Algorithms for Efficiently Learning Low-Rank Neural Networks

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Abstract

We study algorithms for learning low-rank neural networks – networks where the weight parameters are re-parameterized by products of two low-rank matrices. First, we present a provably efficient algorithm which learns an optimal low-rank approximation to a single-hidden-layer ReLU network up to additive error $\epsilon$ with probability $\geq 1 - \delta$, given access to noiseless samples with Gaussian marginals in polynomial time and samples. Thus, we provide the first example of an algorithm which can efficiently learn a neural network up to additive error with respect to a strictly smaller hypothesis class. To solve this problem, we introduce an efficient SVD-based Nonlinear Kernel Projection algorithm for solving a nonlinear low-rank approximation problem over Gaussian space. Inspired by the efficiency of our algorithm, we propose a novel low-rank initialization framework for training low-rank deep networks, and prove that for ReLU networks, the gap between our method and existing schemes widens as the desired rank of the approximating weights decreases, or as the dimension of the inputs increases (the latter point holds when network width is superlinear in dimension). Finally, we validate our theory by training ResNet and EfficientNet models [He et al., 2016, Tan and Le, 2019] on ImageNet [Russakovsky et al., 2015].

1 Introduction

Training deep networks is a canonical task in modern machine learning. Training and serving deep networks with very large parameter counts efficiently is of paramount importance in recent years, since significant performance gains on a variety of tasks are possible simply by scaling up parameter counts [Rae et al., 2021, Shin et al., 2021, Henighan et al., 2020, Gordon et al., 2021, Sharma and Kaplan, 2020, Kaplan et al., 2020]. Further theoretical evidence suggests that requiring the resulting learned networks to be smooth functions (and therefore, in some sense, robust to perturbations) entails even larger parameter counts [Bubeck and Sellke, 2021].

However, there are significant computational difficulties with both training and deploying such large models. Most existing works focus on efficiently deploying trained deep networks and uses a variety of approaches including sparsifying neural network weights [Reed, 1993, Blalock et al., 2020, LeCun et al., 1990, Hassibi and Stork, 1993, Mozer and Smolensky, 1989, Dong et al., 2017, Han et al., 2016, Lewis et al., 2021, Yang et al., 2019, Su et al., 2020, Frankle et al., 2020, Fischer and Burkholz, 2021], model distillation [Heo et al., 2019, Hinton et al., 2015], low-rank post-processing [Anonymous, 2022, Idelbayev and Carreira-Perpinán, 2020, Tukan et al., 2021], and mixtures thereof [Chen et al., 2021a]. Unfortunately, these methods do not address the question of efficient training.

1.1 Training-Time Efficient Deep Networks

Another general approach to improving speed and memory at both train and inference time is to replace each weight matrix $W \in \mathbb{R}^{d \times m}$ with a computationally efficient representation which improves the training speed of standard gradient-based optimization methods, while ideally not losing out on the representation capacity too much. A variety of papers have taken this approach with varying techniques including fast Fourier transform-inspired sparse matrix decompositions, low-rank factorizations, orthogonal basis kernel

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approximations, and sketching-based approaches [Dao et al., 2020, Khodak et al., 2021, Vahid et al., 2020, Wang et al., 2021, Dusenberry et al., 2020, Romero et al., 2014, Zhang et al., 2015, Choromanski et al., 2020, Chen et al., 2021b, Panigrahy et al., 2021]. In the sparse deep network literature, there also exist methods to perform pruning before or during training (to also get efficiency gains during training) [Wang et al., 2019, Mostafa and Wang, 2019, He et al., 2021, Su et al., 2020, Frankle et al., 2020, Mussay et al., 2020].

1.2 Low-Rank Factorized Networks

Given the broad spectrum of proposed methodologies, it may be unclear to practitioners which families of methods are most practical to use. Two recently popular approaches are unstructured sparse pruning and low-rank factorization. Low-rank methods do not require specialized hardware to convert smaller parameter counts into compute savings, unlike the sparse methods [Paszke et al., 2019, NVIDIA, 2020, Mishra et al., 2021].

For a fully-connected layer, the basic idea of a low-rank layer (or a factored layer) is to parameterize the network weights $W \in \mathbb{R}^{d \times m}$ with a low-rank matrix product $UV^\top$, where $U \in \mathbb{R}^{d \times r}$, $V \in \mathbb{R}^{m \times r}$ and $r$ is the (user-selected) rank. Simple generalizations exist for other standard layers including convolution and attention layers [Khodak et al., 2021]. Low-rank deep networks reduce parameter counts (thus saving memory) as well as the number of ops required for matrix-vector multiplication: $(d + m) \cdot r$ vs. $d \cdot m$.

Khodak et al. [2021] demonstrate that if one pays attention to proper initialization and regularization, low-rank methods outperform sparse pruning approaches in many domains, contrary to existing beliefs that sparse methods outperform low-rank methods in parameter count savings. In particular, a low-rank initialization scheme called spectral initialization is crucial to achieve better performance – initialization schemes are in general quite important for achieving good performance in neural network training [Bachlechner et al., 2020, Choromanski et al., 2018, Dauphin and Schoenholz, 2019, Hu et al., 2020, Huang et al., 2020, Mishkin and Matas, 2015, Pennington et al., 2017, Xiao et al., 2018, Zhang et al., 2021]. Spectral initialization samples a full-rank matrix $W \in \mathbb{R}^{d \times m}$ from a known init distribution, factorizes $W$ as $A \Sigma^{1/2} \Sigma^{1/2} B^\top$ via singular value decomposition (SVD), and initializes $U$ and $V^\top$ with these factors.

However, there are no explanations for why this approach yields improved performance beyond the zeroth-order justification that it well-approximates the parameters of the full-rank weights at initialization. Thus, it is a natural next step to develop better theoretical understanding of the properties of the low-rank network learning problem, with the hope that it will aid us in finding improved methods for training low-rank versions of deep networks and in uncovering the principles of learning low-rank network approximations.

1.3 Contributions

We study the problem of learning low-rank neural networks in this paper and ask two questions:

(A) What are the statistical and computational complexities of learning one-hidden-layer fully-connected low-rank neural networks from noiseless samples?

(B) Are there better algorithms for initializing low-rank deep neural networks that improve post-training generalization error?

Our contributions are as follows:

1. We provide theoretical results closing an open learning theory problem regarding the tractability of learning an optimal low-rank approximation to a one-hidden-layer, fully-connected ReLU network over the standard assumption of Gaussian marginals. In particular, we present a provably efficient algorithm (Algorithm 2) which learns the optimal low-rank approximation up to additive error $\epsilon$ with probability at least $1 - \delta$, given access to noiseless samples in polynomial (in the relevant parameters) time and samples (Theorem 2.8). Our learning algorithm crucially depends on a novel computationally efficient subroutine— the Nonlinear Kernel Projection algorithm (see Theorem 2.10 and Algorithm 1)— which solves a nonlinear low-rank factorization problem. Thus, we provide the first example of an algorithm which can efficiently learn a neural network up to additive error with respect to a strictly smaller hypothesis class.
2. We introduce a novel initialization framework for low-rank deep learning which we call function approximation at initialization (Definition 3.2). We use Nonlinear Kernel Projection to implement the layer-wise distributed case (Definition 3.3) of our low-rank initialization framework, and also provide an empirical method which applies more generally beyond the settings under theoretical study.

3. For the ReLU activation in the fully-connected one-hidden-layer setting over Gaussian marginals, we prove lower bounds on the sub-optimality of spectral initialization for matching the function output. In particular, the sub-optimality of spectral initialization grows as the rank decreases, or if the width is super-linear in the input dimension, also as the dimension grows (Corollary 4.5).

4. Finally, we empirically evaluate our novel initialization scheme on the popular ResNet and EfficientNet architectures [He et al., 2016, Tan and Le, 2019] applied to the ImageNet dataset [Russakovsky et al., 2015], and demonstrate that our proposed method significantly improves over other initialization schemes (Tables 1 and 2), and validate predictions of our theory (Figures 1 and 2).

1.4 Paper Outline

In Section 2, we present an efficient algorithm (Algorithm 2) for learning low-rank networks, which uses the Nonlinear Kernel Projection algorithm (Algorithm 1) as a subroutine. In Section 3, we introduce our novel initialization framework (Definition 3.2) and present a special case (Definition 3.3), which Nonlinear Kernel Projection efficiently solves. We also provide empirical heuristics for more general settings. In Section 4, we lower bound the gap in performance between the optimal and spectral initialization, and thereby demonstrate cases where the spectral initialization method fails to perform nonlinear low-rank function approximation. In Section 5, we analyze our experimental results, and we conclude in Section 7.

2 Theory for Learning Low-Rank Networks

In this section we consider the problem of learning optimal low-rank approximations to fully-connected, shallow neural networks. We study this problem in a simple setting to gain insight into methods for learning low-rank deep networks in general, and because it is an interesting open learning theory problem. It is of particular interest since in the literature, the only computationally tractable cases for learning even simple neural networks requires assuming that the true signal is in the hypothesis class (possibly perturbed by some additive 0-mean noise). All positive results for computationally tractable learning up to (non-approximate) additive error requires making these assumptions, and various hardness results (for instance, statistical queries (SQ) lower bounds [Feldman, 2016]) are known for a variety of more general agnostic settings. In our case, since we wish to learn a low-rank approximation, we are automatically not in the realizable setting: however, we know a lot more structure about the responses than in the arbitrary agnostic setting, so it is plausible that our learning problem is tractable.

2.1 Problem Statement and Assumptions

Problem 2.1 (Shallow Low-Rank Learning Problem). Consider the objective

$$\mathcal{R}(Y) := \mathbb{E}_{x \sim \mathcal{N}(0,I)} \left[ \| \sigma_{\text{ReLU}}(x^\top Y) - \sigma_{\text{ReLU}}(x^\top W) \|^2 \right]$$

(1)

where $\sigma_{\text{ReLU}}(x) = \max(0, x)$ is the ReLU activation, $W, Y \in \mathbb{R}^{d \times m}$, and $W$ are fixed ground-truth full-rank weights. Let $\text{opt} := \mathcal{R}(Y^*)$, where $Y^*$ is the argmin over matrices of rank $r$. If a learner is only given samples $\{(x, \sigma_{\text{ReLU}}(x^\top W))\} \sim \mathcal{N}(0,I)$, what are the computational and sample complexities of finding the optimal rank $r$ matrix $\hat{Y}$, such that with probability at least $1 - \delta$, $\mathcal{R}(\hat{Y}) < \text{opt} + \epsilon$?

Remark 2.2 (Recovering Low-Rank Factors). Note that we have framed the learning problem in terms of recovering a low-rank matrix $Y^*$. To fulfill the promise of improved computational efficiency, the original motivation for considering this learning problem, we would apply a final post-processing step after learning $Y^*$ by exactly decomposing it into the product of two rank $r$ matrices using SVD.
Remark 2.3 (Convolutional Architecture). In this problem we only consider fully-connected architecture. However, since a convolution is a linear operator, we can make use of results which efficiently learn one-layer convolutional ReLU networks [Du et al., 2018] to first recover the convolutional filters before reducing to our low-rank recovery procedure.

We also remark upon when activation functions satisfy easy invertibility (Definition 2.7):

Remark 2.4 (Examples of Easily Invertible Activations). We mention a few classes which satisfy Definition 2.7:

1. Even activation functions do not satisfy this condition.
2. All odd activations satisfy this condition.

Concretely, ReLU, Tanh, Leaky ReLU [Maas et al., 2013], Swish [Ramachandran et al., 2017], SoftPlus, SmeLU [Shamir et al., 2020] all satisfy these conditions. Sigmoid also satisfies the condition despite being neither even nor odd. On the other hand, the quadratic activation, some parameter choices for GSmeLU [Shamir et al., 2020], and CReLU [Shang et al., 2016] do not satisfy Definition 2.7.

2.2 Related Work

Many papers have studied related problems in a variety of settings [Goel et al., 2016, 2019, Soltanolkotabi, 2017, Chen et al., 2021c, Diakonikolas et al., 2020, Goel et al., 2020b,a, Bakshi et al., 2019, Ge et al., 2019]. Compared to previous work, the setting we study is a) not realizable but, b) there is significant structure on the outputs, and there is no noise. Our results diverge from previous work like Bakshi et al. [2019] and Ge et al. [2019], which consider a two-layer network recovery problem over structured data distributions and additive mean-zero noise, in that we are not trying to recover the ground truth: we are learning over a restricted hypothesis class (low-rank approximations of the ground-truth). We assume Gaussian marginals, similarly to previous work. See Section 6 and also Ch. 3 of Chen [2021] for a thorough discussion of recent related work in statistics and deep learning theory.

It is thus currently open whether there exists an algorithm that runs in polynomial time and sample complexity to solve this problem; it is also open whether we can solve this using a gradient (or any SQ) method, as existing lower bounds do not directly rule out such an algorithm for this setting.

We prove that for the shallow low-rank learning problem with the ReLU activation, there is a computationally efficient SQ algorithm. The full proofs are in Section 8.3 of the Appendix. In the following sections we briefly sketch the key features of the arguments.

2.3 The Algorithm

First we present an efficient algorithmic framework called Nonlinear Kernel Projection (NKP) for computing the optimal low-rank matrix given knowledge of the full-rank weights for a broad family of nonlinearities. Using Nonlinear Kernel Projection for ReLU, we give the first efficient learning algorithm for the shallow low-rank ReLU learning problem. A few definitions will be useful first.

Definition 2.5 (Nonlinearity Kernel). Given a univariate activation function $\sigma$, define the associated nonlinearity kernel$^1$ by: $k_\sigma(x, y) := \mathbb{E}_{z \sim \mathcal{N}(0, 1)}[(\sigma(x^T z), \sigma(y^T z))]$.

Note this is a positive semi-definite kernel [Schölkopf et al., 2002, Martens et al., 2021].

Lemma 2.6 (Feature Map for Nonlinearity Kernels). Given the Hermite coefficients [O’Donnell, 2014] for a nonlinearity $\sigma$, it is easy to construct the feature map $\phi : \mathbb{R}^d \rightarrow \mathcal{L}_2(\mathcal{N}(0, I))$ such that $k_\sigma(x, y) = \langle \phi(x), \phi(y) \rangle$.

See Section 8.1 for more details.

We also define a family of activation functions which satisfy an inversion condition on $\phi$, which is necessary for Nonlinear Kernel Projection to work.

$^1$In prior literature, this function is highly related to the C-Map concept derived and applied in Saxe et al. [2014], Poole et al. [2016], Martens et al. [2021], and is identical up to normalization. It is worth noting that the setting in which these works derive the C-Map is considerably different from ours: normality arises due to taking infinite-width limits of deep networks and assumptions on weight initialization distributions, rather than an assumption on the input data distribution.
Complexity of learning rank-
\( r \) and additive generalization error is a bound on the \( \ell_2 \)-norm of the columns of the input matrix \( Y \). In Remark 8.15, we mention other avenues for improving the degrees in the bounds.

To prove this theorem, we put together 1) a computationally and statistically efficient method for estimating the kernel matrix up to additive Frobenius error (Corollary 8.11); 2) a computationally and statistically efficient method for estimating the optimal low-rank matrix up to additive Frobenius error \( \epsilon \) with probability at least \( 1 - \delta \); and 3) a computationally efficient algorithm for recovering the best low-rank approximation \( Y^* \) given knowledge of \( W \) and the kernel matrix \( K_{\text{ReLU}} \) (NKP Algorithm, Theorem 2.10).

Proof Sketch. To prove this theorem, we put together 1) a computationally and statistically efficient method for estimating the kernel matrix up to additive Frobenius error (Theorem 2.11); 2) a computationally and statistically efficient method for estimating the optimal low-rank matrix up to additive Frobenius error \( \epsilon \) with probability at least \( 1 - \delta \); and 3) a computationally efficient algorithm for recovering the best low-rank approximation \( Y^* \) given knowledge of \( W \) and the kernel matrix \( K_{\text{ReLU}} \) (NKP Algorithm, Theorem 2.10).

