\rho,p}^+ \) is not dense in \( V_{\rho,p}^+ \), where we defined

\[
V_{\rho,p}^+ = \{ \Phi(\cdot; \theta) : \theta \in [0,\infty)^p \times \mathbb{R}^{p \times n} \} \subseteq L_2 \bar{X}
\]

(see the remark at the end of the proof). The r.v. \( Y \) is taken to be \( Y = g_1(X) - g_2(X) \), where \( g_2 = \beta \psi_{\rho,\nu} \in V_{\rho,1}^+ \), \( \beta > 0 \), \( \nu = e_n \), and \( g_1 = \sum_{i=1}^p \alpha_i \psi_{\rho,\nu_i} \in V_{\rho,p}^+, \alpha \in (0,\infty)^p, \nu_i \in \{e_n\}^\perp, \) \( i \in [p] \), is such that

\[
\inf_{f \in V_{\rho,p-1}^+} E|f(X) - g_1(X)|^2 = \epsilon > 0
\]
We define
\[ V_{\rho,(p-1,1)} = \left\{ f = f_1 - f_2 : f_1 \in V_{\rho,p-1}^+, f_2 \in V_{\rho,1}^+ \right\} \]

Notice that, for every path \( \theta : t \in [0,1] \mapsto \theta_t \in \Theta \) such that \( \Phi(\cdot;\theta_0) \in V_{\rho,p}^+ \) and \( \Phi(\cdot;\theta_1) \in V_{\rho,(p-1,1)} \), there exists \( t_0 \in (0,1) \) such that \( \Phi(\cdot;\theta_{t_0}) \in V_{\rho,p}^+ \). Consider the lifted square loss function \( L : V_{\rho,p} \to [0,\infty) \) defined as
\[ L(f) = \mathbb{E}[f(X) - g(X)]^2 \quad \text{for } f \in V_{\rho,p} \]

We want to show that
\[ L_{(p-1,0)} = \min_{f \in V_{\rho,p-1}^+} L(f) > L_{(p,0)} = \min_{f \in V_{\rho,p}^+} L(f) > L_{(p-1,1)} = \min_{f \in V_{\rho,(p-1,1)}^+} L(f) \]

It holds that
\[ L_{(p-1,0)} = \min_{f \in V_{\rho,p-1}^+} \left\{ \mathbb{E}[f(X) - g_1(X)]^2 \right\} + 2 \min_{f \in V_{\rho,p}^+} \left\{ \mathbb{E}[f(X)g_2(X)] \right\} 
+ \mathbb{E}[g_2(X)]^2 - C\rho(0) 
\geq \epsilon + L_{(p,0)} - C\rho(0) \]

where \( C = \mathbb{E}[g_1(X)] + \mathbb{E}[g_2(X)] \), and that
\[ L_{(p,0)} = \min_{f \in V_{\rho,p}^+} \left\{ \mathbb{E}[f(X) - g_1(X)]^2 \right\} + 2 \min_{f \in V_{\rho,p}^+} \left\{ \mathbb{E}[f(X)g_2(X)] \right\} 
+ \mathbb{E}[g_2(X)]^2 - C\rho(0) 
\geq \beta^2 \mathbb{E}[\psi_{\rho,n}(X_n)]^2 - C\rho(0) \]

Finally, it holds that
\[ L_{(p-1,1)} \leq \min_{i \in [1,p]} \alpha_i^2 \mathbb{E}[\psi_{\rho,v_i}(X)]^2 \]

Given \( M > 0 \), up to multiply \( g_1 \) by a positive constant, it holds that
\[ \epsilon \geq M + C\rho(0) \]
\[ \beta^2 \geq \frac{M + C\rho(0) + \min_{i \in [1,p]} \alpha_i^2 \mathbb{E}[\psi_{\rho,v_i}(X)]^2}{\mathbb{E}[\psi_{\rho,v}(X_n)]^2} \]

This implies that the sets \( \Omega_1 = \{ \theta = (u, W) \in \Theta : u \in (0,\infty)^p \} \) and \( \Omega_2 = \{ \theta = (u, W) \in \Theta : u \in (-\infty,0)^p \times (0,\infty) \} \) satisfy the statement of the theorem. \( \square \)

