Learning Single-Index Models with Shallow Neural Networks

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Abstract

Single-index models are a class of functions given by an unknown univariate "link" function applied to an unknown one-dimensional projection of the input. These models are particularly relevant in high dimension, when the data might present low-dimensional structure that learning algorithms should adapt to. While several statistical aspects of this model, such as the sample complexity of recovering the relevant (one-dimensional) subspace, are well-understood, they rely on tailored algorithms that exploit the specific structure of the target function. In this work, we introduce a natural class of shallow neural networks and study its ability to learn single-index models via *gradient descent*. More precisely, we consider shallow networks in which biases of the neurons are frozen at random initialization. We show that the corresponding optimization landscape is benign, which in turn leads to generalization guarantees that match the optimal sample complexity of dedicated semi-parametric methods.

1 Introduction

High-dimensional learning with both computational and statistical guarantees remains an outstanding challenge, with even more relevance in the face of current scaling trends. One important question which has seen considerable attention recently is to understand the advantages brought by non-linear learning models, such as neural networks, over more mature (from a theoretical standpoint) counterparts, such as kernel methods [32, 33, 49, 13], even in their simplest shallow instantiations.

While approximation benefits of shallow neural networks over non-adaptive kernels have been known for decades [8, 40], an important piece of this theoretical puzzle was provided by the *statistical* analysis of [5], which hinted at an inherent advantage of neural networks for extracting information from high-dimensional data with a "hidden" low-dimensional structure. Alas, the remaining piece of this puzzle, namely providing *computational* guarantees, is still mostly unresolved.

Several computational *hardness* results for learning functions that can be efficiently approximated by shallow neural networks [18, 26, 45, 17] have been established in the literature, which rule out positive results in the general setting. On the other hand, progress has been made on the positive side [1, 2, 43] by focusing on function classes with strong structural properties, thereby showcasing the adaptive representation learning capabilities of neural networks.

This work aligns with the latter effort, and focuses on the class of *single-index models*. Single-index models are high-dimensional functions $F : \mathbb{R}^d \to \mathbb{R}$ of the form $F_*(x) = f_*(\langle \theta^*, x \rangle)$, where *both* the univariate "link" function $f_* : \mathbb{R} \to \mathbb{R}$ and relevant (one-dimensional) subspace $\theta^* \in \mathbb{S}^{d-1}$ are unknown. These models have been extensively studied in the statistics literature [16, 28, 19], leading to dedicated algorithmic procedures, and can be provably approximated with shallow neural networks without incurring in a curse-of-dimensionality [5]. In contrast, the analysis of neural

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network learning using gradient-descent techniques has been more heavily focused on the so-called "Teacher-Student" setup [27, 24, 50, 51, 3], where the link function f is assumed to be known.

The mix of a high-dimensional parametric component (the hidden direction) with a low-dimensional non-parametric one (the link function) in single-index models naturally suggests a shallow neural network architecture where the inner weights are "active", while the biases are "lazy" [14]. We instantiate such an architecture by *freezing* the biases at their random initialization, and analyze gradient descent dynamics on the remaining free parameters in the continuous-time limit.

Our main results establish that as soon as the width N of the network is bigger than a quantity, which depends solely on the smoothness properties of the link function f_*[1], gradient descent recovers the unknown direction θ^* and approximates the univariate link function f_* with optimal sample and time complexity $O(d^s)$ (Theorem 5.1), where s is the so-called *information-exponent* of the link function [3]. The information exponent roughly captures the signal strength, which here refers to the alignment between the network direction θ and the hidden direction θ^*, at typical initializations.

The success of gradient descent relies on the benign optimization landscape of the empirical loss, though the presence of degenerate saddles requires a careful convergence analysis leveraging uniform convergence results for the empirical landscape [36, 20]. We show that gradient descent over our proposed neural network architecture solves two distinct problems–univariate non-parametric kernel ridge regression and non-convex optimization in high dimension–*simultaneously* and *efficiently*, cementing its role as a versatile algorithm for high-dimensional learning. We illustrate our theoretical results with experiments in Appendix D.

2 Related Work

Our work builds upon methods from different areas in statistics, optimization, and machine learning.