In Remark 8.15, we suggest that if we assume an average case setting over \( W \), we can make use of random matrix theory to replace the eigenvalue gap and spectral norm terms as well as improve the degrees in the bounds. Given Theorem 2.8, we broadly note where the difficulties in Problem 2.1 lie:

Definition 2.7 (Family of Easily Invertible Activation Functions). We define a family of easily invertible activations \( \mathcal{A} \) as: \( \mathcal{A} := \{ \sigma : \mathbb{R} \to \mathbb{R} : \mathbb{E}_{z \sim N(0,1)}[\sigma(z)] > 0 \} \).

Algorithm 1 Nonlinear Kernel Projection (NKP) Algorithm

Require: \( W \in \mathbb{R}^{d \times m} \), optional \( K \in \mathbb{R}^{m \times m} \), rank \( r < d < m \), easily invertible activation function \( \sigma \)
1. Compute kernel \( K = k_\sigma(W, W) \) if not given.
2. Compute \( VAV^\top = \text{SVD} (K, r) \). // rank-\( r \) SVD
3. Return: \( Y^* = WVV^\top \in \mathbb{R}^{d \times m} \).

Our shallow low-rank ReLU learning algorithm consists of recovering \( W \) approximately from samples using gradient descent (which is efficient in the realizable setting [Soltanolkotabi, 2017]), recovering the kernel matrix \( K_\sigma \) approximately from samples with an empirical estimate, and then applying NKP with the ReLU activation.

Algorithm 2 Shallow Low-Rank ReLU Learning

Require: Sample access to \( \{(x, \sigma_{\text{ReLU}}(x^\top W)) \}_{x \sim \mathcal{N}(0, I)} \) for unknown \( W \in \mathbb{R}^{d \times m} \), \( r < d < m \)
1. Use gradient descent to recover \( \hat{W} \) up to Frobenius error \( \epsilon_W \) with probability \( \geq 1 - \delta_W \) by learning the ReLU for all \( m \) columns using \( n_W(\epsilon_W, \delta_W) \) samples.
2. Compute \( \hat{K} = \frac{1}{N} \sum_{i=1}^N \sigma(x_i^\top W)\sigma(x_i^\top W)^\top \) up to Frobenius error \( \epsilon_K \) with probability \( \geq 1 - \delta_K \) using \( N = n_K(\epsilon_K, \delta_K) \) samples.
3. Return: \( \hat{Y} = \text{NKP} (\hat{W}, \hat{K}, r, \sigma_{\text{ReLU}}) \).

2.4 Analysis

Now we prove our main theorem: Algorithm 2 efficiently solves Problem 2.1.

Theorem 2.8 (Shallow Low-Rank ReLU Learning is Computationally and Statistically Efficient). Consider Problem 2.1, where \( W \in \mathbb{R}^{d \times m} \) is the matrix of full-rank parameters defining the one-hidden-layer ReLU function. Algorithm 2 is an efficient learning algorithm for recovering the optimal low-rank matrix up to additive generalization error \( \epsilon \) with probability at least \( 1 - \delta \). Both the sample complexity and computational complexity of learning rank-\( r \) ReLU approximation are \( \text{poly} \left( R, d, m, \frac{1}{\epsilon}, \log \left( \frac{1}{\delta} \right), \|W\|_2, \lambda_r, \lambda_{r-1}, r \right) \), where \( R \) is a bound on the \( \ell_2 \) norms of the columns of \( W \), \( \|W\|_2 \) is the spectral norm of \( W \), and \( \lambda_r, \lambda_{r-1} \) are the \( r \)th and \( (r - 1) \)st eigenvalues of \( K_{\text{ReLU}} \) respectively.

Proof Sketch. To prove this theorem, weopted together 1) a computationally and statistically efficient method for estimating the kernel matrix up to additive Frobenius error (Theorem 2.11); 2) a computationally and statistically efficient method for estimating \( W \) up to additive Frobenius error \( \epsilon \) with probability at least \( 1 - \delta \); and 3) a computationally efficient algorithm for recovering the best low-rank approximation \( Y^* \) given knowledge of \( W \) and the kernel matrix \( K_{\text{ReLU}} \) (NKP Algorithm, Theorem 2.10).

In Remark 8.15, we suggest that if we assume an average case setting over \( W \), we can make use of random matrix theory to replace the eigenvalue gap and spectral norm terms as well as improve the degrees in the bounds. Given Theorem 2.8, we broadly note where the difficulties in Problem 2.1 lie:
Corollary 2.9 (Reduction to Realizable Learning and Kernel Learning). Learning shallow, low-rank, easily invertible activation functions over Gaussian data up to additive error is computationally efficient given an efficient learning algorithm for noiseless realizable activation learning over Gaussian data and an efficient algorithm for learning the nonlinearity kernel matrix given i.i.d. samples.

Now we proceed to provide the key non-trivial theorems required for the proof of Theorem 2.8. First we prove the correctness of NKP for any activation function satisfying the easily invertible condition (Definition 2.7), though it is likely possible to extend beyond this condition (see Remark 8.9).

Theorem 2.10 (Correctness & Efficiency of NKP). The NKP algorithm optimizes the population objective of Problem 2.1 for any easily invertible activation function, given \( W \in \mathbb{R}^{d \times m} \) and target rank-\( r \), in \( \mathcal{O}(m^3 + m^2 \cdot (r + d)) \) time.

Proof Sketch. The key idea is to apply kernel PCA to the full-rank parameter matrix \( W \in \mathbb{R}^{d \times m} \), noting that \( W \) is not a data matrix. Then, we need to invert the feature map of the nonlinearity kernel in order to recover the best low-rank parameter matrix \( Y \in \mathbb{R}^{d \times m} \) (we are left with a matrix in \( \mathbb{R}^{r \times m} \) after kernel PCA). This step is possible if the kernel is easily invertible (Definition 2.7). See the full proof in Section 8.3 in the Appendix.

We also require the following non-trivial result on the sample complexity of learning the ReLU nonlinearity kernel (it is necessary to learn the kernel separately, see Remark 8.17):

Theorem 2.11 (ReLU Kernel Learning Sample Complexity). Let \( \hat{K}_\sigma = \frac{1}{N} \sum_{k=1}^N \sigma(x_k^T W)\sigma(x_k^T W)^T \), where the columns of \( W \in \mathbb{R}^{d \times m} \) satisfy \( \|W_i\|_2 \leq R \) for \( i \in [m] \), \( \sigma(a) = \max(0, a) \) for \( a \in \mathbb{R} \) is the ReLU activation function and where we draw \( N \) samples from the data distribution \( \{ (x_k, \sigma(x_k^T W)) \}_{k=1}^N \) with \( x_k \sim \mathcal{N}(0, I_{d \times d}) \) i.i.d. for all \( k \in [N] \). Now suppose \( N \geq \Omega \left( R^4 \cdot d^2 \cdot m^2 \cdot \frac{1}{\epsilon^2} \cdot \min \left\{ d \log^2 \left( \frac{1}{\delta} \right), \frac{1}{\delta} \right\} \right) \), with probability \( \geq 1 - \delta \), we have \( \| \hat{K}_\sigma - K_\sigma \|_F \leq \epsilon \).

Proof Sketch. We proceed by analyzing the concentration of the individual kernel values, followed by a union bound over a discretization of the compact space of possible \( W \) (Lemma 8.13). This analysis is very similar to the analysis in Rahimi and Recht [2008]; however, we must make use of a more involved argument involving the dependent Hanson-Wright inequality (Lemma 8.12). The key challenge is that our kernel estimate is not a bounded or Lipschitz function in the random samples and has complicated dependencies. The full proof is in Section 8.3 in the Appendix.

3 Function Approximation at Initialization

In this section, we propose a general framework for initializing low-rank deep networks given a full-rank initialization scheme. Inspired by Algorithm 1, a central component of our efficient shallow low-rank learning algorithm, we describe a special case of our framework which is provably efficient to implement for many settings.

3.1 Framework

The key idea behind our approach is to mimic the full-rank initialization distribution as closely as possible. Khodak et al. [2021] follows this principle to argue for the spectral initialization approach to initialize the low-rank weights: the idea is to match the weight matrices in Frobenius norm as closely as possible using SVD. More precisely:

Definition 3.1 (Spectral Initialization). Given a full-rank weight \( W \in \mathbb{R}^{d \times m} \) initialized according to distribution \( \mathcal{D} \), spectral initialization with rank \( r \) is the following procedure:

1. Sample \( W \sim \mathcal{D} \).
2. Factorize \( U \Sigma V^T = W \) via singular value decomposition, where \( U \in \mathbb{R}^{d \times r}, \Sigma \in \mathbb{R}^{r \times r}, V \in \mathbb{R}^{m \times r} \).
3. Output factor initialization \( \hat{U} = U \Sigma^{1/2}, \hat{V} = V \Sigma^{1/2} \).
However, it is not clear that this metric for matching low-rank to full-rank functions accurately captures what is important in the approximation: Ultimately, we are initializing highly nonlinear functions, and various terms in the weights may be less important than others (in a post-training setting, Anonymous [2022] demonstrates the efficacy of taking nonlinearities into account). Thus, we consider a function-approximation viewpoint rather than a weight-approximation viewpoint at initialization:

**Definition 3.2** (Function Approximation at Initialization). Given a full-rank weight distribution \( D \), we find a low-rank weight matrix of rank \( r \) for initialization as follows:

1. Sample \( W = [W_1, \ldots, W_k] \sim D \) with \( W_i \in \mathbb{R}^{d_i \times m_i} \).
2. Solve \( \hat{U}, \hat{V} = \arg \min_{U,V} \mathbb{E}_{x \sim \mathcal{N}(0, I)} [(f_{U,V}(x) - f_W(x))^2] \), where \( f \) denotes the deep network class we consider, and \( \hat{U} = [\hat{U}_1, \ldots, \hat{U}_k] \) and \( \hat{V} = [\hat{V}_1, \ldots, \hat{V}_k] \), where \( \hat{U}_i \in \mathbb{R}^{d_i \times r} \) and \( \hat{V}_i \in \mathbb{R}^{m_i \times r} \).
3. Use \( \hat{U}, \hat{V} \) as the initialization for the low-rank weights.

Thus, we attempt to match the function values of the networks, rather than simply the weights, making our approach *nonlinearity-aware*. Here we have chosen to measure the similarity of the network outputs over a standard Gaussian input distribution; however, this aspect can easily be modified to be samples over a particular distribution of interest.

Since this approach is essentially function approximation of the initialization network (rather than the trained network, as in other work), we refer to our general approach as *function approximation at initialization*. To implement this approach, one can optimize the low-rank parameters with a gradient-based method with some automatic differentiation framework like Tensorflow [Abadi et al., 2015]. We now proceed to outline a simplification to this general approach which is more tractable and easier to use in practice.

### 3.2 Layerwise Function Approximation at Initialization

Given our result in Theorem 2.10, we know that for a broad family of activation functions, and given the full-rank weights, it is possible to efficiently solve the function approximation at initialization problem for each layer individually. Thus we propose a simplification to the general approach: keep the relevance of the non-linearity, but instead approximate each layer separately rather than the entire network. This approach has the benefits of a) being a simpler problem to solve, and b) being embarrassingly parallel to distribute. Thus, we can obtain a significant speedup in the initialization method compared to the full function approximation at initialization approach.

To adapt to more general layer definitions, we also propose an empirical sample-based stochastic optimization approach for solving the problem using gradient methods. Concretely:

**Definition 3.3** (Layerwise Function Approximation at Initialization). Given a deep neural network \( f \), define the function corresponding to the \( i \)th layer with weights \( W_i \) as \( f_{W_i} \). Then, given a full-rank weight distribution \( D \), we find a low-rank weight matrix of rank \( r \) for initialization as follows:

1. Sample \( W_i \sim D \);
2. Solve \( \hat{U}_i, \hat{V}_i = \arg \min_{U_i,V_i} \mathbb{E}_{x \sim \mathcal{N}(0, I)} [(f_{U_i,V_i}(x) - f_{W_i}(x))^2] \) for all layers \( i \) in parallel;
3. Use \( \hat{U}_i, \hat{V}_i \) as the low-rank initialization for layer \( i \).

If the \( i \)th layer \( f_{W_i} \) is sufficiently simple and the activation function is easily invertible (Definition 2.7), we can solve the layerwise function approximation problem using Algorithm 1 and then apply SVD to factorize the low-rank output into matrices \( \hat{U}_i, \hat{V}_i \), since we have access to \( W_i \) — in these cases, this initialization scheme is efficient. From a practical standpoint, the kernels for various activation functions are easy to compute given recent code for implementing the Q-map calculations [Martens et al., 2021] (which correspond to the same nonlinearity kernels we use in Algorithm 1).

In cases where Algorithm 1 does not apply, we can instead optimize the parameters directly using some gradient-based method over the samples. In this case, we are essentially throwing out information about \( W_i \), since we mainly access information about \( W_i \) via samples which are fed into the gradient-based method (note the similarity to Algorithm 2). To further improve efficiency, we can feed this learning method some prior
information about $W$ by initializing the low-rank weights with spectral initialization (Definition 3.1) – we call this step the “spectral warm start,” and observe that it helps with learning empirically (see Section 5). Also, we note in Remark 5.1 that other input distributions than the standard Gaussian are plausible to use.

4 Nonlinear Low-Rank Approximation

In this section, we demonstrate settings in which we can expect the results of using layer-wise function approximation at initialization for the ReLU activation to be significantly different from using spectral initialization. Throughout this section, we will refer to $\sigma_{\text{ReLU}}$ as $\sigma$ for simplicity. To that end, we lower bound the gap between the quality of the spectral solution (linear approximation) and the quality of the (optimal) nonlinear low-rank approximation with respect to the nonlinear error measure (Problem 2.1). Using our analysis, we uncover some conditions on the full-rank matrix which yield a more significant gap. In particular, as the rank gets smaller or as the dimension of the inputs increases (while the width is super-linear in the input dimension), the gap between the initialization methods blows up with dimension (Theorem 4.4 and Corollaries 8.25, 8.27). It is also the case that full-rank matrices $W \in \mathbb{R}^{d \times m}$ with more approximately orthogonal columns yields a larger gap. As a technical tool, we prove a different characterization of the nonlinear function approximation problem (Theorem 4.2), which applies specifically to one-hidden-layer ReLU networks (rather than easily invertible activations). We then exploit the properties of this characterization to prove Theorem 4.4. Some of our intermediate results are also useful proving Theorem 2.8. We defer all proofs and full theorem statements to Section 8.4 of the Appendix. Despite the restriction to ReLU, we believe our results to be characteristic for other activation functions, as we empirically demonstrate for the Swish activation in Section 5.

These results only apply to the difference between SVD (the spectral solution) and the optimal nonlinear low-rank approximation. While this result is useful for understanding what properties of the full-rank matrix $W$ govern the extreme cases where the two initialization approaches are very similar or very different, these initialization results do not directly prove anything about downstream generalization error, except in the setting where the true optimal weights are close to the initialization distribution. Nevertheless, we empirically demonstrate the connection between good nonlinear low-rank approximation and improved downstream generalization error for deep low-rank models in Section 5.