Remark 2. In the proof of Theorem 12 we used the fact that, if \( p \geq 1 \) verifies \( p \leq \frac{1}{2} \text{dim}_s(\rho,n) \), then there exist \( X \in \mathcal{R}_d(\rho,n) \) such that \( V_{\rho,p-1}^+ \) is not dense in \( V_{\rho,p}^+ \) (in the \( L_2^X \) metric). Assume \( X \) is a \( n \)-dimensional standard Gaussian variable. If \( \rho \) is non-polynomial, this can be verified in the same way as in Remark 3. The only other case that we need to consider is \( \rho(z) = z^{2k} \) for \( k \geq 1 \) integer. If \( k = 1 \), then
\[ V_{\rho,p}^+ \simeq \{ M \in S^2(\mathbb{R}^n) : M \text{ is PSD} \} \]
In particular, this implies that $V^+_{\rho,p-1}$ is not dense in $V^+_{\rho,p}$ if $p \leq n = \dim_*(\rho, n)$ (which justifies the statement of Corollary 13). If $k > 1$, let $p \leq \frac{1}{2} \dim_*(\rho, n)$ and assume that $V^+_{\rho,p-1}$ is dense in $V^+_{\rho,p}$. This implies that every tensor $T = \sum_{i=1}^{p} \psi_i^{2k}$ can be written as $T = \sum_{i=1}^{p-1} \psi_i^{2k}$ for some $\psi_1, \ldots, \psi_{p-1} \in \mathbb{R}^n$. But this also implies that every tensor $T \in \mathbb{S}^{2k}(\mathbb{R}^n)$ has rank $\mathrm{rk}_S(T) \leq 2(\frac{1}{2} \dim_*(\rho, n) - 1) = \mathrm{rk}_S(2k, n) - 2$, which contradicts the definition of $\mathrm{rk}_S(2k, n)$.

C Proof of Theorem 15

Proof. With abuse of notation, we write $\langle w, x \rangle \triangleq \langle w(n) \rangle + w_{n+1}$ for $w \in \mathbb{S}^n, x \in \mathbb{R}^n$, where $w(n) = (w_1, \ldots, w_n)$ represents a neuron and $w_{n+1}$ a bias term. If we denote by $d\mu$ the probability distribution of $X$, the continuous function

$$\psi : (w, x) \in \mathbb{S}^n \times \mathbb{R}^n \mapsto \psi_w(x) = \rho(\langle w, x \rangle)$$

belongs to $L^2(\mathbb{S}^n \times \mathbb{R}^n, d\tau \otimes d\mu)$. We consider the kernel associated with the neural network architecture

$$k(x, y) = \int_{\mathbb{S}^n} \psi_w(x)\psi_w(y) \, d\tau(w) \quad (15)$$

The above defines a continuous symmetric, positive semi-definite kernel $k$, along with $\mathbb{H}$, the RKHS associated, and the integral operator $\Sigma : L^2(\mathbb{R}^n, d\mu) \to \mathbb{H} \subseteq L^2(\mathbb{R}^n, d\mu)$ defined as

$$f \mapsto \left( \Sigma f : x \mapsto \int_{\mathbb{R}^n} f(y)k(x, y) \, d\mu(y) \right)$$

The operator $\Sigma$ admits a spectral decomposition in $L^2(\mathbb{R}^n, d\mu)$: $\Sigma e_k = \lambda_k e_k$ for an orthonormal basis $\{e_k\}_{k \geq 1}$ of $L^2(\mathbb{R}^n, d\mu)$ and non-increasing sequence of non-negative eigenvalues $\{\lambda_k\}_{k \geq 1}$. Moreover the RKHS $\mathbb{H}$ is dense in $L^2(\mathbb{R}^n, d\mu)$ (see Lemma 26), which is equivalent to have $\lambda_k > 0$ for all $k \geq 1$. The expectation in $\rho, p$ provides a singular value decomposition for $\Sigma$ in terms of functions in $L^2(\mathbb{S}^n, d\tau)$. Indeed, given $g \in L^2(\mathbb{S}^n, d\tau)$, the linear operator $T : L^2(\mathbb{S}^n, d\tau) \to L^2(\mathbb{R}^n, d\mu)$ defined as