Single–index and multi-index models. A useful modeling assumption in high-dimensional regression is that the regression function $F(x) = \mathbb{E}[y|x]$ only depends on one or a few directions. This leads to the single-index model $F(x) = f_*(\langle\theta^*, x\rangle)$, and multi-index model $F(x) = f_*(\langle\theta_1^*, x\rangle, \ldots, \theta_k^*, x\rangle)$, with k typically much smaller than the dimension. Such models have a long history in the statistics literature and different methods exist for various estimation problems, including projection pursuit [21], slicing [30], gradient-based estimators [31], and moment-based estimators [16]. When the function f_* is also to be estimated, we face a semi-parametric problem involving parameter recovery of θ^* and non-parametric estimation of f_*. Our work is closely related to [19], which also characterizes the population landscape of certain objectives by leveraging Gaussian data. Single and multi-index models are also studied in [5] in the context of shallow neural networks, where it is shown that certain models of infinite-width shallow networks can adapt to such low-dimensional structure, though no tractable algorithms are introduced. Finally, [1] studies the learnability of functions on the hypercube by shallow neural networks and stochastic gradient descent and introduces the *merged staircase property*, which provides necessary and sufficient conditions for learnability with linear sample complexity $n = O(d)$. While they learn a broader class of functions (including multi-index model) for a more efficient sample complexity regime ($O(d)$ vs $O(d^s)$), our work captures the regime of semi-parametric estimation by considering Gaussian data without the sparsity constraints restrictions on F implied by their merged staircase property.

Teacher–student models. In the context of neural networks, several works have considered the teacher–student setting, where the target function F takes the form of a neural network with the same activation as network used for learning [27, 24, 50, 51, 3]. In this case the problem does not involve non-parametric estimation as in our setup, but this line of work often involves studying optimization landscapes similar to ours for estimating hidden directions.

Kernels and random features. Our work builds on the kernel methods literature for approximation and non-parametric regression [44, 7], their links with neural networks [15, 5], and in particular on random feature approximation [41, 6, 42, 37].

[1] Note that this quantity is independent of the input dimension d as the link function f_* is univariate.

Non-convex optimization landscapes. There is a vast literature studying tractable non-convex optimization landscapes, arising from high-dimensional statistics and statistical physics [35, 34, 22, 4, 46, 10, 24]. A particular aspect of our setup is that the optimization landscape does *not* have the strict saddle property, which is often leveraged to establish global convergence [29].

3 Preliminaries

We focus on regression problems under a single-index model with Gaussian input data. Specifically, we assume d-dimensional inputs $x \sim \gamma_d := \mathcal{N}(0, I_d)$, and labels

$$y = F^*(x) + \epsilon = f_*(\langle \theta^*, x \rangle) + \epsilon,$$

where $\theta^* \in \mathbb{S}^{d-1}$ and ϵ is random noise such that $\mathbb{E}[\epsilon|x] = 0$, $\mathbb{E}[\epsilon^2|x] \leq \sigma^2$.

Shallow networks and random features. We consider learning algorithms based on shallow neural networks of the form

$$G(x; c, \theta) = c^\top \Phi(\langle \theta, x \rangle) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} c_i \phi(\langle \theta, x \rangle - b_i),$$

with $\theta \in \mathbb{S}^{d-1}$, where $\phi(u) = \max\{0, u\}$ is the ReLU activation, $b_i \sim \mathcal{N}(0, \tau^2)$ (we assume $\tau > 1$) are random "bias" scalars that are frozen throughout training, and $\Phi(u) = \frac{1}{\sqrt{N}}(\phi(u - b_i))_{i \in [N]}$ is the vector of random features. If we also fix the direction θ, learning c alone may be seen as a random feature model [41] that approximates a kernel method with the following kernel:

$$\kappa(u, v) = \mathbb{E}_{b \sim \gamma_\tau}[\phi_b(u)\phi_b(v)] \ , \tag{1}$$

where $\phi_b(u) := \phi(u - b)$ and $\gamma_\tau = \mathcal{N}(0, \tau^2)$ is the Gaussian measure on $\mathbb{R}$ with mean zero and variance τ^2. The kernel κ corresponds to an RKHS $\mathcal{H}$, which we precisely define as

$$\mathcal{H} := \left\{ f : \mathbb{R} \to \mathbb{R} \mid \ f(u) = \int c(b)\phi(u - b) d\gamma_\tau(b), \ c \in L_2(\gamma_\tau) \right\} \ .$$

The following lemma characterizes the corresponding RKHS norm $\| \cdot \|_{\mathcal{H}}$.

Lemma 3.1 (RKHS Sobolev Representation, [48, Theorem 5])**.** *The RKHS norm in $\mathcal{H}$ is given by*

$$\|f\|_{\mathcal{H}}^2 = \begin{cases} \int \frac{|f''(u)|^2}{\gamma_\tau(u)} du & \text{if } \lim_{u \to -\infty} f(u) = \lim_{u \to -\infty} f'(u) = 0, \\ \infty & \text{otherwise} \ . \end{cases} \tag{2}$$

where f'' is defined in the generalised (Sobolev) sense.

Remark 3.2. *The boundary conditions for this RKHS can be relaxed by symmetrizing the kernel, ie $\kappa_s(u, v) = \frac{1}{2}(\kappa(u, v) + \kappa(-u, -v))$, but we will keep the original boundary conditions and assume them on f_* for simplicity and w.l.o.g.*

Hermite decompositions. Given that our data is normally distributed, we consider the family of (normalized) Hermite polynomials $\{h_j\}_{j \in \mathbb{N}}$, which form an orthonormal basis of $L^2(\gamma)$, the space of squared-integrable function under the Gaussian measure $\gamma := \mathcal{N}(0, 1)$. We will denote by $f_* = \sum_j \alpha_j h_j$ the Hermite decomposition of the target link function.