4.1 An Alternative View of NKP for ReLU Networks

We prove a lower bound on the gap between the output of spectral initialization and our NKP method for one-hidden-layer ReLU network. To achieve this bound, we further develop theory characterizing the optimal low-rank matrix for Problem 2.1 for the ReLU activation. We begin with a useful definition:

**Definition 4.1** (ReLU Kernel: 1st-Order Arc-Cosine Kernel). For the ReLU activation, the associated nonlinearity kernel (Definition 2.5) is known as the first-order arc-cosine kernel [Cho and Saul, 2009], defined by $k(x, y) := \|x\|_2\|y\|_2 \cdot \sqrt{h}(\rho_{xy})$, where $\rho_{xy} := \frac{x^Ty}{\|x\|_2\|y\|_2}$ and $\sqrt{h}(\rho_{xy}) = \left(\sqrt{1 - \rho_{xy}^2} + (\pi - \cos^{-1}(\rho_{xy}))\rho_{xy}\right)/\pi$.

Now we present an alternative algorithm to compute the result of NKP, which works only for the ReLU activation. This algorithm is not always efficient; however, its utility comes from the characterization of the optimal solution to the ReLU NKP problem – in particular, it reveals more structure of the ReLU kernel which allows us to easily lower bound the sub-optimality of standard Frobenius low-rank approximation computed using SVD. It also provides useful insights into the structure of the solution which we use in the proof of Theorem 2.8.

**Theorem 4.2** (ReLU SVD). Consider the goal of finding the optimal rank-r solution to the objective $R(Y)$ in Problem 2.1 with known $W \in \mathbb{R}^{d \times m}$. Suppose we solve the following problem:

$$
\Lambda^* = \arg\max_{\Lambda \in (0, 1)^d, \|\Lambda\|_1 = r} \sum_{i=1}^m \|W_i\|_2^2 \cdot h \left( \frac{\|\Sigma \text{ diag}(\Lambda) V_i\|_2}{\|\Sigma V_i\|_2} \right)
$$

where $W = U\Sigma V^\top$ with $U \in \mathbb{R}^{d \times d}$, $\Sigma \in \mathbb{R}^{d \times d}$ is diagonal, and $V \in \mathbb{R}^{m \times d}$, with $U^\top U = I_{d \times d}$, $V^\top V = I_{d \times d}$ and $V_i \in \mathbb{R}^d$ is the $i$th column of $V^\top$, and where $h$ is defined in Definition 2. Then, the optimal rank-r matrix
Figure 1: We plot the gap growth $\frac{1}{2d} \sqrt{h(\rho) - \rho_0^2}$ (see Theorem 4.4) for $W \in \mathbb{R}^{d \times m}$ with $m = n^{1.5}$ and $d = 0.2n$ with respect to the ReLU nonlinearity. Note the width is super-linear in dimension: $m = \Omega(n^{1+\epsilon})$ for all $\epsilon > 0$. The entries of ground truth matrix $W$ are drawn from $\mathcal{N}(0, 1)$, and then we normalize $\|W_i\|_2 = 1, \forall i \in [m]$. We observe that the gap increases with increasing dimension and decreasing rank scale. Note that the behavior demonstrated matches the theoretical predictions: the gap increases as $\Theta((d^{1/2} \cdot (1 - \sqrt{r/d})^2)$ as per Corollary 4.5.

$Y^* \in \mathbb{R}^{d \times m}$ minimizing the initial objective Eq. (1) is given by $Y^* = U \text{gnorm} \big( \text{diag}(\Lambda^*) \Sigma V^T \big)$, where $\text{gnorm}(A)_i := A_i \cdot \frac{\sqrt{h(\|A_i\|_2)}}{\|A_i\|_2}$ for the $i$th column of matrix $A$.

4.2 Lower Bounding the Gap: SVD vs. NKP

We now use the developed theory to prove a lower bound on the sub-optimality of using the SVD to optimize the objective of Problem 2.1 when given $W$.

**Lemma 4.3** (Relationship between SVD and ReLU SVD). Suppose $W = U \Sigma V^T \in \mathbb{R}^{d \times m}$. Consider the solution for rank-$r$ ReLU SVD (given by $Y^*$) as described in Theorem 4.2. If $h(\rho)$ is replaced with $\rho_0^2$, and we always choose $\Lambda^*$ to correspond to the top $r$ singular values of $\Sigma$, then $Y^*$ is the standard SVD solution.

**Theorem 4.4** (Lower Bound on Suboptimality of SVD). Recall the objective $R(Y)$ from Problem 2.1, where we require that $Y \in \mathbb{R}^{d \times m}$ is a rank-$r$ matrix. Let $W \in \mathbb{R}^{d \times m}$. Define $\rho_0^s \in \mathbb{R}^m$ as the correlations $\|\Sigma \text{diag}(\Lambda^*) V_i\|_2/\|\Sigma V_i\|_2$, where $\Lambda^* \in \{0, 1\}^d$ is the solution to the optimization problem posed in Theorem 4.2. As shorthand, denote $Y(\rho)$ as the associated low-rank matrix for correlation vector $\rho \in \mathbb{R}^m$ (computed as described in Theorem 4.2). Denote $\rho_0^s \text{SVD}$ to be the optimal correlations in the case where we pick $\Lambda^*$ to correspond to the top $r$ singular values, as in SVD. Then, we have the following lower bound for the suboptimality of the SVD solution $Y_{\text{SVD}}$: $\frac{1}{2d} (R(Y_{\text{SVD}}) - R(Y(\rho_0^s))) \geq \frac{1}{2d} \|w \odot \sqrt{h(\rho_0^s)} - \rho_0^s \|_2^2$, where $h$ is defined in Definition 2; $w = \|[W_1\|_1 \cdots \|W_m\|_2\|$ is a vector of column norms of $W$ with $W_i$ being the $i$th column of $W$, and $\odot$ is the elementwise product. We normalize by $d$ to get an average over the entry-wise error of the approximated output.

Using the lower bound in Theorem 4.4, we can now characterize the conditions on the full-rank matrix $W \in \mathbb{R}^{d \times m}$, where the solution to Problem 2.1 and the SVD solution are significantly different. First, smaller correlations $\rho_0^s \text{SVD}$ result in better solutions – this case roughly corresponds to the columns of $W$ being approximately orthogonal (Corollary 8.25, Remark 8.26). When $\max_i \rho_0^s \text{SVD}(i) < 1$, we can prove that if the
width $m$ is super-linear in $d$, the sub-optimality gap grows as $d$ increases, and furthermore the sub-optimality gap is monotone non-decreasing as $r$ decreases (Corollary 8.27). Finally, we prove a stronger version of Corollary 8.27 under the assumption of Gaussian distributed columns of $W \in \mathbb{R}^{d \times m}$, and recover the actual dependence on the rank scale $r/d$:

**Corollary 4.5 (Spherical Weights).** Suppose the columns of $W \in \mathbb{R}^{d \times m}$ are drawn from the uniform distribution over the surface of the unit sphere\(^2\). Consider target rank $r \leq d$. Assume that $r \gg \Theta(\log(m))$. Then with probability at least constant, $\rho_{\text{max}} \leq \sqrt{\frac{1}{\pi}}$, and thus $\frac{1}{d} (R(Y_{\text{SVD}}^*)(Y(Y_{\text{SVD}}^*))) \geq \Omega \left( d^d \cdot \left( \frac{1}{\pi} - \frac{1}{2} \sqrt{\frac{1}{\pi}} \right)^2 \right)$, assuming that $m = d^{1+\delta}$ for some $\delta > 0$ and that $\sqrt{\frac{d}{r}} < \frac{2}{\pi}$.

Therefore, in the case of spherical $W$, the sub-optimality gap increases as either the dimension increases (when width is super-linear in dimension) or as the rank scale decreases.

## 5 Experiments and Discussion

We present some empirical results for our low-rank initialization scheme for training EfficientNets [Tan and Le, 2019] and ResNets [He et al., 2016] on the ImageNet dataset [Russakovsky et al., 2015] with stochastic gradient descent and momentum, with tuned parameters and learning rate schedule. We study low-rank variants of these networks for various choices of rank scale – for parameter matrix $W \in \mathbb{R}^{d \times m}$, the rank scale is the fraction of $\min(d, m)$ that we require for our low-rank factorization $UV^T$. We compare the following initialization methods: 1) Baseline Low-Rank – apply the full-rank init distribution for $W$ to low-rank factors $U \in \mathbb{R}^{m \times r}, V \in \mathbb{R}^{d \times r}$; 2) Spectral (Definition 3.1); 3) Nonlinear Kernel Projection (NKP) – general version of our proposed layerwise init, implemented with Adam [Kingma and Ba, 2014]; 4) WS-Nonlinear Kernel Projection (WS-NKP) – NKP except we initialize with a warm start corresponding to spectral initialization.

### 5.1 Details on Main Experimental Setup

We train ResNet50 [He et al., 2016] and EfficientNet [Tan and Le, 2019] models with stochastic gradient descent and momentum on the 2012 ImageNet dataset [Russakovsky et al., 2015], with tuned parameters and learning rate schedule. The low-rank version of this model simply replaces the convolution layers with low-rank convolutions, as described in Khodak et al. [2021]. The full-rank weight initialization is a truncated normal distribution $\mathcal{N}(0, 1/d)$, where $d$ is the number of input units for the layer, and where “truncation” refers to discarding and re-sampling any samples which are more than two standard deviations from the mean.

We also consider two kinds of regularization on the objective:

1. **Weight decay:** This method is the standard Frobenius norm regularization on the weights of the layers. In the low-rank setting, instead of penalizing $\|W\|_F$, we penalize $\|U\|_F + \|V\|_F$.

2. **Frobenius decay:** This regularization approach is demonstrated by Khodak et al. [2021] to outperform weight decay in several settings they consider. Instead of separately regularizing the low rank factors, this approach penalizes $\|UV^T\|_F$.

We tune the regularization strength separately for both approaches and report the performance of the best regularization strength. Tuning the Frobenius decay regularization strength did not succeed for the EfficientNet models due to divergence during training. Thus we only report the weight decay results for the EfficientNet models. For ResNet-50, for Frobenius decay, we use a regularization strength of 0.3. For ResNet-50 weight decay, we use a regularization strength of $10^{-4}$. For the EfficientNet models with weight decay, we use a regularization strength of $10^{-5}$. We compare across multiple choices of rank scale $\frac{d}{r}$: 0.05, 0.1, 0.15, 0.2.

We run each experiment three times for three different random seeds and average the results and include the standard error up to one standard deviation on the mean performance. The differences across each experiment instance are due to the changes in random seeds used in both sampling at initialization and for sampling batches during optimization. We trained the models on TPU hardware.

---

\(^2\)This assumption is reasonable, given the many similar init distributions used in practice (e.g., He and Glorot inits [He et al., 2015, Glorot and Bengio, 2010]).
For NKP-based approaches, we choose the standard Gaussian as the input distribution. However, other choices are also feasible:

**Remark 5.1 (On the Choice of Input Distribution).** Motivated by our theoretical results, we minimize the function approximation loss over the Gaussian distribution. Our theory suggests that this problem is likely computationally tractable to solve for more general layer architectures as well. However, in practice, we may view this choice as a hyper-parameter to tune. For instance, another reasonable (but computationally expensive) approach is to minimize the function approximation loss over the real data distribution (after being transformed by the previous input layers).

### 5.1.1 Model Architecture

The EfficientNet architecture for b0, b3, and b7 is standard and available in libraries such as Tensorflow [Abadi et al., 2015]. See for instance https://github.com/keras-team/keras/blob/v2.7.0/keras/applications/efficientnet.py. For EfficientNet-b9, we define the width scale parameter to be 3.0, and the depth-scale parameter to be 3.2. For both architectures, we used the Swish nonlinearity [Ramachandran et al., 2017]. For ResNet-50, we also simply use the standard available architecture in Tensorflow.

### 5.1.2 Hyperparameters for Layerwise Initialization

In our experiments, we implement both NKP and WS-NKP using the Adam optimizer [Kingma and Ba, 2014]. Since our networks consist of low-rank convolutional layers (see Khodak et al. [2021] for guidance on how to efficiently define a low-rank convolutional layer), sample 1000 Gaussian vectors in the shape (64, 64, num. input filters) – we arbitrarily choose 64 × 64 patches since the specific dimension of the “image” does not matter too much, and we want to avoid making the dimension of our training problem too large. The number of input filters is determined by the layer and the architecture – for the first layer, there are 3 input filters.

For Adam, we set the learning rate to $5 \times 10^{-3}$, the batch size to 512, and the number of steps per epoch to 128 after hyper-parameter searching over these parameters to determine the quickest convergence rate. With these parameters, Adam converges to the optimum for all low-rank layerwise optimization problems we tried within 6 epochs.

We reported results both for initializing Adam with spectral initialization (WS-NKP) and with baseline initialization (NKP) – almost universally WS-NKP is better.

### 5.1.3 Hyperparameters for Post-Initialization Optimization

For ResNet-50 and each EfficientNet model, we trained the network for 62000 epochs using Stochastic Gradient Descent (SGD) with Momentum. We set the batch size to 4096. We set the momentum parameter to 0.9 and the learning rate schedule to follow a linear warm-up schedule for 1560 steps (choose values for the learning rate from 0 to an initial rate of 1.6), followed by a cosine curve with an initial rate of 1.6, decaying over the remaining 60440 steps (see the CosineDecay learning rate schedule in Tensorflow). We did not modify this training scheme across our experiments for simplicity (our goal was to compare the performance of different init schemes rather than to attain the optimal performance), explaining why our full-rank EfficientNet numbers do not match the numbers in the original EfficientNet paper [Tan and Le, 2019].

### 5.2 Results

It turns out that either WS-NKP or NKP typically outperform the other initialization schemes across multiple rank scales and architecture widths. On average across all experiments, our method gains on the order of 0.3% in accuracy, though the gain is larger for smaller rank scales and larger width networks. These results are also significant – we demonstrate a clear separation of our approach compared to others in 1-standard deviation confidence intervals, and our method tends to have lower variance in performance. Furthermore, we also find empirical evidence of our theoretical claims in Section 4, despite the fact that we use the Swish activation while our theory was ReLU-based: we see the trend that as the rank-scale decreases, or as the widths of the...
Table 1: The reported metrics are average top-1 accuracy as a percent on EfficientNet models of increasing width and depth, trained with Weight Decay regularization. We report standard error over three samples up to one standard deviation. The EfficientNet model variants we consider have width and depth scale parameters set to be (1, 1); (1.2, 1.4); (2.0, 3.1); (3.0, 3.2), corresponding to the b0, b3, b7, and b9 variants respectively. We see the empirical effect described in Section 4 – our NKP method has more significant improvements for smaller rank scales and larger width models.

| Rank Scale | Method        | EfficientNet-b9 | EfficientNet-b7 | EfficientNet-b3 | EfficientNet-b0 |
|------------|---------------|-----------------|-----------------|-----------------|-----------------|
| 0.05       | Baseline      | 66.36 ± 0.23    | 58.61 ± 0.45    | 37.34 ± 0.29    | 31.22 ± 0.62    |
|            | Spectral      | 66.64 ± 0.23    | 58.84 ± 0.38    | **38.3 ± 0.09** | 30.96 ± 0.32    |
|            | NKP           | 65.84 ± 0.28    | 59.00 ± 0.18    | **38.22 ± 0.28**| **32.39 ± 0.26**|
|            | WS-NKP        | 66.90 ± 0.11    | 59.63 ± 0.37    | 38.04 ± 0.03    | 30.8 ± 0.19     |
| 0.10       | Baseline      | 71.67 ± 0.19    | 68.89 ± 0.07    | **57.06 ± 0.24**| **48.24 ± 0.13**|
|            | Spectral      | 72.07 ± 0.15    | 68.83 ± 0.16    | 56.66 ± 0.35    | 47.79 ± 0.17    |
|            | NKP           | 71.02 ± 0.32    | 68.52 ± 0.04    | **56.96 ± 0.19**| 47.42 ± 0.30    |
|            | WS-NKP        | **72.28 ± 0.04**| **69.09 ± 0.16**| 56.76 ± 0.11    | 47.84 ± 0.24    |
| 0.15       | Baseline      | 73.20 ± 0.05    | 71.67 ± 0.19    | 62.56 ± 0.07    | 54.99 ± 0.05    |
|            | Spectral      | **73.55 ± 0.15**| 71.55 ± 0.20    | 63.02 ± 0.07    | 54.97 ± 0.10    |
|            | NKP           | 72.70 ± 0.18    | 71.25 ± 0.12    | 62.86 ± 0.12    | 54.85 ± 0.09    |
|            | WS-NKP        | 73.31 ± 0.04    | **71.74 ± 0.02**| **63.55 ± 0.16**| **55.19 ± 0.10**|
| 0.20       | Baseline      | 73.84 ± 0.04    | 72.16 ± 0.27    | 66.05 ± 0.23    | **59.78 ± 0.17**|
|            | Spectral      | **74.14 ± 0.19**| 72.45 ± 0.17    | 65.96 ± 0.29    | 59.42 ± 0.32    |
|            | NKP           | 73.91 ± 0.09    | 72.32 ± 0.18    | 65.93 ± 0.06    | 59.20 ± 0.11    |
|            | WS-NKP        | **74.01 ± 0.11**| **72.72 ± 0.03**| **66.32 ± 0.02**| 59.38 ± 0.18    |
| 1.0        | Full-Rank     | 79.62 ± 0.05    | 78.70 ± 0.02    | 76.63 ± 0.19    | 74.50 ± 0.13    |

While Frobenius Decay outperforms Weight Decay for smaller rank scales, the advantage erodes for larger rank scales. This effect was not observed by Khodak et al. [2021], possibly because we study larger models and datasets. We note that our method improves over other initialization methods regardless of the regularization scheme.