$$g \mapsto \left( Tg : x \mapsto \int_{\mathbb{S}^n} g(w)\psi_w(x) \, d\tau(w) \right)$$

satisfies $\Sigma = TT^*$. It follows that there exists an orthonormal basis of $L^2(\mathbb{S}^n, d\tau)$, $\{f_k\}_{k \geq 1}$ such that $Tf_k = \lambda_k^{1/2} e_k$ and therefore $\psi_w = \sum_{k=1}^{\infty} \lambda_k^{1/2} f_k(w)e_k$. Finally, it can be shown [1] that in fact $\mathbb{H} = \text{Im}(T)$, and thus $\mathbb{H}$ consists of functions $f$ that can be written, for some $g \in L^2(\mathbb{S}^n, d\tau)$ as

$$f(x) = \int_{\mathbb{S}^n} g(w)\psi_w(x) \, d\tau(w) = \langle g, \psi(\cdot, x) \rangle_{L^2(\mathbb{S}^n, d\tau)} \quad \text{for } x \in \mathbb{R}^n$$

For an account of these properties, we refer to Bach [2]. Thanks to the density of $\mathbb{H}$ in $L^2(\mathbb{R}^n, d\mu)$, we can assume, without loss of generality, that

$$f^*(x) = \int_{\mathbb{S}^n} g^*(w)\psi_w(x) \, d\tau(w)$$
for some $g^* \in L^2(S^n, d\tau)$. Now, given an initial set of first layer weights $w_1, \ldots, w_p \in S^n$ sampled i.i.d. from $d\tau$, and $W = [w_1, \ldots, w_p]^T$, we define the empirical kernel

$$k_W(x, y) = \frac{1}{p} \sum_{i=1}^{p} \rho((x, w_i))\rho((y, w_i))$$

which in turn defines an empirical RKHS $\mathbb{H}_W$. Keeping the first layer weights fixed and optimizing the second layer weights thus gives us the ability to find a function $f^*_W \in \mathbb{H}_W$ that best approximates $f^*$:

$$\|f^*_W - f^*\|_{L^2(\mathbb{R}^n, d\mu)} = \min_{f \in \mathbb{H}_W} \|f - f^*\|_{L^2(\mathbb{R}^n, d\mu)} = R(W)$$

Given an initial parameter parameter value $\tilde{\theta} = (\tilde{u}, \tilde{W})$ (here we incorporated $\tilde{b}$ in $\tilde{W}$) as in the statement, consider the path

$$\theta_t = (tq(\tilde{W}) + (1-t)\tilde{u}, \tilde{W}) \quad \text{where} \quad q(\tilde{W}) = \arg\min_{u \in \mathbb{R}^p} L(\theta)|_{\theta=(u, \tilde{W})}$$

By convexity of $L$, the function $t \in [0, 1] \mapsto L(\theta_t)$ is non-increasing and it holds that

$$L(\theta_1) \leq R(X, Y) + R(\tilde{W})$$

Applying Proposition 1 from Bach [2], it holds that

$$R(\tilde{W}) \leq 4\lambda \quad \text{if} \quad p \geq 5d(\lambda) \log(16d(\lambda)/\delta)$$

with probability greater or equal than $1 - \delta$, where

$$d(\lambda) = \max_{w \in S^n} \mathbb{E}[\varphi_w(X)((\Sigma + \lambda I)^{-1}\psi_w)(X)]$$

$$= \max_{w \in S^n} \sum_{k=1}^{\infty} \frac{\lambda_k}{\lambda_k + \lambda} f_k(w)^2 \leq \lambda^{-1} \max_{w \in S^n} \sum_{k=1}^{\infty} \lambda_k f_k(w)^2 = \lambda^{-1} \max_{w \in S^n} \|\psi_w\|_{L^2(\mathbb{R}^n, d\mu)}^2$$