We apply the following useful properties of Hermite polynomials [39]:

$$h_j' = \sqrt{j} h_{j-1} \quad \text{and} \quad \langle h_j(\langle \theta, \cdot \rangle), h_{j'}(\langle \theta', \cdot \rangle) \rangle_{\gamma_d} = \delta_{j,j'} \langle \theta, \theta' \rangle^j,$$

where $\langle \cdot, \cdot \rangle_{\gamma_d}$ is the inner product in $L^2(\gamma_d)$ and δ the Kronecker delta. We will assume throughout that $\|f_*\|_\gamma^2 = \sum_j \alpha_j^2$, $\|f_*'\|_\gamma^2 = \sum_j j\alpha_j^2$, and $\|f_*''\|_\gamma^2 = \sum_j j(j-1)\alpha_j^2$ are all finite (see Assumption 4.1).

Definition 3.3 (Population loss)**.** *We define the L_2-regularized population loss by*

$$L(c, \theta) = \mathop{\mathbb{E}}_{x \sim \gamma_d}[(F_{\theta^*}(x) - G(x; c, \theta))^2] + \lambda \|c\|^2 \ .$$

From features to Hermite coefficients. To precisely characterize the landscape of $L(c, \theta)$, we introduce notation to represent the relationship each student feature ϕ_b in terms of Hermite polynomials h_j. We define the linear integral operator $\mathcal{T} : L_2(\gamma) \to \mathbb{R}^N$ by

$$(\mathcal{T} f)_i := \frac{1}{\sqrt{N}} \langle f, \phi_{b_i} \rangle_\gamma \ . \tag{3}$$

Note that the operator $\mathcal{T}$ has rank N almost surely. We abuse notation to equivalently let $\mathcal{T}(j, b_i) := \frac{1}{\sqrt{N}} \langle h_j, \phi_{b_j} \rangle_\gamma = (\mathcal{T} h_j)_i$ and observe that $(\mathcal{T} f)_i = \sum_j \mathcal{T}(j, b_i)$. Observe that $\mathcal{T}$ has an adjoint $\mathcal{T}^* : \mathbb{R}^N \to L_2(\gamma)$ defined as $(\mathcal{T}^* c)(u) = \frac{1}{\sqrt{N}} \sum_{i=1}^N c_i \phi(u - b_i) = c^\top \Phi(u)$. Let $\mathcal{T}_j := \mathcal{T} h_j = (\mathcal{T}(j, b_i))_{i=1 \dots N} \in \mathbb{R}^N$. We can then write down the Hermite expansion of the student network:

$$G(x; c, \theta) = c^\top \Phi(\langle \theta, x \rangle) = \sum_{j \geq 0} \langle c, \mathcal{T}_j \rangle h_j(\langle \theta, x \rangle).$$

Denoting $m := \langle \theta, \theta^* \rangle$, this allows us to rewrite the regularized objective as

$$L(c, \theta) = \sum_j \alpha_j^2 + \sum_j \langle c, \mathcal{T}_j \rangle^2 - 2 \sum_j \alpha_j \langle c, \mathcal{T}_j \rangle m^j + \lambda \|c\|^2,$$

where the term $\sum_j \alpha_j^2$ is a constant that can be ignored. Let $Q := \mathcal{T}\mathcal{T}^* \in \mathbb{R}^{N \times N}$ be a feature covariance matrix and $Q_\lambda = Q + \lambda I$. Note that Q_λ is positive semi-definite for $\lambda > 0$. We define the regularized projection $\hat{P}_\lambda = \hat{\Sigma}(\hat{\Sigma} + \lambda I)^{-1}$ onto the random feature space $\hat{\mathcal{H}}$ for $\hat{\Sigma} = \mathcal{T}^* \mathcal{T}$. Observe that $(\hat{P}_\lambda f)(u) = c^{*\top} \Phi(u)$, where $c^* \in \mathbb{R}^N$ is the solution to the following objective:

$$\min_{c \in \mathbb{R}^N} \left\| f - c^\top \Phi \right\|_\gamma^2 + \lambda \|c\|_2^2 \ . \tag{4}$$

Geometry on the sphere. Because the direction θ is constrained to lie on the sphere, our optimization algorithms rely on spherical (Riemannian) gradients, which are defined as follows:

$$\nabla_\theta^{\mathbb{S}^{d-1}} L(c, \theta) = \mathrm{Proj}_{\theta^\perp} \nabla_\theta L(c, \theta) \ ,$$

where $\mathrm{Proj}_{\theta^\perp} v = v - \langle \theta, v \rangle \theta$. We say that (c, θ) is a *critical point* of L if $\nabla_\theta^{\mathbb{S}^{d-1}} L(c, \theta) = 0$ and $\nabla_c L(c, \theta) = 0$.