We also note that in our EfficientNet experiments (Table 1), the effect of width does not appear to be as strong as the effect of the rank scale – loosely using the intuition built by our theory, this empirical result makes sense: We are likely not in a setting where the width is super-linear in the input dimension. In fact, we are likely in the linear regime, where $m = O(d)$. Since the networks are deep, it is difficult to directly use the 1-hidden-layer metaphor from our theory – nevertheless, for many of the layers in the network, the difference between input and output dimension is typically not more than a factor of 2 – even for the EfficientNet architecture which we scale increasingly with depth. Thus, we do not expect as dramatic gains when we scale up the widths of the networks, though we do see some mild gain. On the other hand, the effect of the smaller rank scale is quite apparent in our experiments. It would be interesting to develop a more thorough characterization of the impact of the ratios of the inputs and outputs of layers in a deep architecture on the effectiveness of the NKP framework – it seems plausible that we would have to take into account some notion of average ratio between input and output sizes, and possibly the structure of the architecture itself as well.

We include some more tables in the Appendix in Section 9: In Tables 3, 4, 5, 6, 7, and 8, we summarize the performance of our best initialization method compared to the others.

### 5.3 Downstream Generalization Error

While existing literature has studied the effects of various initializations on optimization, no results as far as we are aware connect the choice of initialization to downstream generalization performance, though this effect has been demonstrated empirically. Thus, we empirically justify the benefits of function approximation at initialization for low-rank networks. We fix rank scale 0.10, EfficientNet-b7 and initialization algorithm...
Table 2: Average Top-1 accuracy on ResNet-50 with different regularization methods. Note that our method tends to outperform the baselines regardless of whether Weight Decay or Frobenius Decay is used. For each rank scale, we display in bold all methods whose confidence intervals overlap.

| Rank Scale | Method   | Weight Decay | Frobenius Decay |
|------------|----------|--------------|-----------------|
| 0.05       | Baseline | 56.92 ± 0.14 | 57.73 ± 0.23    |
|            | Spectral | 56.28 ± 0.39 | 57.42 ± 0.38    |
|            | NKP      | 56.55 ± 0.04 | 57.61 ± 0.15    |
|            | WS-NKP   | **57.37 ± 0.08** | **58.22 ± 0.31** |
| 0.10       | Baseline | 64.09 ± 0.12 | 65.61 ± 0.09    |
|            | Spectral | 64.06 ± 0.19 | 65.69 ± 0.12    |
|            | NKP      | 64.02 ± 0.17 | 65.55 ± 0.05    |
|            | WS-NKP   | **64.74 ± 0.04** | **65.93 ± 0.05** |
| 0.15       | Baseline | 67.58 ± 0.15 | 68.15 ± 0.20    |
|            | Spectral | 66.95 ± 0.16 | 68.21 ± 0.08    |
|            | NKP      | 67.24 ± 0.26 | 67.13 ± 0.51    |
|            | WS-NKP   | **67.74 ± 0.03** | **67.83 ± 0.42** |
| 0.20       | Baseline | 69.04 ± 0.33 | 69.22 ± 0.05    |
|            | Spectral | 68.59 ± 0.19 | 69.04 ± 0.14    |
|            | NKP      | 68.93 ± 0.20 | 68.87 ± 0.10    |
|            | WS-NKP   | **69.37 ± 0.07** | **69.47 ± 0.09** |
| 1.0        | Full-Rank| 78.1         | 78.1            |

WS-NKP, and investigate the effect of layerwise function approximation at initialization on downstream generalization. We implement layerwise function approximation with Adam, as mentioned above. We train the network on ImageNet training data starting from the initialization produced after $0 - 6$ epochs of running Adam starting from the spectral initialization, and measure the top-1 validation accuracy. For each number of epochs of training, we run the experiment 3 times and take the average.

Then, on the $x$-axis, for each number of initialization training epochs, we plot the average multiplicative error across the 107 layers of EfficientNet-b7, paired with the corresponding downstream generalization error. In particular, if the optimum value of our objective (defined in Problem 2.1) at a given layer (at init) is opt, and we have reached $(1 + \epsilon_{layer_i}) \cdot opt$, then we record the average $\epsilon$ across all layers for that number of epochs, and plot alongside it the corresponding average over downstream top-1 validation accuracy. We find that after 4 epochs, training converges and the optimization procedure has reached the optimum.

In Figure 2, we observe that as WS-NKP optimizes, accuracy improves, demonstrating that optimal function approximation at initialization improves downstream generalization.
Figure 2: We vary the number of optimization steps used to implement WS-NKP and plot the average normalized error across layers against the average downstream validation top-1 accuracy for training an EfficientNet-b7 model on ImageNet. Decreasing the function approximation error at init is beneficial for top-1 accuracy.

6 Related Work

Here we fill in some of the related work not previously described in the paper.

6.1 Single-Index Models

Results for efficiently learning realizable activations directly provides one of the ingredients for efficient learning results like Theorem 2.8 (see Corollary 2.9), so we might wonder for what activations other than ReLU it is possible to efficiently solve the problem.

The general problem of learning an activation is known as learning a single-index model in the statistics community (see Dudeja and Hsu [2018] for a comprehensive review of this body of work).

Many existing works have studied the problem of properly learning various activations in the realizable setting [Klivans et al., 2004, Kalai and Sastry, 2009, Kakade et al., 2011, Ge et al., 2018, Zhong et al., 2017, Janzamin et al., 2015, Dudeja and Hsu, 2018], and if those activations also satisfy our easily invertible condition, we can efficiently learn a low-rank approximation for these activations as well (simply replacing gradient descent with whatever the efficient realizable learning algorithm is).

Notably, the conditions often require monotonicity and Lipschitz assumptions, smoothness assumptions, Fourier-theoretic low-degree polynomial approximation assumptions, or are for specific activations, most commonly the ReLU, sigmoid, and tanh activations. The GLMtron algorithm of Kakade et al. [2011] and the tensor-recovery initialized gradient methods of Zhong et al. [2017] in particular apply to broad classes of activation functions.

Most of the methods for learning non-linear activations do not apply to learning the Swish activation, which is non-monotonic and non-symmetric about the origin. Since Swish is smooth, however, we can adapt methods from the literature on single-index models to learn a single Swish function. In particular, the single-index algorithm of Dudeja and Hsu [2018] applies to our setting which has a poly($N,d$) runtime, where $N$ is the number of samples, though the sample complexity is $O(1/\epsilon^2)$ and poly($d$).

The square activation corresponds to the extremely well-studied phase retrieval problem. Our Nonlinear Kernel Projection algorithm does not apply (the square activation is even), but existing work has studied low-rank phase retrieval in different settings [Vaswani et al., 2017, Nayer et al., 2020].
6.2 Computational Learning Theory for Neural Networks

Several works [Goel et al., 2019, 2020b,a, Soltanolkotabi, 2017, Goel et al., 2016] derive the computational and statistical hardness of learning a single ReLU function $\sigma(w^T x)$ in various settings. Such works typically assume the data distribution is marginally Gaussian on the examples, and focus on definitions of generalization error with respect to square loss. There is a significant difference in attainable results in the agnostic learning setting compared to the realizable setting. In the realizable setting, where the noiseless labels come from a planted model $\sigma(w^* T x)$, the results are positive: Soltanolkotabi [2017] proved that projected gradient descent, initialized at 0, converges at a linear rate (in square loss) to the planted $w^*$ with optimal sample complexity. Bakshi et al. [2019] and Ge et al. [2019] provide polynomial time algorithms for learning a two-layer network, while assuming structured data distributions and additive mean-zero noise – this setting is not realizable, but is far more structured than the agnostic learning setting (over, say, Gaussian marginals). This form of non-realizable learning differs from ours in that it only considers additive noisy perturbations of the signal, which is assumed to come from the hypothesis class used by the learning algorithm. In our setting, the hypothesis class we consider is far more restricted: even without noise we cannot hope to reconstruct the ground-truth full-rank network.

In various other settings, hardness results exist. In the agnostic learning setting with Gaussian marginals, Goel et al. [2020b] demonstrates that any statistical-query (SQ) based algorithm — which includes most known learning algorithms including stochastic gradient descent — requires exponential in dimension many statistical queries to learn a ReLU up to additive error $1/10$ with respect to the squared loss.

On the other hand, Goel et al. [2019] gives an efficient approximation algorithm with runtime poly($d, 1/\epsilon$) for finding the best fitting ReLU in an agnostic learning setting which achieves error $O(\text{opt}^{2/3}) + \epsilon$, where opt is the square loss of the best fitting ReLU, when the marginal distribution of the features is log-concave. Diakonikolas et al. [2020] significantly improves this result by providing an algorithm which has runtime poly($d, 1/\epsilon$) which, under the assumption of marginal log-concavity (and no assumptions on the noise/response), is able to recover a vector $w$ such that the corresponding ReLU function has square loss at most $O(\text{opt}) + \epsilon$. Note that Goel et al. [2019] proved that achieving opt + $\epsilon$ is computationally hard (via reduction to learning sparse parities with noise), so this is essentially the best result we can hope for. Also, some assumption on the marginal distribution of the features is necessary, otherwise the problem is NP-hard [Diakonikolas et al., 2020].

In the average case PAC learning setting, Daniely and Vardi [2020] showed that learning a randomly initialized two-layer network with a single output neuron in square loss reduces to refuting random k-SAT formulas, a computational hardness assumption known as RSAT, for various natural choices of initialization distributions. This paper shows that it is often average-case computationally hard to learn a randomly initialized two-layer network over arbitrary data distributions.

Thus, taken separately, both the Gaussian marginals assumption and the average case weights assumption can still lead to hardness for additive approximation in square loss for various simple neural networks, though we can evade such issues if we are willing to give up a constant factor in the optimal error. It is quite reasonable to hope to avoid such constant factors from a practical standpoint, and the existing computational hardness results do not apply to our setting.

In our setting, we consider both these assumptions simultaneously, and while our hypothesis class does not contain the ground-truth function (and thus we are not in the realizable setting), the ground-truth function is also not arbitrary: It is a full-rank variant of our function, and our setting is noiseless. Furthermore, we are in the setting where the output of our function is not 1-dimensional – none of the existing papers study this case. Furthermore, the distribution of the vector outputs is not arbitrary as is the case in the agnostic PAC setting considered in many papers that consider learnability with respect to Gaussian marginals: We assume that the output is a specific function drawn from a class of specific distributions (but our hypothesis class simply does not contain this function) – we can hope to exploit this extra information about the problem setting to evade existing hardness results. Thus, the existing lower bounds on SQ algorithms (like SGD) do not apply to our setting given the assumptions we make.

There is also recent work [Chen and Meka, 2020] considering the problem of learning low-rank deep networks with respect to Gaussian marginals in the realizable setting; but to the best of our knowledge there are no such other works. They are able to give an algorithm whose running time is polynomial in the dimension (and an exponentially large function in the network’s other parameters as well as in $1/\epsilon$, where $\epsilon$ is
the additive square loss generalization error). Their work does not directly apply to our setting since they are in the realizable setting (we want to learn the best low-rank approximation to the full rank network).

6.3 Low-Rank Approximation Theory

At the heart of Problem 2.1 is the idea that we want to make an alternate (nonlinear) low-rank approximation to a matrix $W$. Low-rank approximation has been long studied in the theoretical computer science literature (see [Woodruff, 2014, Mahoney, 2011] for thorough surveys of the topic). One particularly related line of work is the masked low-rank approximation literature [Musco et al., 2019]. The basic idea of masked low-rank approximation is that we want to find a low-rank $Y$ that minimizes $\|M \circ (W - Y)\|_F^2$, where $M$ is a mask applied as an elementwise product (the Hadamard product). This problem captures many different problems studied in the literature under various structural assumptions on $M$ (for instance, the case where $M$ is a real-valued non-negative is known as weighted low-rank approximation, and was studied by Razenshteyn et al. [2016]). Musco et al. [2019] study the case where $M$ is a binary mask and provide bicriteria approximation guarantees since the problem is hard in general. It is interesting to consider the connection between the binary masked low-rank approximation problem of Musco et al. [2019] and our problem, where we apply ReLU to Gaussian samples and mask only the output — interestingly, in our case, the problem is solvable efficiently. It would be interesting to establish further connections between our problem setting and other low-rank approximation settings, perhaps by adopting our setup from Problem 2.1 but possibly changing the input distribution. It seems plausible that for some choices of input distribution, one could make the problem computationally hard. For more background on the low-rank approximation literature, see the discussion in Musco et al. [2019].

7 Conclusion

We introduced efficient algorithms for learning low-rank neural networks: 1) Algorithm 2 solves an open learning theory question on learning low-rank approximations of ReLUs, and 2) Algorithm 1 (Nonlinear Kernel Projection) serves as a subroutine in both Algorithm 2 and as a step in a novel initialization method for low-rank deep networks. We provide theoretical guarantees and intuition for when our methods should outperform classic approaches (high input dimension and low-rank), and validate our theory with promising empirical results.

We close with a few directions for future work: It would be interesting to 1) provably characterize the impact of initialization schemes on downstream generalization, low-rank or otherwise; 2) identify optimal distributions to sample low-rank weights from without optimization; 3) discover better low-rank training methods; 4) extend our theory beyond 1-hidden-layer ReLU networks to other activations, depths, and architectures; 5) extend our init framework to “efficiently-parameterized” networks beyond low-rank.

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8 Appendix: Proofs

8.1 Background on Hermite Analysis

We present some theory about the Hermite polynomial basis which is useful in the analysis. We take the definition and required basic facts from O’Donnell [2014].

Definition 8.1 (Gaussian Space). $L_2(N(0,1))$ is Hilbert space with respect to the Hermite orthogonal polynomial basis.