This shows part 1 of the statement. To prove part 2, notice that $f^*_W = \Phi(:, \theta)$ with $\theta = (u^*_W, W)$ for some $u^*_W \in \mathbb{R}^p$. By taking $u_k = \frac{1}{p}g^*(w_k)$ for $k \in [p]$ and denoting $Z(w) := g^*(w)\psi_w$ and by $Z$ the r.v. $Z = Z(v)$, for $v \sim d\tau$, with values in $L^2(\mathbb{R}^n, d\mu)$, it holds

$$R(W) \leq \left\| \frac{1}{p} \sum_{k=1}^{p} Z(w_k) - \mathbb{E}_r[Z] \right\|_{L^2(\mathbb{R}^n, d\mu)}$$

Note that $C \doteq \sup_{w \in S^n} \|Z(w)\|_{L^2(\mathbb{R}^n, d\mu)} \leq \|g^*\|_{L^\infty(S^n, d\tau)} \max_{w \in S^n} \|\psi_w\|_{L^2(\mathbb{R}^n, d\mu)} < \infty$ if $\|g^*\|_{L^\infty(S^n, d\tau)} < \infty$. Then, applying Lemma 23 to the bound (16), we get that

$$\mathbb{P}_r\{R(W) \leq \varepsilon\} \geq 1 - \exp\left\{-\left(\varepsilon - \sqrt{v(p)}\right)^2/(2v(p))\right\}$$

for every $\varepsilon \geq \sqrt{v(p)}$, with $v(p) = C^2/p$. The result follows by taking $\varepsilon = v(p)^{1/2} + p^{1/2-1/2}$.
D Proofs of Section 2.1

Proof of Lemma 3. If \( \rho \) is a polynomial of any degree \( d \), then it holds that \( \dim^* (\rho, n) < \infty \). Indeed, let \( \rho(z) = a_0 + a_1 z + \cdots + a_d z^d \), for some \( a_k \in \mathbb{R} \). If \( I = \{k \in [0, d] : a_k \neq 0\} \), then

\[
V_\rho \subseteq \mathbb{R}_I[x] \triangleq \{ z \mapsto \sum_{k \in I} \alpha_k z^k : \alpha \in \mathbb{R}^{|I|} \}
\]

It follows that

\[
\dim^* (\rho, n) = \dim(V_\rho) \leq \dim(\mathbb{R}_I[x]) = \sum_{k=0}^{d} \binom{n + k - 1}{k} 1_{\{a_k \neq 0\}} = O(n^d)
\]

This proves one implication. We prove the other one by contradiction. Assume now that \( \rho \) is not a polynomial and that \( \dim(V_\rho) = q < \infty \). Thanks to Theorem 1 in Leshno et al. [30], for every continuous function \( g : \mathbb{R}^n \to \mathbb{R} \), any compact set \( K \subset \mathbb{R}^n \), and any \( \varepsilon > 0 \) there exist \( h \in V_\rho \) such that

\[
\sup_{x \in K} |h(x) - g(x)| < \varepsilon \tag{17}
\]

Now, let \( g : \mathbb{R}^n \to \mathbb{R} \) be a continuous function supported on a compact set \( C \subset \mathbb{R}^n \). We call \( C_c(\mathbb{R}^n) \) the set of the real-valued continuous functions from \( \mathbb{R}^n \) with compact support. Thanks to (17), we can find a sequence of compact sets \( \{K_m\}_{m \geq 1} \) of \( \mathbb{R}^n \) such that

\[
C \subseteq K_1 \subseteq K_2 \subseteq \cdots \subseteq K_m \subseteq \cdots \subseteq \bigcup_{m=1}^{\infty} K_m = \mathbb{R}^n
\]

and a sequence of functions \( \{h_m\}_{m \geq 1} \subseteq V_\rho \) such that

\[
\|g - h_m 1_{K_m}\|_{L^2_K} = \|(g - h_m) 1_{K_m}\|_{L^2_K} < 2^{-m}
\]

In particular this implies that

\[
\|h_n 1_{K_n} - h_m 1_{K_m}\|_{L^2_K} < 2^{1-\min\{n,m\}} \to 0
\]

as \( n, m \to \infty \), i.e. \( \{h_m 1_{K_m}\}_{m \geq 1} \) is a Cauchy sequence in \( L^2_K \) and therefore it admits a limit

\[
\lim_{n \to \infty} h_m 1_{K_m} = g \in L^2_K.
\]