4 Population Landscape under Frozen Random Biases

In order to understand the optimization and generalization properties of applying gradient descent to the empirical loss $L_n(c, \theta)$, we first the study optimization landscape of the population loss $L(c, \theta)$. We precisely characterize the critical points of the population loss in order to show that a gradient-based optimizer of a student neural network of sufficient width N converges only when its direction vector θ is either parallel or orthogonal to the teacher direction θ^*. In the subsequent section, we show that having sufficiently many training samples n provides a similar optimization landscape and has favorable generalization properties for most initializations.

We will make the following regularity assumptions on the teacher link function f_*, in order to ensure small approximation error from random features, and a benign empirical landscape.

Assumption 4.1 (Regularity of f_*)**.** *Let $f_*^{(p)}$ be the pth derivative of f_*. We assume that $f_*^{(p)} \in L^2(\gamma)$ (i.e. $\|f_*^{(p)}\|_\gamma < \infty$) for all $p \leq 6$, that f_* is Lipschitz and that f_* is polynomially bounded.*

The index of the first non-zero Hermite coefficient α_j of f_* is referred to as the information exponent *and is given by $s := \min\{j : \alpha_j \neq 0\}$.*

To consider the critical points of $L(c, \theta)$, we introduce the *projected population loss* at a given student direction θ:

$$\bar{L}(\theta) := \min_c L(c, \theta) \ .$$

Crucially, the sufficient number of features N depends on the regularization parameter $\lambda \in (0, 1)$, the variance $\tau^2 > 1$ of the random biases, and the teacher link function f_*, but *not* on the input dimension d.

Theorem 4.2 (Critical Points of Population Loss)**.** *For $\tau > 1$, and $\delta \in (0,1)$, there exist constants C_τ and C_{f_*} depending only on τ and the teacher link function f_* respectively such that if*

$$\lambda < C_{f_*}^{-(2+1/\tau^2)} \qquad \text{and} \qquad N \geq \frac{C_\tau}{\lambda} \ln\left(\frac{1}{\lambda\delta}\right) \tag{5}$$

then with probability $1-\delta$ over the random biases $b_1, \ldots, b_N$, the set of first-order critical points $\mathcal{C}_L := \{(c,\theta) : \nabla_\theta^{\mathbb{S}^{d-1}} L(c,\theta) = 0,\ \nabla_c L(C,\theta) = 0\}$ satisfies:

1. *(orientation relative to θ^*) if $(c,\theta) \in \mathcal{C}_L$, then either $\theta \in \{\pm\theta^*\}$ or $\langle \theta, \theta^* \rangle = 0$; and*
2. *(existence and uniqueness of c) if $\nabla_\theta^{\mathbb{S}^{d-1}} \bar{L}(\theta) = 0$, then there exists a unique c such that $(c,\theta) \in \mathcal{C}_L$.*

Theorem 4.2 thus establishes a benign optimization landscape in the population limit, rejoining several known non-convex objectives with similar behavior, such as tensor decomposition [25] or matrix completion [23]. Importantly, this optimization landscape has the same topology as if one were using Hermite basis functions rather than random scalar features [19, Theorem 5], the tailored choice that exploits the knowledge that the data is being generated by a single-index model. We view this as an interesting robustness property of shallow neural networks – at least in the regime where biases are randomly frozen.

We now outline the analysis that leads to the proof of the theorem before proving it formally in Section 4.3.

4.1 Exact expression of first-order critical points

The first step is to characterize the critical points of the regularized population loss. This is described in the following result.

Claim 4.3 (Critical point equation)**.** *Let $g_m, \bar{g}_m \in L_2(\gamma)$ be defined by*

$$g_m = \sum_j \alpha_j m^j h_j \ , \ \bar{g}_m = \sum_j \alpha_j j m^{j-1} h_j \ , \tag{6}$$

where $m = \langle \theta, \theta^* \rangle$. Then, the critical points of $L(c,\theta)$ satisfy the following equations:

$$c = Q_\lambda^{-1} \sum_j \alpha_j m^j \mathcal{T}_j \ ,$$

$$\sum_j \alpha_j^2 j m^{2j-1} - \langle (I - \hat{P}_\lambda) g_m, \bar{g}_m \rangle_\gamma = 0 \ .$$

Remark 4.4 (Infinite-width student networks)**.** *If the kernel is universal and $N \to \infty$, then P_λ is the identity operator when $\lambda = 0$. Hence, $\langle h_j, P_\lambda h_{j'} \rangle = \delta_{j,j'}$ in this limit and the teacher can be exactly represented when $m = 1$.*

We prove Claim 4.3 in Appendix B.1 by exactly computing the gradients and relating the critical points of $\bar{L}(\theta)$ and $L(c,\theta)$.