Definition 8.2 (Hermite orthogonal polynomial basis). The Hermite basis is an orthogonal basis over $L_2(N(0,1))$. In particular, we can write

$$f(a) = \sum_{\ell=0}^{\infty} c_\ell H_\ell(a)$$

where $H_\ell(a)$ is the $\ell^{th}$ Hermite basis function, and $c_\ell = \mathbb{E}_a[f(a)H_\ell(a)]$. We define

$$H_0(a) = 1, \quad H_1(a) = a,$$

and compute the rest by applying Gram-Schmidt over the function space. We have the following definition for the $\ell^{th}$ Hermite basis function:

$$H_\ell(a) := \frac{1}{\sqrt{\ell!}} \frac{(-1)^\ell}{\varphi(a)} \frac{d^\ell}{da^\ell} \varphi(a).$$

We also have the recurrence relation

$$H_{\ell+1}(a) = \frac{1}{\sqrt{\ell+1}} \left(a H_\ell(a) - \frac{d}{da} H_\ell(a)\right)$$

and derivative formula

$$\frac{d}{da} H_\ell(a) = \sqrt{\ell} H_{\ell-1}(a).$$

The following important lemma provides a rule for calculating $\mathbb{E}_{a,a'}[f(a)f(a')]$ when $a, a'$ are correlated standard Gaussian random variables.

Lemma 8.3. Let $a, a'$ be standard Gaussian random variables with correlation $\rho$. Then, we have

$$\mathbb{E}_{a,a'}[H_\ell(a)H_{\ell'}(a')] = \begin{cases} \rho^\ell & \text{if } \ell = \ell' \\ 0 & \text{otherwise.} \end{cases}$$

and

$$\mathbb{E}_{a,a'}[f(a)f(a')] = \sum_{\ell,\ell'=1}^{\infty} c_\ell c_{\ell'} \mathbb{E}_{a,a'}[H_\ell(a)H_{\ell'}(a')]$$

$$= \sum_{\ell=0}^{\infty} c_\ell^2 \rho^\ell.$$

8.2 Hermite Decomposition of ReLU

Goel et al. [2019] derives properties of the Hermite expansion for the univariate ReLU:

Lemma 8.4 (Hermite Expansion Properties for Univariate ReLU [Goel et al., 2019]). Let $\{c_i\}_{i=0}^{\infty}$ be the Hermite coefficients for ReLU. Then,

$$c_k = \begin{cases} 1/\sqrt{2\pi} & \text{if } k = 0 \\ 1/2 & \text{if } k = 1 \\ \frac{1}{\sqrt{2\pi}k!} (H_k(0) + kH_{k-2}(0)) & \text{if } k \geq 2 \end{cases}$$
Figure 3: $\sqrt{h(\rho)}$ (see Definition 4.1) plotted against the linear function $\rho$. Here, $\rho$ is a correlation between the inputs to the arc-cosine kernel.

Using the above properties, we can derive the explicit form of the Hermite coefficients for the ReLU activation:

**Lemma 8.5 (Hermite Coefficients for ReLU).** Let $\{c_i\}_{i=0}^{\infty}$ be the Hermite coefficients for ReLU. Then,

$$c_k = \begin{cases} 
1/\sqrt{2\pi} & \text{if } k = 0 \\
1/2 & \text{if } k = 1 \\
0 & \text{if } k = 2m + 1, m \geq 1 \\
\frac{1}{2\pi} \frac{1}{4^m} \cdot \frac{(2m)!}{m!} \cdot \frac{1}{(2m-1)!} & \text{if } k = 2m, m \geq 1 
\end{cases}$$

**Proof.** First we show that $c_k = 0$ for odd $k > 1$. This is easy to check since if $k$ is odd, so is $k - 2$ and checking that there is no constant term for odd Hermite polynomials $H_k$ yields that the whole expression is 0.

For the rest of the even terms, plug in the standard formula $H_{2m}(0) = (-1)^m \frac{(2m)!}{m! \cdot 2^m}$ to the recurrence given in the expansion properties and simplify using $\frac{(2m)!}{m! \cdot 2^m}$.

**Lemma 8.6 (Hermite Analysis of ReLU Correlation).** Suppose we have univariate standard Gaussians $g_1, g_2$ which are $\rho$-correlated ($\rho \in [0, 1]$). Let $\sigma(x) = \max(0, x)$ be the ReLU activation. Then,

$$2\mathbb{E}_{g_1, g_2}[\sigma(g_1)\sigma(g_2)] = \frac{1}{\pi} \left( 1 + \frac{\pi}{2} \rho + \sum_{\ell=1}^{\infty} \frac{1}{4^\ell} \cdot \left( \frac{2\ell}{\ell} \right) \cdot \frac{1}{(2\ell - 1)!} \rho^{2\ell} \right)$$

(2)

**Proof.** Apply Lemma 8.3 and Lemma 8.5 and simplify the algebra.

**Lemma 8.7 (Convexity and Monotonicity of $\sqrt{h}$).** The function $\sqrt{h}$ defined by Definition 2 is both convex and monotone increasing on $[0, 1]$, and is also bounded between $[0, 1]$ for inputs in $[0, 1]$.

**Proof.** First we compute the derivative:

$$\frac{d\sqrt{h}(\rho)}{d\rho} = \frac{1}{2} + \sum_{\ell=1}^{\infty} \frac{1}{4^\ell} \left( \frac{2\ell}{\ell} \right) \frac{2\ell}{(2\ell - 1)!} \rho^{2\ell - 1}$$

25
Observe the derivative is positive for \( \rho \in [0, 1] \); thus \( \sqrt{h}(\rho) \) is monotone increasing. Since \( \sqrt{h}(\rho) \) is a positive combination of convex functions (linear functions and even powers are convex), it is also convex. To prove it is bounded, using monotonicity, we only need consider the extremes at \( \rho = 0, 1 \). We have \( h(0) = \frac{1}{\pi} \), and we have (using the closed form given by Definition 4.1)

\[
h(1) = \frac{(\sqrt{1-1^2} + (\pi - 0) \cdot 1)}{\pi} = 1
\]

which proves the statement.

**Remark 8.8 (Convexity and Monotonicity of C-Maps).** It is worth noting that the analysis in Martens et al. [2021] proves that a wide variety of related functions to \( \sqrt{h} \) are convex and monotone.

### 8.3 Proofs for Section 2

First we prove the correctness of NKP.

**Theorem 2.10 (Correctness & Efficiency of NKP).** The NKP algorithm optimizes the population objective of Problem 2.1 for any easily invertible activation function, given \( W \in \mathbb{R}^{d \times m} \) and target rank-\( r \), in \( \mathcal{O} \left( m^3 + m^2 \cdot (r + d) \right) \) time.

**Proof.** We have

\[
\mathbb{E}_{x \sim N(0, I)} \left[ \| \sigma(x^\top Y) - \sigma(x^\top W) \|^2 \right] = k_\sigma(Y, Y) + k_\sigma(W, W) - 2k_\sigma(Y, W) \tag{3}
\]

where \( \phi \) is the feature map defining \( k_\sigma(x, y) \), applied column-wise to \( Y, W \). Then, we can perform the standard manipulations to recover the kernel SVD objective, by writing \( \phi(Y) = UU^\top \phi(W) \) for \( U \) orthogonal rank-\( r \):

\[
\arg \min_Y \| \phi(Y) \|^2_2 - 2\text{Tr} \left( \phi(Y)^\top \phi(W) \right) = \arg \max_{U^\top U = I_{r \times r}} 2\text{Tr} \left( (I - UU^\top) \phi(W) \phi(W)^\top (I - UU^\top) \right) \tag{4}
\]

Now we can write the kernel form of the optimization problem to get the dependence on \( K = \phi(W)^\top \phi(W) \in \mathbb{R}^{m \times m} \), which we also note is a positive semi-definite symmetric matrix. We now reproduce the standard ideas of Schölkopf et al. [1998, 2002]. Note we can write \( U = \phi(W)A \) for \( A \in \mathbb{R}^{m \times r} \), since we have \( \phi(W) \phi(W)^\top U = U \Sigma \) and thus \( U = \phi(W) \left( \phi(W)^\top U \Sigma^{-1} \right) \). Let \( Z = U^\top \phi(W) = A^\top \phi(W)^\top \phi(W) = A^\top K_\phi \).

Finally, noting that our current objective is maximizing \( \text{Tr} \left( ZZ^\top \right) \), we write

\[
ZZ^\top = U^\top \phi(W) \phi(W)^\top U = A^\top K_\phi^2 A \tag{5}
\]

and thus get

\[
\arg \max_{A^\top K_\phi A = I_{r \times r}} \text{Tr} \left( A^\top K_\phi^2 A \right)
\]

Writing \( B = \sqrt{K_\phi} A \), we get

\[
\arg \max_{B^\top B = I_{r \times r}} \text{Tr} \left( B^\top K_\phi B \right)
\]

Then \( B^* = V \in \mathbb{R}^{m \times r} \), where \( V \) corresponds to the top \( r \) eigenvectors of \( K_\phi \). We can then write \( Z^* = A^\top^* K_\phi = V^\top \sqrt{K_\phi} = V^\top \Sigma V^\top = \Sigma V^\top \in \mathbb{R}^{r \times m} \), the resultant optimal low-dim projection.
However, we want to actually recover $Y^*$. Thus, we write in the expanded feature space
\begin{align}
\phi(Y^*) &= U\Sigma V^T \\
Y^* &= \phi^{-1}(U\Sigma V^T)
\end{align}
(6)

We have written $\phi^{-1}$ to refer to a column-wise inverse transformation – in order for this step to be valid, such a column-wise inverse has to exist. In our case, this is guaranteed by the fact that the activation is easily invertible (Definition 2.7). Since the Hermite coefficient $c_1 := E_{d \sim N(0,1)}[|\sigma(z)|]$ is positive by easy invertibility, for some column vector $x \in \mathbb{R}^d$, the associated feature map $\phi(x)$ has $d$ rows which correspond to $c_1 \ast x$. We only need to identify those rows and divide by $c_1$ to recover $x$; thus the operation $\phi^{-1}$ is well-defined (even if the feature-map is a mapping to Hilbert space!). However, we want to avoid computing $U$, the corresponding top eigenvectors of $\phi(W)\phi(W)^T$ which lie in the feature map space, since this can be expensive (or impossible in the case of Hilbert space feature maps). Again easy invertibility saves us: We only care about the relevant $d$ rows of the feature map corresponding to the entries of $Y^*$. Thus, we have
\[ Y^* = \frac{1}{c_1}U\Sigma V^T \]
where $U \in \mathbb{R}^{d \times r}$ is the low-rank approximation of $U$ localized to the correct $d$ rows. However, we still need to calculate $U$. Notice that considering the full-rank case, we get
\begin{align}
W &= \phi^{-1}(U_{\dim(\phi) \times m}V_{m \times m}^T) \\
&= \frac{1}{c_1}U_{d \times m}V_{m \times m}^T
\end{align}
(7)

We emphasize here that this expression is not the standard singular value decomposition of $W$ – in particular, $U$ does not have orthogonal columns, and $\Sigma, V$ are already defined by the kernel SVD. However, we then get the following expression:
\[ U_{d \times m} = c_1 \cdot WV_{m \times m}\Sigma^{-1}_{m \times m} \]

To get the corresponding low-rank approximation $U$, we simply choose the top singular values according to $\Sigma$ and their corresponding singular vectors in $V$:
\[ U = c_1 \cdot WV_{m \times r}\Sigma^{-1}_{r \times r} \]

Then, we can plug this expression back into $Y^*$:
\[ Y^* = \frac{1}{c_1}U\Sigma V^T = WVV^T \]

where $V$ is the top $r$ eigenvectors of $K_\phi$, thus proving the result.

Since the algorithm only requires taking the SVD of the $m \times m$ kernel matrix and some matrix multiplications, the algorithm is poly($d, m$) time.

\[ \square \]

Remark 8.9 (Easy Invertibility Is Possibly Not Necessary). Here, we have made the easily invertible assumption which is necessary for the Nonlinear Kernel Projection framework to work, namely that we can efficiently recover $x$ given $\phi(x)$. However, it is plausible that a variant of NKP works for other activation functions, namely modifying the recovery step. One can write down a set of nonlinear equations in $x$ based on the non-zero coefficients of $\phi$ to recover the input (the number of coefficients you need and the nonlinearities involved impact the feasibility and efficiency of NKP).

Now we prove that Algorithm 2 efficiently solves the shallow low-rank ReLU learning problem.

**Theorem 2.8 (Shallow Low-Rank ReLU Learning is Computationally and Statistically Efficient).** Consider Problem 2.1, where $W \in \mathbb{R}^{d \times m}$ is the matrix of full-rank parameters defining the one-hidden-layer ReLU function. Algorithm 2 is an efficient learning algorithm for recovering the optimal low-rank matrix up to additive generalization error $\epsilon$ with probability at least $1 - \delta$. Both the sample complexity and computational complexity of learning rank-$r$ ReLU approximation are poly $\left(R, d, m, \frac{1}{\epsilon}, \log(\frac{1}{\delta}), \|W\|_2, \frac{1}{\lambda_r - \lambda_{r-1}}, r\right)$, where $R$ is a bound on the $L_2$ norms of the columns of $W$, $\|W\|_2$ is the spectral norm of $W$, and $\lambda_r, \lambda_{r-1}$ are the $r^{th}$ and $(r-1)^{st}$ eigenvalues of $K_{\text{ReLU}}$ respectively.
Proof. To prove this theorem, we put together 1. a computationally and statistically efficient method for estimating the kernel matrix up to additive Frobenius error; 2. a computationally and statistically efficient method for estimating $W$ up to additive Frobenius error; 3. a computationally efficient algorithm for recovering the best low-rank approximation $Y^*$ given knowledge of $W$ and the kernel matrix $K_{ReLU}$; 4. perturbation bounds on the eigenvectors of an approximate kernel matrix combined with perturbation bounds on approximate $W$ to get a perturbation estimate of the final $Y^*$. Putting all these elements together yields the result.

First we define

$$
\epsilon_K := \left\| K_{ReLU} - \hat{K}_{ReLU} \right\|_F
$$

and

$$
\epsilon_W := \|W - \hat{W}\|_F
$$

We now list the various results we need:

1. Theorem 2.11 gives an algorithm which requires $N = \mathcal{O}\left(\frac{R^4 \cdot d^2 \cdot m^2}{\epsilon_K^2} \cdot \min\left(d \log^2 \left(\frac{1}{\delta_K}\right), \frac{1}{\epsilon_K}\right)\right)$ samples and runtime $\mathcal{O}(N \cdot d \cdot m)$ to learn the kernel $K_\sigma$ up to additive Frobenius error $\epsilon_K$ with probability at least $1 - \delta_K$.

2. Corollary 8.11 due to Soltanolkotabi [2017] gives an algorithm which requires $N = \mathcal{O}(d + \log(m/\delta_W))$ samples and runtime $\mathcal{O}(N \cdot d \cdot m \cdot \log \left(\frac{R \cdot \sqrt{m}}{\epsilon_W}\right))$ to learn the matrix $W$ up to additive Frobenius error $\epsilon_W$ with probability at least $1 - \delta_W$.

3. Algorithm 1 finds the optimal rank $r$ $Y^*$ given exact $W$ and $K_{ReLU}$ in time $\mathcal{O}(m^3 + m^2 \cdot (r + d))$ (though see Allen-Zhu and Li [2016] for faster methods than $\mathcal{O}(m^3)$ for SVD depending on other parameters of the matrix).

4. Algorithm 2 uses Algorithm 1 as a subroutine applied to estimates of the kernel matrix $\hat{K}_{ReLU}$ and the parameter matrix $\hat{W}$, which have time and sample complexities given directly above.