Since \( \dim(V_\rho) = q < \infty \), there exists \( w_1, \ldots, w_q \in \mathbb{R}^n \) such that every \( h \in V_\rho \) can be written as

\[
h(x) = \langle u, \gamma(x) \rangle
\]

for some \( u \in \mathbb{R}^q \), where \( \gamma(x) = (\rho(\langle w_1, x \rangle), \ldots, \rho(\langle w_q, x \rangle)) \). Let \( \{u_m\}_{m \geq 1} \subseteq \mathbb{R}^q \) such that \( h_m(x) = \langle u_m, \gamma(x) \rangle \). Thanks to the above calculations, we know that the sequence \( \{\|h_m 1_K\|_{L^2_K}\}_{m \geq 1} \) is bounded for any arbitrary compact set \( K \subseteq \mathbb{R}^n \). Since

\[
\|h_m 1_K\|_{L^2_K}^2 = u_m^T M u_m
\]

where \( M = \mathbb{E}[\gamma(X) \gamma(X)^T 1_{\{X \in K\}}] \in \mathbb{R}^{q \times q} \), this implies that the sequence \( \{u_m\}_{m \geq 1} \) is bounded (unless \( g = 0 \)). Therefore (up to extracting a sub-sequence) we can assume that it has a limit \( u \in \mathbb{R}^q \). If we call \( h \in V_\rho \) the function defined as \( h(x) = \langle u, \gamma(x) \rangle \), it is easy to check (from the above calculations) that \( h = g \in L^2_K \). This shows that \( C_c(\mathbb{R}^n) \subseteq V_\rho \), which in turn implies that \( V_\rho \) is dense in \( L^2_K \) (since \( C_c(\mathbb{R}^n) \) is dense in \( L^2_K \)). But this is impossible, since \( \dim(V_\rho) = q < \infty = \dim(L^2_K) \). Therefore, it must hold \( \dim(V_\rho) = \infty \). \qed
Proof of Lemma 3. Let $\theta = (u, W) \in [0, \infty)^p \times \mathbb{R}^{p \times n}$. For every $x \in \mathbb{R}^n$ it holds

$$
\Phi(x; \theta) = \sum_{i=1}^{p} u_i (\langle w_i, x \rangle)^k = \sum_{i=1}^{p} u_i \langle w_i^\otimes k, x^\otimes k \rangle_F = \langle \sum_{i=1}^{p} u_i w_i^\otimes k, x^\otimes k \rangle_F
$$

For any $p \geq 1$ and $(u, W) \in [0, \infty)^p \times \mathbb{R}^{p \times n}$, $\sum_{i=1}^{p} u_i w_i^\otimes k \in S^k(\mathbb{R}^n)$. By definition of $\text{rk}_S(k, n)$, it follows that there exists $q \leq \text{rk}_S(k, n)$ and $\hat{\theta} = (\hat{u}, \hat{W}) \in [0, \infty)^q \times \mathbb{R}^{q \times n}$ such that

$$
\sum_{i=1}^{p} u_i w_i^\otimes k = \sum_{i=1}^{q} \tilde{u}_i \tilde{w}_i^\otimes k \implies \Phi(; \theta) = \Phi(; \hat{\theta})
$$

By definition of $\dim_s(\rho, n)$, this implies that $\dim_s(\rho, n) \leq \text{rk}_S(k, n)$. The equality follows by choosing $(u, W) \in [0, \infty)^p \times \mathbb{R}^{p \times p}$ such that $\text{rk}_S(\sum_{i=1}^{p} u_i w_i^\otimes k) = \text{rk}_S(k, n)$.

\[\square\]

Proof of Lemma 4. If $\rho$ is polynomial, then one implication follows by Lemma 3. Now, assume that $\rho \in L^2(\mathbb{R}, e^{-x^2/2} \, dx)$ is a continuous non-polynomial activation and let $X \sim N(0, I)$ be a r.v. in $\mathcal{R}_2(\rho, n)$. Then, we can write $\rho(z) = \sum_{k=0}^{\infty} \hat{\rho}_k h_k(z)$, where $h_k$ is the $k$-th Hermite polynomial. It follows that, for $\theta = (u, W)$,

$$
E|\Phi(X; \theta)|^2 = \sum_{k=1}^{\infty} \hat{\rho}_k^2 \left\| \sum_{i=1}^{p} u_i w_i^\otimes k \right\|_F^2
$$