4.2 Controlling random feature approximation

We now consider (finite) random feature approximations to functions in the RKHS. We show that the best possible loss of a linear combination of sufficiently many finite features is bounded above by the best approximation with infinitely many features with high probability.

Let $A(f,\lambda)$ be the (regularized) L_2 approximation error for functions in the space $\mathcal{H}$ with respect to the target function f and measure γ. Formally,

$$A(f,\lambda) := \min_{g \in \mathcal{H}} \|f - g\|_\gamma^2 + \lambda \|g\|_{\mathcal{H}}^2 \ .$$

Lemma 4.5 (Random features approximation, adapted from [6])**.** *Let $\delta \in (0,1)$, $\tau > 1$, and $f \in L^2(\gamma)$. There exists a constant $C_\tau > 0$ such that if $N \geq \frac{C_\tau}{\lambda} \ln \frac{1}{\lambda\delta}$, then with probability at least $1-\delta$,*

$$\|(I - \hat{P}_\lambda) f\|_\gamma^2 \leq 4A(f,\lambda). \tag{7}$$

Proof. The claim is immediate from Lemmas B.5 and B.6 in Appendix B.2. □

Next, we show that the approximation error of the RKHS corresponding to an infinite number of random features can be bounded in terms of the regularization λ and the γ-norm of the second derivative of the target function. The bound is independent of d, as we consider τ and λ fixed as d grows.

Lemma 4.6 (RKHS approximation error)**.** *Assume $f \in L^2(\gamma)$ is in the weighted Sobolev space $H^2(\gamma)$ and has polynomial growth (i.e. there exist $C > 0$ and $M > 0$ such that $|f(u)| \leq C(u^M + u^{-M})$). Then,*

$$A(f, \lambda) = O\left(\lambda^\beta \|f''\|_\gamma^2\right), \tag{8}$$

with $\beta := \frac{\tau^2}{\tau^2+2}$.

The proof appears in Appendix B.3.

4.3 Proof of Theorem 4.2

Proof. For (c, θ) to be a critical point of L, it must satisfy $\nabla_\theta^{\mathbb{S}^{d-1}} L(c, \theta) = 0$ and $\nabla_c L(\theta, c) = 0$. According to Claim 4.3, every fixed θ has a unique complementary c such that $\nabla_c L(\theta, c) = 0$, and $\nabla_\theta^{\mathbb{S}^{d-1}} L(c, \theta) = 0$ if and only if $\theta \in \{-\theta^*, \theta^*\}$ or

$$\sum_j \alpha_j^2 j m^{2j-1} = \langle (I - \hat{P}_\lambda) g_m, \bar{g}_m \rangle_\gamma. \tag{9}$$

The remainder of the proof involves showing that the latter condition is true only if $m = 0$. We derive a contradiction whenever $m \neq 0$. Let $\beta := \frac{\tau^2}{\tau^2+2}$ and take $N \geq \frac{C_\tau}{\lambda} \ln \frac{1}{\lambda\delta}$ and

$$\lambda < \left(\frac{C' \|f_*''\|_\gamma \sqrt{\|f_*''\|_\gamma^2 + \|f_*'\|_\gamma^2}}{\alpha_s^2 s} \right)^{-2/\beta}$$

for sufficiently large C' and C_τ. We contradict the equality with probability at least $1 - \delta$ over the randomly sampled biases $b_1, \ldots, b_N$:

$$\begin{aligned}
\left| \langle (I - \hat{P}_\lambda) g_m, \bar{g}_m \rangle_\gamma \right| &\leq \|(I - \hat{P}_\lambda) g_m\|_\gamma \|\bar{g}_m\|_\gamma \\
&\leq 2\sqrt{A(g_m, \lambda)} \|\bar{g}_m\|_\gamma && \text{[Lemma 4.5]} \\
&\leq C' \lambda^{\beta/2} \|g_m''\|_\gamma \|\bar{g}_m\|_\gamma && \text{[Lemma 4.6]} \\
&\leq C' \lambda^{\beta/2} |m|^{2s-1} \|f_*''\|_\gamma \sqrt{\|f_*''\|_\gamma^2 + \|f_*'\|_\gamma^2} && \text{[Lemma B.7]} \\
&< \alpha_s^2 s |m|^{2s-1} \leq \sum_{j=0}^\infty \alpha_j^2 j |m|^{2j-1} = \left| \sum_{j=0}^\infty \alpha_j^2 j m^{2j-1} \right|. \ \square
\end{aligned}$$

5 Empirical Landscape and Generalization Guarantees

Now that we have established that the population landscape $L(c, \theta)$ has a particularly simple structure given sufficiently many random features $N \gtrsim O(1)$, we study the optimization properties of its finite-sample counterpart. For training samples $\{(x_i, y_i)\}_{i \in [n]}$ generated by independently drawn $x_i \sim \mathcal{N}(0, I)$ and $y_i = f_*(\langle x_i, \theta^* \rangle)$ [2] and random features $\Phi : \mathbb{R} \to \mathbb{R}^N$ with $\Phi(u)_j = N^{-1/2} \phi(u - b_j)$, we define the *empirical risk* as

$$L_n(c, \theta) := \frac{1}{n} \sum_{i=1}^n \left(c^\top \Phi(\langle x_i, \theta \rangle) - y_i \right)^2 + \lambda \|c\|^2. \tag{10}$$

[2] For simplicity of the analysis and exposition, we assume clean labels without additive noise, but note we may incorporate additive noise to our analysis in a straightforward manner.