5. Lemma 8.19 bounds the gap in population error between the optimal rank-$r$ matrix $Y^*$ and the estimated matrix $\hat{Y}$ which is the output of Algorithm 2 in terms of the Frobenius norms of the additive approximation errors of the estimates of $\hat{K}_{ReLU}$ and $\hat{W}$ used by Algorithm 2:

$$
\mathcal{R}(\hat{Y}) - \mathcal{R}(Y^*) \leq 8R^2 \cdot m \cdot \sqrt{\epsilon_K \cdot \frac{\|W\|_2}{\lambda_r - \lambda_{r-1}}} + \epsilon_W
$$

All that remains is to plug in the error estimates and take union bounds across the kernel learning subroutine and the $W$-learning subroutine to get the overall additive generalization error bound. First we set

$$
\epsilon = 8R^2 \cdot m \cdot \sqrt{\epsilon_K \cdot \frac{\|W\|_2}{\lambda_r - \lambda_{r-1}}} + \epsilon_W
$$

Let $\epsilon_W = \frac{1}{2} \gamma^2$ and $\epsilon_K = \frac{1}{2} \gamma^2 \cdot \frac{\lambda_r - \lambda_{r-1}}{\|W\|_2}$. Then, $\epsilon = 8R^2 \cdot m \cdot \gamma$ and we choose

$$
\epsilon_W = \frac{1}{2} \left(\frac{\epsilon}{8R^2 \cdot m}\right)^2
$$

and

$$
\epsilon_K = \frac{1}{2} \left(\frac{\epsilon}{8R^2 \cdot m}\right)^2 \cdot \frac{\lambda_r - \lambda_{r-1}}{\|W\|_2}
$$

to give us total generalization error $\epsilon$.

Now we take union bounds across kernel learning and $W$-learning and simply set probability of failure for kernel learning and the probability of failure for $W$-learning to both equal $\delta/2$ – this step just adds a constant factor to the bound and does not affect the asymptotic complexity. So, the total sample complexity...
across both kernel and $W$-learning is dominated by the kernel learning sample complexity and is thus overall bounded by

$$N = O\left(\frac{R^{12} \cdot d^2 \cdot m^6 \cdot \|W\|^2_2}{\epsilon^4 \cdot (\lambda_r - \lambda_{r-1})^2} \cdot \min\left(d \log^2 \left(\frac{1}{\delta}\right), \frac{1}{\delta}\right)\right)$$

The overall time complexity is bounded by

$$O\left(N \cdot d \cdot m \cdot \log\left(\frac{R^5 \cdot m^{2.5}}{\epsilon^2}\right) + m^3 + m^2 \cdot (r + d)\right)$$

Thus, both the time complexity and the sample complexity are $poly\left(R, d, m, \frac{1}{\delta}, \|W\|_2, \frac{1}{\lambda_r - \lambda_{r-1}}, r\right)$.

Now we proceed with the development of the required lemmas to prove Theorem 2.8. First we restate the main theorem of Soltanolkotabi [2017] for reference:

**Lemma 8.10** (Learning Realizable ReLU with Gradient Descent [Soltanolkotabi, 2017]). Consider the setting of learning a single ReLU $max(0, w^\top x)$ from noiseless samples (e.g., one column of $W$, so $w^* \in \mathbb{R}^d$) over standard Gaussian marginals. Assume $\|w^*\|_2 \leq R$. Then if we run projected gradient descent initialized from 0 over a batch of size $n$, where $n \geq d$, with probability at least $1 - 9 \exp(-\Theta(n))$, we have that the gradient descent updates $w_t$ satisfy

$$\|w_t - w^*\|_2 \leq 2^{-t} \cdot R$$

Or, defining $\epsilon = \|w_t - w^*\|_2$,

$$t \geq \log\left(\frac{R}{\epsilon}\right)$$

giving the required number of iterations of gradient descent to reach $\ell_2$ error $\epsilon$ for learning $w^*$, thus giving a total computational complexity $poly\left(n, d, \log\left(R/\epsilon\right)\right)$.

**Corollary 8.11** (Learning $W$ from Samples). We can run gradient descent $m$ times - once for each column of $W$ - so the guarantee holds simultaneously over all $m$ learning problems. So the probability of failure is set to be $\delta$, we choose $n = \Theta\left(d + \log\left(\frac{m}{\delta}\right)\right)$ (via union bound). Then, to ensure that $\|W^* - \hat{W}\|_F \leq \epsilon$, we choose $t = \log\left(\frac{R \cdot \sqrt{m}}{\epsilon}\right)$ and run that many steps for each of the $m$ columns of $W$. Thus, the sample complexity is $n = poly\left(d, \log(m), \log(1/\delta)\right)$ and the computational complexity is $poly\left(m, d, n, \log\left(R/\epsilon\right)\right)$.

We will make use of a dependent random variables version of the Hanson-Wright inequality for quadratic forms, which yields sub-exponential tails:

**Lemma 8.12** (Dependent Hanson-Wright over Sub-Gaussians [Zajkowski, 2020]). Suppose $x \in \mathbb{R}^d$ is a sub-gaussian random variable satisfying $E_x[\exp(t \cdot x)] \leq \exp\left(K^2 t^2 / 2\right)$ for all $t \in \mathbb{R}$. Then for matrix $A \in \mathbb{R}^{d \times d}$, we have

$$\mathbb{P}\left(\|x^\top A x - E_x[x^\top A x]\| > t\right) \leq 2 \exp\left(-\min\left\{\frac{t^2}{16C^2 K^4 \|A\|^2_{\text{nuclear}}}, \frac{t}{4 C K^2 \|A\|_{\text{nuclear}}}\right\}\right)$$

where $C$ is a universal constant and $\|\cdot\|_{\text{nuclear}}$ refers to the nuclear norm defined by the absolute sum of the singular values of the matrix.

Now we prove a learning result for the kernel matrix.

**Theorem 2.11** (ReLU Kernel Learning Sample Complexity). Let $\hat{K}_\sigma = \frac{1}{N} \sum_{k=1}^N \sigma(x_k^\top W)\sigma(x_k^\top W)^\top$, where the columns of $W \in \mathbb{R}^{d \times m}$ satisfy $\|W\|_2 \leq R$ for $i \in [m]$, $\sigma(\alpha) = \max(0, \alpha)$ for $\alpha \in \mathbb{R}$ is the ReLU activation function and where we draw $N$ samples from the data distribution $\{(x_k, \sigma(x_k^\top W))\}_{k=1}^N$ with $x_k \sim \mathcal{N}(0, I_{d \times d})$ i.i.d. for all $k \in [N]$. Now suppose $N \geq \Omega\left(R^4 \cdot d^2 \cdot m^2 \cdot \frac{1}{\epsilon^2} \cdot \min\left(d \log^2 \left(\frac{1}{\delta}\right), \frac{1}{\delta}\right)\right)$, then with probability $\geq 1 - \delta$, we have $\|\hat{K}_\sigma - K_\sigma\|_F \leq \epsilon$. 29
Proof. We proceed by analyzing the concentration of the individual kernel values, followed by a union bound over a discretization of the compact space of possible $W$. This analysis is very similar to the analysis in Rahimi and Recht [2008]; however we must make use of a more involved argument using dependent Hanson-Wright (Lemma 8.12) since our kernel estimate is not a bounded function in the random samples and has more complicated dependencies.

First define the random variable

$$Z(i, j) := \sigma(x^\top W_i)\sigma(x^\top W_j)$$

where $x \sim \mathcal{N}(0, I_{d \times d})$ and $W_i, W_j$ are the $i^{th}$ and $j^{th}$ columns of $W$. Note that by definition,

$$E_x[Z(i, j)] = K\sigma(i, j) = K\sigma(j, i)$$

When we want to refer to the $Z(i, j)$ associated with sample $k \in [N]$, we call it $Z_k(i, j)$. For simplicity, we drop the $i,j$ indexing until it is necessary. Thus, to prove concentration and get a lower bound on the required sample complexity, we want to upper bound

$$\mathbb{P}\left(\left|\sum_{k=1}^{N} Z_k - E[Z_k]\right| > N \cdot t\right)$$

Now note that $Z_k$ is very similar to a quadratic form – we want to take advantage of Hanson-Wright style concentration bounds. The main difference is that we have a non-constant matrix in the quadratic form. In particular, we can write $\sum_{k=1}^{N} Z_k$ as follows:

$$\sum_{k=1}^{N} Z_k = X^\top A(X)X$$

and thus

$$\mathbb{P}\left(\left|\sum_{k=1}^{N} Z_k - E[Z_k]\right| > N \cdot t\right)$$

$$= \mathbb{P}\left(|X^\top A(X)X - E[X^\top A(X)X]| > N \cdot t\right)$$

where we define

$$X = [x_1 \cdots x_N] \in \mathbb{R}^{d \cdot N}$$

for $x \in \mathbb{R}^d$. The variable matrix is defined by

$$A(X) = \begin{bmatrix} B_{ij}(x_1) \\ \vdots \\ B_{ij}(x_N) \end{bmatrix} \in \mathbb{R}^{d \cdot N \times d \cdot N}$$

where the individual blocks on the diagonal are given by

$$B_{ij}(x) := W_i W_j^\top 1(W_i^\top x > 0) 1(W_j^\top x > 0) \in \mathbb{R}^{d \times d}$$

We will also refer to $B_{ij} = W_i W_j^\top$ when there is no $x$.

Thus we can apply Hanson-Wright if we can reduce to the question to bounding the concentration of each of the $2^N$ possible values of $A(X)$. To enact this strategy, we re-write the bound in terms of different random variables which can be bounded with $N$ different Hanson-Wright concentration bounds, after conditioning on which realization of $A(X)$ shows up. We will be able to do this due to the independence of the $x_1, \cdots, x_N$ as well as the fact that the block diagonals are identically distributed (either 0 or $B_{ij}$).

In particular, define the random variable

$$\xi_k := Y_k^\top B_{ij} Y_k \cdot I_k - p_{ij} \cdot E_{Y_k}[Y_k^\top B_{ij} Y_k]$$
where we define $I_k$ as the indicator random variable for the event $B_{ij}(x_k) > 0$, and the probability

$$ p_{ij} = \mathbb{P}_{x \sim \mathcal{N}(0, I)} (B_{ij}(x) \neq 0) \\
= \mathbb{P}_{x \sim \mathcal{N}(0, I)} (W_i^T x \geq 0 \text{ and } W_j^T x \geq 0) $$

(11)

Note that since $I_k$ is i.i.d., $\mathbb{P}(I_k) = p_{ij}$. Let the distribution of $Y_k$ be defined conditionally as $x_k | I_k$.

Now, though $x_k \sim \mathcal{N}(0, I_{d \times d})$ are independent features, dependencies may arise in $Y_k$ as the result of this conditioning. Note that $\xi_k$ are i.i.d. across $k \in [N]$ and also that $\mathbb{E}[\xi_k] = 0$.

With these definitions in hand, we can write

$$ \mathbb{P} \left( \left| X^\top A(X)X - \mathbb{E}[X^\top A(X)X] \right| > N \cdot t \right) $$

$$ = \mathbb{P} \left( \sum_{k=1}^{N} x_k^\top B_{ij} x_k \cdot I_k - \mathbb{E}[x_k^\top B_{ij} x_k | I_k] > N \cdot t \right) $$

$$ = \mathbb{P} \left( \sum_{k=1}^{N} x_k^\top B_{ij} x_k \cdot I_k - p_{ij} \mathbb{E}[x_k^\top B_{ij} x_k | I_k] > N \cdot t \right) $$

(12)

$$ = \mathbb{P} \left( \sum_{k=1}^{N} Y_k^\top B_{ij} Y_k \cdot I_k - p_{ij} \mathbb{E}[Y_k^\top B_{ij} Y_k] > N \cdot t \right) $$

$$ = \mathbb{P} \left( \sum_{k=1}^{N} \xi_k > N \cdot t \right) $$

To bound this probability, we will split the bound into two sub-problems: one bounds the concentration of the indicator variable (scaled by some quantities) and the other applies (dependent) Hanson-Wright to bound the concentration of the quadratic forms. First we need to condition on $Y_k$ to split the problems up:

$$ \mathbb{P} \left( \left| \sum_{k=1}^{N} \xi_k \right| > N \cdot t \right) $$

$$ = \mathbb{E}_{Y_1, \ldots, Y_N} \left[ \mathbb{P} \left( \sum_{k=1}^{N} \xi_k | Y_k > N \cdot t | Y_1, \ldots, Y_N \right) \right] $$

(13)

using the tower property of conditional expectation and the independence of $\xi_k$ to all $Y_j, j \neq k$. Now we focus on the probability to bound inside the expectation. The relevant random variables are now the conditioned versions of $\xi_k$. For notational simplicity, we define $\xi_k := \xi_k | Y_k$. Now we can write down the following decomposition:

$$ \mathbb{P} \left( \left| \sum_{k=1}^{N} \xi_k \right| > N \cdot t \right) $$

$$ = \mathbb{P} \left( \sum_{k=1}^{N} \xi_k - \mathbb{E}_{I_k}[\xi_k] + \sum_{k=1}^{N} \mathbb{E}_{I_k}[\xi_k] > N \cdot t \right) $$

$$ \leq \mathbb{P} \left( \sum_{k=1}^{N} \xi_k - \mathbb{E}_{I_k}[\xi_k] + \sum_{k=1}^{N} \mathbb{E}_{I_k}[\xi_k] > N \cdot t \right) $$

(14)

$$ = \mathbb{P} \left( \sum_{k=1}^{N} \mathbb{E}_{I_k}[\xi_k] > N \cdot (t - s) | J(s) \right) \mathbb{P}(J(s)) $$

$$ + \mathbb{P} \left( \sum_{k=1}^{N} \mathbb{E}_{I_k}[\xi_k] > N \cdot (t - s) | \neg J(s) \right) \mathbb{P}(\neg J(s)) $$

$$ \leq \mathbb{P} \left( \sum_{k=1}^{N} \mathbb{E}_{I_k}[\xi_k] > N \cdot (t - s) \right) + \mathbb{P}(J(s)) $$
where we define the indicator event

\[ J(s) := 1 \left( s \leq \frac{1}{N} \sum_{k=1}^{N} \hat{\xi}_k - \mathbb{E}_{I_k}[\hat{\xi}_k] \right) | Y_1, \cdots, Y_N \]

Now, we can take the expectation over the bounds and finally split up the two terms and apply dependent Hanson-Wright to the first term and Bernoulli concentration to the second term. In particular, we have

\[
P\left( \left| \sum_{k=1}^{N} \xi_k \right| > N \cdot t \right) \\
\leq \mathbb{E}_{Y_1, \cdots, Y_N} \left[ P\left( \left| \sum_{k=1}^{N} \mathbb{E}_{I_k}[\hat{\xi}_k] \right| > N \cdot (t - s) | \neg J(s), Y_1, \cdots, Y_N \right) \right] \\
+ \mathbb{E}_{Y_1, \cdots, Y_N} \left[ P\left( J(s) | Y_1, \cdots, Y_N \right) \right] \\
\leq P\left( \left| \sum_{k=1}^{N} Y_k^T B_{ij} Y_k - \mathbb{E}_{Y_k}[Y_k^T B_{ij} Y_k] \right| > N \cdot t \frac{p_{ij}}{p_{ij}} \right) \\
+ \mathbb{E}_{Y_1, \cdots, Y_N} \left[ P\left( \left| \sum_{k=1}^{N} \hat{\xi}_k - \mathbb{E}_{I_k}[\hat{\xi}_k] \right| \geq s | Y_1, \cdots, Y_N \right) \right] \tag{15}
\]

where we used the fact that
\[ \mathbb{E}_{I_k}[\hat{\xi}_k] = p_{ij} (Y_k^T B_{ij} Y_k - \mathbb{E}_{Y_k}[Y_k^T B_{ij} Y_k]) \]