(see Lemma 1 from Mondelli and Montanari [33]). Since $\rho$ is not polynomial and $n > 1$, $V_{\rho, p} \neq V_{\rho, p+1}$. Indeed, if $V_{\rho, p} = V_{\rho, p+1}$, then $V_{\rho, p} = V_{\rho, q}$ for every $q > p$. Let $k$ be a positive integer such that $\hat{\rho}_k \neq 0$ and such that $\text{rk}_S(k, n) > p$. Let $G = \sum_{i=1}^{q} \alpha_i v_i^\otimes k$ a symmetric tensor with $\text{rk}_S(G) = q = \text{rk}_S(k, n)$ and $g = \sum_{i=1}^{q} \alpha_i \psi_{\rho, v_i}$. If $g \in V_{\rho, p}$, then there exists $\hat{\theta} = (\hat{u}, \hat{W}) \in \Theta = \mathbb{R}^p \times \mathbb{R}^{p \times n}$ such that

$$
0 = E|\Phi(X; \theta) - g(X)|^2 = \sum_{k=1}^{\infty} \hat{\rho}_k^2 \left\| \sum_{i=1}^{p} u_i w_i^\otimes k - \sum_{i=1}^{q} \alpha_i v_i^\otimes k \right\|_F^2
$$

But this would imply that $\text{rk}_S(G) \leq p$, which is a contradiction. This concludes the proof.

\[\square\]

Remark 3. The proof of Lemma 4 can be extended to prove the following (stronger) fact, which we will use to prove Corollary 13. Assume that $\rho \in L^2(\mathbb{R}, e^{-x^2/2} \, dx)$ is a continuous non-polynomial activation and let $X \sim N(0, I)$ be a r.v. in $\mathcal{R}_2(\rho, n)$. Then it holds that

$$
\infty = \max\{p \geq 1 : V_{\rho, p-1} \text{ is not dense in } V_{\rho, p}\} \leq \dim_s(\rho, X)
$$

To prove this, since by the proof of Lemma 3 we know that $V_{\rho, p} \neq V_{\rho, p+1}$, we only need to show that $V_{\rho, p}$ is closed in $L^2_X$ for every $p \geq 1$. To see this, let $\{f_n\}_{n \geq 1}$ be a sequence of functions in $V_{\rho, p}$ which converges in $L^2_X$. Assume that $f_n$ is not zero for infinitely many $n$ (otherwise $\lim_{n \to \infty} f_n = 0 \in V_{\rho, p}$). Then $\|f_n\|^2_{L^2_X}$ is bounded and so, by (13), there exists a bounded sequence $\{\|\theta_n\|\}_{n \geq 1} \subset \Theta$ such that $f_n = \Phi(\cdot; \theta_n)$ for every $n \geq 1$. Therefore (up to extracting a sub-sequence) we can assume that $\lim_{n \to \infty} \theta_n = \hat{\theta}$ exists finite. But this implies that $\lim_{n \to \infty} f_n = \Phi(\cdot; \hat{\theta}) \in V_{\rho, p}$. This shows that $V_{\rho, p}$ is closed and therefore proves (14).

\[\text{Here, dense is meant in the sense of the } L^2_X \text{ norm.}\]
E  Proofs of Additional Lemmas

Lemma 24. Consider the optimization problem

$$\arg \min_{\mathbf{W} \in \mathbb{R}^{m \times n}} \ell(\mathbf{W}) \quad \text{where} \quad \ell(\mathbf{W}) = \mathbb{E} \| \mathbf{WX} - \mathbf{Y} \|^2$$

(20)

for two square integrable r.v.'s $\mathbf{X}$ and $\mathbf{Y}$ with values in $\mathbb{R}^n$ and $\mathbb{R}^m$ respectively. Then one solution to (20) is given by

$$\mathbf{W} = \Sigma_{\mathbf{YX}} \Sigma_{\mathbf{X}}^\dagger$$

(21)