We specifically consider the estimator $\hat{F}(x) := \hat{f}(\langle x, \hat{\theta}\rangle)$, where $(\hat{f}, \hat{\theta})$ are obtained by using gradient descent on c and θ to minimize $L_n(c, \theta)$. Such strategy appears to be reasonable, in light of the properties of the population landscape studied in Section 4, namely that its only local minimisers are also global, and correspond to $\tilde{f} = \hat{P}_\lambda f^*$ and $\tilde{\theta} = \theta_*$. Given a sufficiently large sample size n, one expects the empirical landscape L_n to concentrate around its expectation L and inherit its benign optimization properties. However, the presence of a degenerate saddle at $(c, m) = (0, 0)$ flattens the landscape around the "equator" $\{\theta : \langle \theta, \theta_*\rangle = 0\}$, and a sufficiently large sample complexity is ultimately required to ensure that gradient descent iterates can escape from it, given its dangerously close initialization $|\langle \theta_0, \theta_*\rangle| = \Theta(1/\sqrt{d})$.

Prior works have obtained the optimal sample complexity of $n = O(d^s)$ (recall that s is the information exponent of the teacher function f_*) for recovering the teacher direction θ_* either by employing a learning algorithm that explicitly learns individual harmonic polynomials [19] or by assuming that f^* is known a priori [3]. Their argument goes essentially as follows:

- The empirical optimization landscape (when regarded as a function only of the direction θ) near the equator $|m| \ll 1$ is of the form $L(\theta) = \Theta(m^s)$.
- In order to certify that the optimization does not converge to a suboptimal critical point on the equator (i.e. $\|\nabla L(\theta)\| \gtrsim \epsilon$) one must require that $m \gtrsim \epsilon^{1/(s-1)}$.
- A standard uniform concentration argument of the form $\|\nabla L(\theta) - \nabla L_n(\theta)\| \lesssim \sqrt{\frac{d}{n}}$ and the fact that $m \sim d^{-1/2}$ at initialization together imply that $n = O(d^s)$ samples are sufficient to escape from the "influence" of the equator.

In order to repurpose these arguments to our setting, the relative scaling of the top-layer weights c relative to the direction vector θ will turn out to be crucial, as has also been observed in the literature on *lazy*-vs-*rich* regimes [14, 49] in the context of overparametrized neural networks.

We consider an idealized version of a Gradient Descent algorithm over the empirical loss L_n in the infinitesimally small learning rate regime, resulting in the gradient flow ODE:

$$\begin{aligned} \dot{c}(t) &= -\zeta(t)\nabla_c L_n(c, \theta) \\ \dot{\theta}(t) &= -\nabla_\theta^{\mathbb{S}^{d-1}} L_n(c, \theta)\,, \end{aligned} \tag{11}$$

where ζ is the relative time-scale between first- and second-layer weights, and $\nabla_\theta^{\mathbb{S}^{d-1}}$ is the Riemannian gradient.

Our main result establishes that this gradient flow, under a simple schedule for ζ, efficiently finds an approximate minimiser of the *population* loss, with an error explicitly quantified as a function of n:

Theorem 5.1 (Gradient flow finds approximate minimizers)**.** *Let $0 < \delta < 1/8$ and assume (i) $n \geq C\lambda^{-1} d^s \log \delta^{-1}$, (ii) $N \geq C\lambda^{-1}\log(\lambda^{-1}\delta^{-1})$, (iii) $C_{f_*}\lambda^{\beta/2} < s^2\alpha_s^2/2$, and (iii) a target f_* satisfying the regularity assumptions 4.1. Then with probability (over the empirical data, the randomness of initialization and the draw of the random features) greater than $1/4 - 2\delta$, the output of the procedure 1 with $\rho = \Theta(N^{-1-s})$, $N_0 = O\left(\frac{n}{d}\right)^{\frac{2s}{(2s-1)(s+1)}}$ and $T_0 = \widetilde{\Theta}\left(d^{s/2-1}\right)$ returns (c_T, θ_T) after time $T > T_0$ satisfying*

$$\begin{aligned} \|c_T^\top \Phi - \hat{P}_\lambda f_*\|_\gamma &= O\left(\lambda^{-1}\sqrt{\frac{d}{n}}\right) + O\left(\lambda^{-3}\frac{d}{n}\right) \\ &\quad + \widetilde{O}\left(\lambda^{-1}(T - T_0)^{-1/2}\right) + \widetilde{O}\left(\lambda^{-3}(T - T_0)^{-1}\right)\,, \end{aligned} \tag{12}$$

$$1 - |\langle \theta_T, \theta^*\rangle| \leq O\left(\lambda^{-2}\frac{d}{n}\right) + \widetilde{O}\left(\lambda^{-2}(T - T_0)^{-1}\right)\,. \tag{13}$$