Now define the mean zero random variable (conditioned on \( Y_1, \cdots, Y_k \))

\[ \psi_k := \hat{\xi}_k - \mathbb{E}_{I_k}[\hat{\xi}_k] = Y_k^T B_{ij} Y_k \cdot (I_k - p_{ij}) = Y_k^T B_{ij} Y_k \cdot (I_k - \mathbb{E}[I_k]) \tag{16} \]

so after conditioning on \( Y_k \), we have a centered Bernoulli(\( p \)) scaled by a quadratic form in \( Y_k \). Thus we can apply Bernoulli concentration via the Hoeffding bound [Vershynin, 2018], since the \( \psi_k \) are bounded i.i.d. conditioning on the \( Y_k \). We have that the size of the bound interval on \( \psi_k \) (conditioning on the \( Y_k \)) is:

\[ Y_k^T B_{ij} Y_k \cdot [(1 - p_{ij}) - (-p_{ij})] = Y_k^T B_{ij} Y_k \]

Thus, applying Hoeffding, we get

\[
P\left( \left| \sum_{k=1}^{N} \psi_k \right| \geq N \cdot s | Y_1, \cdots, Y_N \right) \leq 2 \exp \left( -\frac{2(N \cdot s)^2}{\sum_{k=1}^{N} (Y_k^T B_{ij} Y_k)^2} \right) \tag{17} \]

Now plugging in the expectation, we get

\[
\mathbb{E}_{Y_1, \cdots, Y_N} \left[ P\left( \left| \sum_{k=1}^{N} \hat{\xi}_k - \mathbb{E}_{I_k}[\hat{\xi}_k] \right| \geq s | Y_1, \cdots, Y_N \right) \right] \\
\leq 2 \mathbb{E}_{Y_1, \cdots, Y_N} \left[ \exp \left( -\frac{2(N \cdot s)^2}{\sum_{k=1}^{N} (Y_k^T B_{ij} Y_k)^2} \right) \right] \tag{19} \]
Thus, overall, we have the bound
\[
\mathbb{P} \left( \left| \sum_{k=1}^{N} \xi_k \right| > N \cdot t \right) \\
\leq \mathbb{P} \left( \left| \sum_{k=1}^{N} Y_k^\top B_{ij} Y_k - \mathbb{E}_k [Y_k^\top B_{ij} Y_k] \right| > N \cdot t \right) \\
+ 2 \mathbb{E}_{Y_1, \ldots, Y_N} \left[ \exp \left( - \frac{2(N \cdot t)^2}{\sum_{k=1}^{N} (Y_k^\top B_{ij} Y_k)^2} \right) \right] \tag{20}
\]
where we noted that the worst case for the first term is \( p_{ij} = 1 \) and we defined \( s = t \). We bound the second term in the sum first by replacing \( Y_k \) with \( X_k \) (this yields an upper bound since \((Y_k^\top B_{ij} Y_k)^2 \) can only grow larger since it is always positive and because \( Y_k \) has more magnitude 0 terms). Then, simply note that
\[
(Y_k^\top B_{ij} X_k)^2 \leq \|W_i\|_2^2 \cdot \|W_j\|_2 \cdot \|X_k\|_2^4
\]
and we can replace the second term with the upper bound
\[
2 \mathbb{E}_{X_1, \ldots, X_N} \left[ \exp \left( - \frac{2(N \cdot t)^2}{R^4 \sum_{k=1}^{N} \|X_k\|_2^4} \right) \right]
\]
Now we condition on the event
\[
I_2 := \sum_{k=1}^{N} \|X_k\|_2^2 < 2N \cdot d^2
\]
We can therefore bound
\[
\mathbb{E}_{X_1, \ldots, X_N} \left[ \exp \left( - \frac{2(N \cdot t)^2}{R^4 \sum_{k=1}^{N} \|X_k\|_2^4} \right) \right] \\
\leq \mathbb{E}_{X_1, \ldots, X_N} \left[ \mathbb{E}_{X_1, \ldots, X_N} \left[ \exp \left( - \frac{2 \cdot N^2 \cdot t^2}{R^4 \sum_{k=1}^{N} \|X_k\|_2^4} \right) \mid I_2 \right] \right] \cdot \mathbb{P}(I_2) \\
+ \mathbb{E}_{X_1, \ldots, X_n} [\exp(0)] \cdot \mathbb{P}(-I_2) \\
\leq \exp \left( - \frac{N \cdot t^2}{R^4 \cdot d^2} \right) + \mathbb{P}(\neg I_2) \\
\leq \exp \left( - \frac{N \cdot t^2}{R^4 \cdot d^2} \right) + c_1 \cdot \exp \left( -c_2 \cdot d \cdot \sqrt{\frac{N}{2}} \right) \tag{21}
\]
where in the last step we apply Lemma 8.14 and \( c_1, c_2 > 0 \) are universal constants.

Now we apply dependent Hanson-Wright (Lemma 8.12) to finish the concentration analysis for a single \( W_i, W_j \). We first give the Hanson-Wright (sub-exponential) bound for a single block, and then apply Bernstein’s inequality [Vershynin, 2018] for sums of sub-exponential variables to conclude. First we apply Lemma 8.12 to a single block to prove the random variables are sub-exponential:
\[
\mathbb{P} \left( \left| Y_k^\top B_{ij} Y_k - \mathbb{E}_k [Y_k^\top B_{ij} Y_k] \right| > t \right) \\
\leq 2 \exp \left( - \min \left\{ \frac{t^2}{c_3^3 \cdot \|B_{ij}\|_{\text{nuclear}}^2}, \frac{t}{c_3 \cdot \|B_{ij}\|_{\text{nuclear}}} \right\} \right) \\
\leq 2 \exp \left( - \min \left\{ \frac{t^2}{c_3^3 \cdot R^2}, \frac{t}{c_3 \cdot R^2} \right\} \right) \tag{22}
\]
where \( c_3 \) is a universal constant and where the last line directly follows from the definition of the nuclear and Frobenius norms: namely that \( \|M\|_{\text{nuclear}}^2 \leq \text{rank}(M) \cdot \|M\|_F^2 \) – here we used the fact that \( W_i W_j^\top \)
is rank 1 and \( \|W_iW_j^T\|_F^2 \leq \|W_i\|_2^2\|W_j\|_2^2 \leq R^4 \). Thus the sub-exponential norm for all \( k \in [N] \) terms is \( \|Y_k^T(B_{ij} - E[Y_k^T B_{ij} Y_k])\|_{\psi_1} \leq c_3 \cdot R^2 \).

Now we apply standard Bernstein concentration for sums of sub-exponential variables (Theorem 2.8.1 in Vershynin [2018]):

\[
\mathbb{P}\left( \left| \sum_{k=1}^{N} Y_k^T B_{ij} Y_k - E[Y_k^T B_{ij} Y_k] \right| > N \cdot t \right) \\
\leq 2 \exp \left( -c_6 \cdot \min \left\{ \frac{N^2 \cdot t^2}{N \cdot c_3^2 \cdot R^4}, \frac{N \cdot t^2}{c_3 \cdot R^2} \right\} \right) \\
\leq 2 \exp \left( -c_6 \cdot N \cdot \min \left\{ \frac{t^2}{c_3 \cdot R^4}, \frac{t}{c_3 \cdot R^2} \right\} \right) 
\]

Therefore, putting it all together, we get the bound

\[
\mathbb{P}\left( \frac{1}{N} \left| \sum_{k=1}^{N} Z_k(i,j) - E[Z_k(i,j)] \right| > t \right) \\
\leq 2 \exp \left( -c_6 \cdot N \cdot \min \left\{ \frac{t^2}{c_3 \cdot R^4}, \frac{t}{c_3 \cdot R^2} \right\} \right) + 2c_1 \cdot \exp \left( -c_2 \cdot d \cdot \sqrt{N} \right) 
\]

Now we need to uniformly bound over all choices of \( W_i, W_j \) satisfying \( \|W_i\|_2, \|W_j\|_2 \leq R \), so that the above bound holds simultaneously for any pair \( W_i, W_j \). The product of the two \( \ell_2 \) balls \( M := B_{\ell_2}(0,R) \times B_{\ell_2}(0,R) \) forms a compact set, so we will proceed by discretizing and arguing that the discretization provides sufficient approximation. Lemma 8.13 gives the upper bound on the probability for the failure event that the approximation error of the kernel for any choice of \( (W_i, W_j) \in M \) is greater than \( \epsilon \):

\[
\delta = 2 \left( 8R^{2d} \cdot P(\epsilon/2) \right)^{\frac{1}{d+1}} \cdot \left( \frac{8}{N} \cdot \left( \frac{Rd}{\epsilon} \right)^2 \right)^{\frac{d}{d+1}} 
\]

where we previously bounded

\[
P(\epsilon/2) \leq 2 \exp \left( -c_6 \cdot N \cdot \min \left\{ \frac{\epsilon^2}{4c_3^2 \cdot R^4}, \frac{\epsilon}{2c_3 \cdot R^2} \right\} \right) \\
+ 2 \exp \left( -N \cdot \frac{\epsilon^2}{4R^4 \cdot d^2} \right) + 2c_1 \cdot \exp \left( -c_2 \cdot d \cdot \sqrt{N} \right) 
\]

Now we have to choose \( N \) appropriately. Consider each of the three terms of the upper bound on \( P(\epsilon/2) \):

1. For the first term, choosing \( N = O \left( \frac{R^4}{\epsilon^2} \log(6/\delta') \right) \) contributes \( \delta' / 3 \) to \( P(\epsilon/2) \).

2. For the second term, choosing \( N = O \left( \frac{R^4 \cdot \epsilon^2}{d^2} \log(6/\delta') \right) \) also contributes \( \delta' / 3 \) to \( P(\epsilon/2) \).

3. For the third term, choosing \( N = O \left( \frac{1}{\epsilon^2 \cdot d} \log^2(1/\delta) \right) \) also contributes at most \( \delta' / 3 \) to \( P(\epsilon/2) \).

Thus, if we choose

\[
N = O \left( \frac{R^4}{\epsilon^2} \log(6/\delta') + \frac{R^4 \cdot d^2}{\epsilon^2} \log(6/\delta') + \frac{1}{d^2} \log^2(1/\delta') \right) 
\]

34
samples, $P(\epsilon/2) \leq \delta'$. Then we can use the result of Lemma 8.13 to solve for $\delta'$ in terms of the final probability $\delta$:

$$
\delta = 2 \left( (8R)^{2d} \cdot \delta' \right)^{\frac{1}{d+1}} \cdot \left( \frac{8}{N} \cdot \left( \frac{Rd}{\epsilon} \right)^2 \right)^{\frac{1}{d+1}} 
$$

(26)

Note that we can choose $N \geq \frac{R^4 \cdot d^2}{\epsilon^2} \cdot 2048$ (and this is consistent with the previous choice of $N$). This simplifies the equation to

$$
\delta' = \frac{\delta^{d+1} \cdot N^d \cdot \epsilon^2}{210d+1} \cdot R^4 \cdot d^2 \cdot \epsilon^2

\geq \frac{\delta^{d+1} \cdot 2^{d+1}}{1}
$$

(27)

and thus

$$
\log(1/\delta') \leq (d + 1) \log(1/\delta)
$$

Plugging this estimate back in to our sample complexity bound gives us the bound in terms of the overall probability of failure $\delta$:

$$
N = \mathcal{O} \left( \frac{R^4 \cdot d}{\epsilon^2} \log(1/\delta) + \frac{R^4 \cdot d^3}{\epsilon^2} \log(1/\delta) + \log^2(1/\delta) \right)
$$

However, we could have also set $N \geq \frac{R^4 \cdot d^2}{\epsilon^2} \cdot 2048 \cdot \frac{1}{\delta}$ – giving up a logarithmic dependence in $1/\delta$. In this case, we would get $\delta' \geq \delta$, and thus

$$
N = \mathcal{O} \left( \frac{R^4 \cdot d^2}{\epsilon^2} \right)
$$

This bound achieves better dependence on dimension if $\delta > 1/d$. Thus, we can overall summarize the sample complexity as

$$
N = \mathcal{O} \left( \frac{R^4 \cdot d^2}{\epsilon^2} \cdot \min (d \log^2 \left( \frac{1}{\delta} \right), \frac{1}{\delta}) \right)
$$

Finally, if we choose $N$ at least that large, we have that with probability at least $1 - \delta$, $\|K_{ReLU} - \hat{K}_{ReLU}\|_\infty \leq \epsilon$. We want to convert this into a Frobenius norm bound. Directly bounding, we get

$$
\|K_{ReLU} - \hat{K}_{ReLU}\|_F^2 \leq m^2 \cdot \epsilon^2
$$

Therefore, choosing $\epsilon = \epsilon'/m$ and plugging it in to get the bound in terms of $\epsilon'$ gives the desired result.

Lemma 8.13. Define

$$
P(\epsilon) := \mathbb{P} \left( \frac{1}{N} \sum_{k=1}^{N} Z_k(i,j) - \mathbb{E}[Z_k(i,j)] \right) > \epsilon \right)
$$

where $Z_k(i,j) := \sigma(x_k^T W_i) \sigma(x_k^T W_j)$ is defined for $\sigma$ the ReLU activation, $x_k \sim \mathcal{N}(0, I_{d \times d})$, $\|W_i\|_2, \|W_j\|_2 \leq R$, and where $N$ is the number of samples. Then consider the compact set $M := \mathcal{B}_{\epsilon}(0, R) \times \mathcal{B}_{\epsilon}(0, R)$. The probability that the worst error estimate over points $(W_i, W_j) \in M$ of the kernel value $k_{ReLU}(W_i, W_j)$ is worse than $\epsilon$ is at most

$$
\delta := 2 \left( (8R)^{2d} \cdot P(\epsilon)/2 \right)^{\frac{1}{d+1}} \cdot \left( \frac{8}{N} \cdot \left( \frac{Rd}{\epsilon} \right)^2 \right)^{\frac{1}{d+1}}
$$

Proof. To prove this theorem, we adapt the argument of Rahimi and Recht [2008]. We define $k(W_i, W_j) := \mathbb{E}_x[\sigma(x^T W_i) \sigma(x^T W_j)]$, $s(W_i, W_j) := \frac{1}{N} \sum_{k=1}^{N} \sigma(x_k^T W_i) \sigma(x_k^T W_j)$, and $f(W_i, W_j) = s(W_i, W_j) - k(W_i, W_j)$. We want to uniformly bound $f(W_i, W_j) = f \left( \begin{bmatrix} W_i \\ W_j \end{bmatrix} \right)$ over $\begin{bmatrix} W_i \\ W_j \end{bmatrix} \in M$. We will refer to $W = \begin{bmatrix} W_i \\ W_j \end{bmatrix}$. Our strategy will be to first take a $\frac{\epsilon}{2}$-net of $M$ (which is possible since $M$ is a compact set), then bound the
approximation error of a point not in the net to the closest point in the net. To carry out this strategy, we first bound the Lipschitz constant of $f$ (note that $f$ is Lipschitz in $W$, while it is not Lipschitz in $x_k$). First note that the Lipschitz constant is defined as follows:

$$L_f = \max_{W \in M} \|\nabla_W f(W^*)\|_2$$

By linearity of expectation we have $\nabla_W k(W) = E[\nabla_W s(W)]$, and therefore we can use the definition of variance to bound

$$E[L_f^2] = E[\|\nabla_W f(W^*)\|_2^2]$$

$$= E[\|\nabla_W s(W^*) - \nabla_W f(W^*)\|_2^2]$$

$$\leq E[\|\nabla_W s(W^*)\|_2^2]$$

$$\leq 2E[\|\nabla_W s(W^*)\|_2^2]$$

$$= 2E_x \left( \left\| \frac{1}{N} \sum_{k=1}^N x_k 1 \left( W_i^T x_k > 0 \right) \sigma \left( W_j^T x_k \right) \right\|_2^2 \right)$$

$$\leq \frac{2}{N^2} \sum_{k=1}^N E_x \left( \left\| x \cdot 1 \left( W_i^T x > 0 \right) \sigma \left( W_j^T x \right) \right\|_2^2 \right)$$

$$\leq \frac{2}{N} \left[ x W_j^T x \right]$$

$$\leq \frac{2}{N} \cdot \| W_j^* \|_2^2 \cdot E_x[\| x \|_2^2]$$

$$\leq \frac{2}{N} \cdot \| W_j^* \|_2^2 \cdot \frac{R^2}{d}$$

where we previously bounded the fourth power of a standard Gaussian $\ell_2$ norm in Lemma 8.14. For convenience, we define

$$\sigma^2 := \frac{2}{N} \cdot \frac{R^2}{d}$$

Then by Markov’s inequality, we have

$$P(L_f^2 > t) \leq \frac{E[L_f^2]}{t} \leq \frac{\sigma^2}{t}$$

and thus

$$P(L_f > t) \leq \left( \frac{\sigma}{t} \right)^2$$

We choose $t = \frac{\epsilon}{2r}$ in order to ensure only an extra $\frac{\epsilon}{2}$ in approximation error for any point not in the net (here, $r$ is the radius of balls we will choose to determine the size of a cover for the $\frac{\epsilon}{2}$-net). Thus we get

$$P\left(L_f > \frac{\epsilon}{2r}\right) \leq \left( \frac{2r \cdot \sigma}{\epsilon} \right)^2$$