Similarly, one solution to the optimization problem

$$\arg \min_{\mathbf{U} \in \mathbb{R}^{m \times p}} \ell(\mathbf{U}; \mathbf{W}) \quad \text{where} \quad \ell(\mathbf{U}; \mathbf{W}) = \mathbb{E} \| \mathbf{UXW} - \mathbf{Y} \|^2$$

for any $\mathbf{W} \in \mathbb{R}^{p \times n}$ is given by

$$\mathbf{U} = q(\mathbf{W}) \doteq \Sigma_{\mathbf{YX}} \mathbf{W}^T (\mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T)^\dagger$$

(22)

Assuming $\Sigma_{\mathbf{X}}$ invertible, the minimal value obtained by $\ell(\mathbf{U}; \mathbf{W})$ is given by

$$\ell(q(\mathbf{W}); \mathbf{W}) = \text{tr}(\Sigma_{\mathbf{Y}}) - \text{tr}((\mathbf{WK})^\dagger (\mathbf{WK}) \mathbf{M})$$

(23)

where $K = (\Sigma_{\mathbf{X}})^{1/2}$ and $\mathbf{M} = K^{-1} \Sigma_{\mathbf{XY}} \Sigma_{\mathbf{YX}} K^{-1}$. If $\mathbf{M} = \sum_{i=1}^n \lambda_i \mathbf{v}_i \mathbf{v}_i^T$ is the SVD of $\mathbf{M}$, the quantity (23) is minimized over $\mathbf{W}$ for $((\mathbf{WK})^\dagger (\mathbf{WK}))^\dagger = \sum_{i=1}^{p/n} \mathbf{v}_i \mathbf{v}_i^T$.

Proof. The first part of the lemma can be shown by writing problem (20) as

$$\arg \min_{\mathbf{W} \in \mathbb{R}^{m \times n}} \ell(\mathbf{W}) \quad \text{where} \quad \ell(\mathbf{W}) = \text{tr}(\mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T) - 2 \text{tr}(\Sigma_{\mathbf{YX}} \mathbf{W}^T)$$

(24)

and by taking $\mathbf{W}$ as a stationary point of the above $\ell(\mathbf{W})$. Using this fact, one minima of the function $\ell(U; \mathbf{W})$ is given by

$$\mathbf{U} = \Sigma_{\mathbf{YX}} \mathbf{W} (\Sigma_{\mathbf{W}X}^\dagger = \Sigma_{\mathbf{YX}} \mathbf{W}^T (\mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T)^\dagger$$

Now assume that $\Sigma_{\mathbf{X}}$ is invertible; let $K = (\Sigma_{\mathbf{X}})^{1/2}$ and $\mathbf{M} = K^{-1} \Sigma_{\mathbf{XY}} \Sigma_{\mathbf{YX}} K^{-1}$. Then it holds

$$\ell(q(\mathbf{W}); \mathbf{W}) = \text{tr}(q(\mathbf{W}) \mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T q(\mathbf{W})^T) - 2 \text{tr}(\Sigma_{\mathbf{YX}} \mathbf{W}^T) + \text{tr}(\Sigma_{\mathbf{Y}})$$

= $$\text{tr}(\Sigma_{\mathbf{YX}} \mathbf{W}^T (\mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T)^\dagger \mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T (\mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T)^\dagger \mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T)$$

= $$2 \text{tr}(\Sigma_{\mathbf{YX}} \mathbf{W}^T (\mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T)^\dagger \mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T)$$

= $$- \text{tr}(\Sigma_{\mathbf{YX}} \mathbf{W}^T (\mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T)^\dagger \mathbf{W} \Sigma_{\mathbf{X}} \mathbf{W}^T)$$

= $$- \text{tr}(\mathbf{M}(\mathbf{WK})^T ((\mathbf{WK})(\mathbf{WK})^T)^\dagger (\mathbf{WK})) + \text{tr}(\Sigma_{\mathbf{Y}})$$