Corollary 5.2 (Excess risk of Algorithm 1)**.** *Under the assumptions of Theorem 5.1, after optimizing the regularisation parameter λ in the previous estimator, one obtains an excess risk of the form*

$$\|\hat{F} - F_{\theta^*}\|_{\gamma_d}^2 \lesssim \left(\frac{d}{n}\right)^{\frac{\beta}{\beta+1}}\,. \tag{14}$$

Algorithm 1 Gradient Flow

Require: $N_0, \rho, T_0, T_1, N, \lambda$
Initialize $\theta(0) \sim \mathrm{Unif}(\mathbb{S}^{d-1})$, $c(0) \sim \mathrm{Unif}(\{c \in \mathbb{R}^N; \|c\|_2 = \rho; \|c\|_0 = N_0\})$.
Run Gradient Flow (11) with $\zeta(t) = \mathbf{1}(t > T_0)$ up to time $T = T_0 + T_1$.
Set $\hat{\theta} = \theta(T)$, $\hat{c} = c(T)$.

Algorithm 2 Fine-Tuning

Require: $\lambda_{n'}$, $\hat{\theta}$ from Algorithm 1.
Set $\hat{c} = \arg\min_c L'_{n'}(c, \hat{\theta})$ as in (15).

Fine-tuning the second layer. After running Algorithm 1, we may include a final fine-tuning phase of training for second layer weights c alone, using a separate training sample (x'_i, y'_i), $i = 1, \dots, n'$ and a possibly different regularization parameter $\lambda_{n'}$. More precisely, we set

$$\hat{c} = \arg\min_c \left\{ L'_{n'}(c, \hat{\theta}) := \frac{1}{n'} \sum_{i=1}^{n'} (c^\top \Phi(\langle \hat{\theta}, x'_i \rangle) - y'_i)^2 + \lambda_{n'} \|c\|^2 \right\}, \tag{15}$$

where $\hat{\theta}$ denotes the output of the previous gradient descent phase. Note that this is a strongly convex optimization problem, and can thus be optimized efficiently using gradient methods or by solving a linear system. While this may not be needed in practice, we use a different training sample for technical reasons, namely to break the dependence between the data and the kernel, which depends on the initial training sample through $\hat{\theta}$. We note that such sample splitting strategies are commonly used in other contexts in the statistics literature (e.g., [9, 12]). We obtain the following guarantee.

Proposition 5.3 (Excess risk of fine-tuning)**.** *Let $\delta > 0$. Let $m = \langle \hat{\theta}, \theta^* \rangle$, where $\hat{\theta}$ is obtained from the previous gradient descent phase, and let $\hat{c}$ be the ridge regression estimator obtained from a fresh dataset $\mathcal{D}'$ of n' samples, N random features,*[3] *and regularization parameter $\lambda_{n'} := (\sigma^2\tau^2/\|f''_*\|_\gamma^2 n')^{1/(\beta+1)}$, and let $\hat{F}(x) = \hat{c}^\top \Phi(\langle \hat{\theta}, x \rangle)$. Assume*

$$n' \gtrsim \max\left\{ \sigma^2\tau^2/\|f''_*\|_\gamma^2, (\|f''_*\|_\gamma^2/\sigma^2\tau^2)^{1/\beta}, \|f_*\|_\infty^2/(\sigma^2\tau^2)^{\beta/(\beta+1)} \right\}$$
$$N \gtrsim C_\tau \left(n' \|f''_*\|_\gamma^2/\sigma^2\tau^2\right)^{\frac{1}{\beta+1}} \ln\left(n'^{1/(\beta+1)}\delta^{-1}\right)$$

With probability at least $1 - \delta$ over the random features, we have

$$\mathop{\mathbb{E}}_{\mathcal{D}'}[\|\hat{F} - F_{\theta^*}\|_{\gamma_d}^2 | \hat{\theta}] \lesssim \|f''_*\|_\gamma^{\frac{2}{\beta+1}} \left(\frac{\sigma^2\tau^2}{n'}\right)^{\frac{\beta}{\beta+1}} + (1 - |m|)^2(\|f'_*\|_\gamma^2 + \|f''_*\|_\gamma^2) \tag{16}$$

where the expectation is over the n' fresh samples, and is conditioned on the previously obtained $\hat{\theta}$.

Combining the two phases leads to the following generalization guarantee on the excess risk for Algorithm 2.

Corollary 5.4 (Excess risk of Algorithm 2)**.** *Let $0 < \delta < 1/8$ and let $\lambda = (s^2\alpha_s^2/2C_{f_*})^{2/\beta}$, assuming 4.1, with C_{f_*} that depends on regularity of f_*. Assume the following:*

$$n \gtrsim \lambda^{-1} d^s \log \delta^{-1}, \qquad n' \gtrsim \max\left\{ \sigma^2\tau^2/\|f''_*\|_\gamma^2, (\|f''_*\|_\gamma^2/\sigma^2\tau^2)^{1/\beta}, \|f_*\|_\infty^2/(\sigma^2\tau^2)^{\frac{\beta}{\beta+1}} \right\}$$
$$N \gtrsim C_\tau \max\left\{ \left(n' \|f''_*\|_\gamma^2/\sigma^2\tau^2\right)^{\frac{1}{\beta+1}} \ln\left(n'^{1/(\beta+1)}\delta^{-1}\right), \lambda^{-1}\log(\lambda^{-1}\delta^{-1}) \right\}.$$

With probability at least $1/4 - 2\delta$ over the initial n samples, initialization, random features, we have

$$\mathop{\mathbb{E}}_{\mathcal{D}'}[\|\hat{F} - F_{\theta^*}\|_{\gamma_d}^2] \lesssim C_1 \frac{d^2}{n^2} + C_2 \left(\frac{\sigma^2\tau^2}{n'}\right)^{\frac{\beta}{\beta+1}}, \tag{17}$$

where C_1 and C_2 only depend on regularity of f_*, ignoring the optimization error.

[3] These can be the same as in the previous phase.

We can make the following remarks:

- The empirical gradient flow therefore escapes the influence of the degenerate saddle with optimal sample complexity $n = \Theta(d^s)$ [3]. This is an instance of gradient descent successfully optimizing a non-convex objective *without the strict saddle property* as soon as $s > 2$, building from the simpler optimization landscapes of [19, 3]. This is in contrast with e.g. spiked tensor recovery problems [4] where the signal strength is substantially weaker, leading to complexity in the optimization landscape.
- While the recovery of the high-dimensional direction is optimal in statistical terms, the joint recovery of the link function is sub-optimal, by comparing Corollaries 5.2 and 5.4. In this sense, the fine-tuning stage recovers the optimal sample complexity, and where the non-parametric rate no longer depends on the ambient dimension d.
- The time-scale separation scheduling for ζ is sufficient but possibly not necessary. The analysis of vanilla dynamics ($\zeta(t) \equiv 1$) is challenging, since during the initial phase of training there may be adverse interaction effects between c and θ, which under naive analysis lead to sub-optimal sample complexity of $n \geq O(d^{2s})$.
- The time discretisation to turn Procedure 1 into a proper algorithm should follow from standard Euler time discretisation arguments, since L_n has Lipschitz gradients.

6 Conclusions

This work studies the ability of shallow neural networks to learn single-index models with gradient descent. Our main results are positive, and demonstrate their ability to solve a semi-parametric problem with nearly optimal guarantees. Interestingly, this success story combines elements from the feature-learning regime —the ability to efficiently identify the hidden direction in high-dimensions under a non-convex objective, with ingredients from the lazy-regime, which offer better computational tradeoffs to solve low-dimensional non-parametric problems. Our technical analysis leverages tools from high-dimensional probability (such as uniform gradient concentration) and RKHS approximation theory, and complements the growing body of theoretical work certifying the efficiency of gradient methods on non-convex objectives. We have followed the standard approach of first establishing benign topological properties of the population loss, and then extend them to the empirical loss.

That said, there are several unanswered questions that our work has not addressed, such as:

- **Extension to Multi-Index Models.** Multi-index models are natural extensions of single-index models where the hidden direction is replaced by a hidden low-dimensional subspace. They enjoy similar statistical guarantees as single-index models [19, 5], and thus a natural question is whether the same algorithmic tools developed here extend to the multi-index setting.
- **Gradient dynamics without warmstart.** An unsatisfactory aspect of our results is the requirement that the algorithm starts by only optimizing θ for $t < T_0$. It would be interesting to understand whether the vanilla dynamics could also succeed.
- **Trainable biases and untied directions.** Our proposed neural network architecture is non-standard, in the sense that its biases are frozen at initialization and all neurons share the same inner weight. For the purposes of learning single-index models, removing these restrictions would not bring any statistical benefits. However, it would be interesting to extend our analysis to the general setting.

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Checklist

The checklist follows the references. Please read the checklist guidelines carefully for information on how to answer these questions. For each question, change the default **[TODO]** to [Yes] , [No] , or [N/A] . You are strongly encouraged to include a **justification to your answer**, either by referencing the appropriate section of your paper or providing a brief inline description. For example:

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