Finally, we notice that the matrix $(\mathbf{WK})^\dagger (\mathbf{WK})$ is the orthogonal projection on the space spanned by the rows of $\mathbf{WK}$, which we denote by $\mathbf{P}_{\mathbf{WK}}$. In particular $\mathbf{P}_{\mathbf{WK}}$ has the form
\[ P_{W^K} = \sum_{i=1}^{r} w_i w_i^T \] for some \( \{w_1, \ldots, w_r\} \subset \mathbb{R}^n \) orthonormal vectors and \( r \leq p \wedge n \). Therefore, minimize \( \ell(q(W); W) \) over \( W \) it is equivalent to maximize the quantity

\[ \sum_{i=1}^{r} w_i^T M w_i \]

over the sets of \( w_1, \ldots, w_r \) orthonormal vectors of \( \mathbb{R}^n \), \( r \leq p \wedge n \). Clearly, this is for \( w_1 = v_1, \ldots, w_{p \wedge n} = v_{p \wedge n} \). This concludes the proof of the lemma.

**Lemma 25.** Let \( X_1, \ldots, X_n \) be independent zero-mean r.v.’s taking values in a separable Hilbert space such that \( \|X_i\| \leq c_i \) with probability one and denote \( v = \sum_{i=1}^{n} c_i^2 \). Then, for all \( t \geq v \), it holds

\[ \Pr\left\{ \left\| \sum_{i=1}^{n} X_i \right\| > t \right\} \leq e^{-(t-\sqrt{n})^2/(2v)} \]

**Proof.** The proof can be found in Boucheron et al. [8], Example 6.3.

**Lemma 26.** Be \( \mathbb{H} \subset L^2_X \) the RKHS defined in the proof of Theorem 15. Then \( \mathbb{H} \) is dense in \( L^2_X \).

**Proof.** First, note that the function \( x \in \mathbb{R}^n \mapsto k(x, x) \) is in \( L^1(\mathbb{R}^n, d\mu) \). Indeed

\[
\int_{\mathbb{R}^n} \int_{\mathbb{S}^n} \psi_w(x)^2 \, d\tau(w) \, d\mu(x) = \int_{\mathbb{R}^n} (1 + \|x\|^2) \int_{\mathbb{S}^n} \psi_w(x/\|x\|)^2 \, d\tau(w) \, d\mu(x) \\
\leq (1 + \mathbb{E}\|X\|^2) \max_{w,y \in \mathbb{S}^n} \psi_w(y)^2 
\]

This implies that \( \mathbb{H} \subseteq L^2(\mathbb{R}^n, d\mu) \). Now, we would like to show that \( V_\rho \) is dense in \( \overline{\mathbb{H}} \), where

\[ V_\rho = \left\{ \sum_{i=1}^{k} u_i \psi_{w_i} : u \in \mathbb{R}^k, \{w_1, \ldots, w_k\} \subseteq \mathbb{S}^n, k \geq 1 \right\} \]

It suffices to show that, for every \( w \in \mathbb{S}^{n-1} \), there exists a sequence \( \{f_n\}_{n \geq 1} \subseteq \mathbb{H} \) such that

\[ f_n \to \psi_w \text{ in } L^2_X. \]

Choose \( g_k \in L^2(\mathbb{S}^n, d\tau) \) such that \( \text{supp}(g_k) \subseteq B_{1/k}(w) = \{v \in \mathbb{S}^n : \|v-w\| \leq 1/k\} \), \( \int_{\mathbb{S}^n} g(v) \, d\tau(v) = 1 \) and \( g_k \geq 0 \), and define \( f_k \in \mathbb{H} \) as \( f_k(x) = \int_{\mathbb{S}^n} g_k(v) \psi_V(x) \, d\tau(x) \).

Then

\[ \|f_k - \psi_w\|_{L^2(\mathbb{R}^n, d\mu)}^2 = \int_{\mathbb{R}^n} \left( \int_{\mathbb{S}^n} g_k(v)(\psi_V(x) - \psi_w(x)) \, d\tau(v) \right)^2 \, d\mu(x) \\
\leq (1 + \mathbb{E}\|X\|^2) \max_{v \in B_{1/k}(w)} \max_{y \in \mathbb{S}^n} (\psi_V(y) - \psi_w(y))^2 \to 0 \]

as \( k \to \infty \). This shows that \( V_\rho \) is dense in \( \overline{\mathbb{H}} \). Thanks to Theorem 1 in Hornik [27], it holds that \( V_\rho \) is dense in \( L^2(\mathbb{R}^n, d\mu) \). This implies the statement of the lemma.