Then we can apply the union bound over the net of size $T$ to get a uniform bound over the elements of the net:

$$P\left( \bigcup_{S=1}^T \{ f(W_s) \geq \epsilon/2 \} \right) \leq T \cdot P\left( \epsilon \right)$$

We combine this estimate using another union bound with the bad event that the error for points off the
\( \frac{\epsilon}{2} \) -net is worse than \( \frac{\epsilon}{2} \) to bound the probability that the error of the worst \( W \in M \) is more than \( \epsilon \):

\[
P \left( \sup_{W \in M} |f(W)| \geq \epsilon \right) \leq T \cdot P \left( \frac{\epsilon}{2} \right) + \left( \frac{2r \cdot \sigma}{\epsilon} \right)^2 \tag{29}
\]

where we used standard upper bounds for the number of \( r \)-balls which can fit in a compact space with a given diameter in dimension 2 (recall \( W \in \mathbb{R}^{2d} \) since it is a concatenation of vectors). Here the bound is of the form

\[
\alpha \cdot r^{-2d} + \beta \cdot r^2
\]

where \( \alpha := (8R)^{2d} \cdot P \left( \frac{\epsilon}{2} \right) \) and \( \beta := \frac{8}{N} \left( \frac{Rd}{r} \right)^2 \). Here, we have let \( r \) be a free parameter. First applying the bound

\[
\text{diam} (M) = \sup \{\|x - y\|_2 : x, y \in M\} \leq 2R + 2R = 4R
\]

and then optimizing over \( r \) yields

\[
r^* = \left( \frac{\alpha}{\beta} \right)^{\frac{1}{2d + 2}}
\]

Plugging this optimal choice of \( r \) back in yields the bound

\[
2\alpha \beta^{\frac{1}{2d + 2}}
\]

Plugging in the values of \( \alpha, \beta \) yields the desired result. \( \Box \)

**Lemma 8.14.** Assume \( X_1, \cdots, X_N \in \mathbb{R}^d \) are i.i.d. standard Gaussians drawn from \( N(0, I_{d \times d}) \). Then

\[
P \left( \frac{1}{N} \sum_{k=1}^{N} \|X_k\|_4^4 > 2d^2 \right) \leq c_1 \cdot \exp \left( -c_2 \cdot d \cdot \sqrt{N} \right)
\]

where \( c_1, c_2 > 0 \) are universal constants.

**Proof.** First we need to show that

\[
P \left( \|X_k\|_2^4 - \mathbb{E} \|X_k\|_2^4 > t \right) \leq c_1 \cdot \exp \left( -c_2 \cdot \sqrt{t} \right)
\]

Then, by Theorem 3 of Talagrand [1989] (in particular see the second equation in the proof of Theorem 3 starting on pg. 1555), we get the concentration bound

\[
P \left( \sum_{k=1}^{N} \|X_k\|_2^4 - \mathbb{E} \|X_k\|_2^4 > N \cdot t \right) \leq c_1 \cdot \exp \left( -c_2 \cdot \sqrt{N \cdot t} \right) \tag{30}
\]

which completes the desired result.

Thus, we proceed by showing the first statement for the \( X_k \). First we bound the concentration probability of the squared norm of a standard \( d \)-dimensional Gaussian (see Theorem 3.1.1 in Vershynin [2018]):

\[
P \left( \|x\|_2^2 \geq t \cdot d \right) \leq 2 \exp \left( -c_5 \cdot d \cdot \min(t, t^2) \right)
\]

Then we have

\[
P \left( \|x\|_2^2 > (1 + t) \cdot d \right) \leq 2 \exp \left( -c_5 \cdot d \cdot \min(t, t^2) \right)
\]

\[
P \left( \|x\|_2^4 > (1 + t^2) \cdot d^2 \right) \leq 2 \exp \left( -c_5 \cdot d \cdot \min(t, t^2) \right)
\]

\[
P \left( \|x\|_2^4 - d^2 > (2t + t^2) \cdot d^2 \right) \leq 2 \exp \left( -c_5 \cdot d \cdot \min(t, t^2) \right) \tag{31}
\]

37
Then note that

$$
\begin{align*}
\mathbb{P} \left( \|x\|_2^4 - d^2 > (2t + t^2) \cdot d^2 \right) \\
&\geq \mathbb{P} \left( \|x\|_2^4 - d^2 > 3 \max (t, t^2) \cdot d^2 \right) \\
&\geq \mathbb{P} \left( \|x\|_2^4 - E[\|x\|_2^4] > 3 \max (t, t^2) \cdot d^2 \right)
\end{align*}
$$

(32)

since by Jensen’s inequality, the convexity of the square function, and the fact that $E[\|x\|_2^4] = d$, we have

$$E[\|x\|_2^4] \geq E[\|x\|_2^2]^2 = d^2$$

Now we have two cases: $t < 1$ and $t \geq 1$. In the first case, $t^2 < t$ and we can plug in our estimates to get the bound

$$\mathbb{P} \left( \|x\|_2^4 - E[\|x\|_2^4] > 3t \cdot d^2 \right) \leq 2 \exp \left( -c_5 \cdot d \cdot t^2 \right)$$

In the second case, $t^2 \geq t$ and we plug in our bounds to get

$$\mathbb{P} \left( \|x\|_2^4 - E[\|x\|_2^4] > 3t^2 \cdot d^2 \right) \leq 2 \exp \left( -c_5 \cdot d \cdot t \right)$$

or after variable replacement $s = 3t^2 \cdot d^2$

$$\mathbb{P} \left( \|x\|_2^4 - E[\|x\|_2^4] > s \right) \leq 2 \exp \left( - \left( c_5 / \sqrt{3} \right) \cdot \sqrt{s} \right)$$

Thus for any $t > 0$ we have proven the bound

$$
\begin{align*}
\mathbb{P} \left( \|x\|_2^4 - E[\|x\|_2^4] > 3t \cdot d^2 \right) \\
&\leq 2 \exp \left( -c_5 \cdot d \cdot \min (t^2, \sqrt{t}) \right)
\end{align*}
$$

(33)

and thus Theorem 3 of Talagrand [1989] applies. Then, in the context of the bound

$$\mathbb{P} \left( \|X_k\|_2^4 - E[\|X_k\|_2^4] > t \right) \leq c_1 \cdot \exp \left( -c_2 \cdot \sqrt{t} \right),$$

We choose $t = 2d^2$ for the statement we want, so we end up using the second case version of the bound. □

Remark 8.15 (Normalized Gaussian Setting). One relevant “average-case” setting which is common in practice chooses the $m$ entries of $W$ from a normalized Gaussian $\mathcal{N}(0, \frac{1}{d} I_{d \times d})$ (e.g. He and Glorot initialization [Glorot and Bengio, 2010, He et al., 2015]). In this case, we have $R = \max_{i \in [m]} \|W_i\|_2 = O(1)$ with high probability via standard argument (see Theorem 3.1.1 in Vershynin [2018]) as long as $d \gg \log(m)$ (for union bound purposes), and we can also bound the spectral norm using Marčenko-Pastur [Marčenko and Pastur, 1967] (or more crudely, with another Frobenius norm bound). Marčenko-Pastur tells us that we can upper bound $\|W\|_2 \leq \left( 1 + \sqrt{d/m} \right)^2$, essentially by a constant. We can also bound the eigenvalue gaps using Theorem 2.6 of Nguyen et al. [2017]: with probability at least $1 - O(m^{-A})$ for $A > 0$, the $r^{th}$ eigenvalue gap of kernel matrix $K_\sigma$ satisfies $\lambda_r - \lambda_{r-1} \geq m^{-B}$. For our case, we can choose to $A$ to be some positive constant and then $B$ can be chosen to be a linear function of $A$. If we factor in this event to the bound (and union bound over this possibility as well), we therefore only experience some additional polynomial blow-up with regards to the dependence on $m$ in Theorem 2.8.

Remark 8.16 (Improvements in Polynomial Degrees). It is likely that one can reduce the polynomial powers of the $R$, $m$, and $\epsilon$ terms in our bounds in Theorem 2.8 by more carefully bounding in Lemmas 8.19, 8.20, and 8.21. Additionally, we can probably remove many factors of $R$ and $m$ by replacing Frobenius norm bounds with spectral norm bounds and working in a setting where the spectral norm is bounded by a constant.

Remark 8.17 (Why Learn the Kernel Matrix Separately from $W$?). Another approach to running the algorithm is to use the estimated $\tilde{W}$ (from gradient descent) in order to calculate an approximate $\tilde{K}$ – in this way, we could potentially avoid the analysis of the concentration of the kernel matrix. However, this approach does not work (at least directly) – if we try to analyze the resultant kernel matrix values, we can only get multiplicative approximations of the error rather than additive (if we try to convert into additive errors, the bounds blow up). This difficulty arises due to having to estimate the cosine of the angles between columns of $W$ – dealing with estimating the normalization is not easy. Since we are trying to get additive approximations of the error, this approach is not sufficient.
Since Algorithm 2 outputs $\hat{W}\hat{V}\hat{V}^\top$, we only care about the terms $\hat{W}$ and $\hat{V}\hat{V}^\top$. We already have a perturbation bound on $\hat{W}$ for free. Thus it remains to get a perturbation bound on $VV^\top$. To get this result, we restate a useful variant of the classic Davis-Kahan $\sin(\Theta)$ theorem:

**Lemma 8.18** (Davis-Kahan $\sin(\Theta)$ Theorem as stated in Yu et al. [2015]). Let $K, \hat{K} \in \mathbb{R}^{m \times m}$ be a real-valued, symmetric with the eigenvalues of $K$ given by $\lambda_1 \geq \cdots \geq \lambda_m$. Since $K$ is real symmetric we can write $K = V\Sigma V^\top$. Suppose we take the top $r < m$ eigenvectors $V \in \mathbb{R}^{m \times r}$, which form an orthonormal eigenbasis. Then

$$\left\| VV^\top - \hat{V}\hat{V}^\top \right\|_F \leq \frac{2\sqrt{2}\|K - \hat{K}\|_F}{\lambda_r - \lambda_{r-1}}$$

The key lemma tying everything together bounds the suboptimality with respect to opt in generalization error of the output of Algorithm 2.

**Lemma 8.19** (Perturbation Bound I). Suppose we learn $\hat{W} = W + E$ and $\hat{K}_{\text{ReLU}} = K_{\text{ReLU}} + H$ from samples, and $VV^\top = \hat{V}\hat{V}^\top + F$ where $V$ and $\hat{V}$ are the top-$r < m$ eigenvectors of $K_{\text{ReLU}}$ and $\hat{K}_{\text{ReLU}}$ respectively, and $\lambda_r, \lambda_{r-1}$ are the $i$th and $(r-1)$st eigenvalues of $K_{\text{ReLU}}$. Then, we bound the perturbation error

$$\mathcal{R}(\hat{Y}) - \mathcal{R}(Y^*) \leq 8R^2 \cdot m \cdot \sqrt{\|H\|_F \|W\|_2 + \|E\|_F}$$

assuming that we will choose the number of samples to produce $\hat{Y}$ so that $\|F_t\|_F < 1$.

**Proof.** First note that since $\|F\|_2 < 1$ we have

$$\mathcal{R}(\hat{Y}) - \mathcal{R}(Y^*) \leq 4R^2 \cdot \sum_{i=1}^m \sqrt{\|F_i\|_2 \|W\|_2 + \|E\|_F}$$

using Lemma 8.20 and Lemma 8.21 and assuming that we will choose the number of samples so that $\|F_t\|_F < 1$. Now we want to get the dependence on properties of $H$ rather than $F$, via Davis-Kahan. By Davis-Kahan we have

$$\|F\|_F \leq \frac{2\sqrt{2}\|H\|_F}{\lambda_r - \lambda_{r-1}}$$

Then we can naively bound $\|F_i\|_2 \leq \|F\|_F$, and so we get

$$\mathcal{R}(\hat{Y}) - \mathcal{R}(Y^*) \leq 8R^2 \cdot m \cdot \sqrt{\|F\|_F \|W\|_2 + \|E\|_F}$$

$$\leq 8R^2 \cdot m \cdot \sqrt{H \|W\|_2 + \|E\|_F}$$

First we relate the generalization gap to the cosine of the angles between the optimum $Y^*$ and the sample optimum $\hat{Y}$:

**Lemma 8.20** (Perturbation Bound II). Let $R = \max_{i \in [m]} \|W_i\|_2$. For the objective defined in Problem 2.1, we have that for $\hat{Y}$ which minimize the population version of the objective with $\hat{W}, \hat{K}$ as the ground truth (e.g. the output of Algorithm 1 on the sample versions of $W$ and $K$) that

$$\mathcal{R}(\hat{Y}) - \mathcal{R}(Y^*) \leq \sqrt{2} \cdot R^2 \cdot \sum_{i=1}^m \sqrt{1 - \cos\left(\Theta(Y^*_i, \hat{Y}_i)\right)}$$
Proof. Using the representation from Theorem 4.2, we write
\[
\mathcal{R}(\hat{Y}) - \mathcal{R}(Y^*) = \frac{1}{2} \sum_{i=1}^{m} (\hat{h}(\rho_i^*) - h(\hat{\rho}_i)) \|W_i\|_2^2 \\
\leq \frac{R^2}{2} \sum_{i=1}^{m} (\sqrt{h}(\rho_i^*) + \sqrt{\hat{h}}(\rho_i)) \cdot (\sqrt{h}(\rho_i^*) - \sqrt{\hat{h}}(\rho_i)) \\
\leq R^2 \sum_{i=1}^{m} (\sqrt{\hat{h}}(\rho_i^*) - \sqrt{\hat{h}}(\rho_i)) \\
\leq R^2 \sum_{i=1}^{m} \left( \frac{1}{2} (\rho_i^* - \hat{\rho}_i) + \frac{1}{\pi} \sum_{t=1}^{\infty} c_t^2 (\rho_i^{2t} - \hat{\rho}_i^{2t}) \right) \\
\leq R^2 \sum_{i=1}^{m} \left( \frac{1}{2} + \frac{1}{\pi} \right) \left( \rho_i^* - \hat{\rho}_i \right) \\
\leq R^2 \|\rho^* - \hat{\rho}\|_1
\]
since $\sqrt{\hat{h}} \in [1/\pi, 1]$ for $\rho \in [0, 1]$. Now we write
\[
\theta_i^* := \arccos \left( \frac{Y_i^{*\top} W_i}{\|Y_i^*\|_2 \|W_i\|_2} \right) \\
\hat{\theta}_i := \arccos \left( \frac{\hat{Y}_i^{\top} W_i}{\|\hat{Y}_i\|_2 \|W_i\|_2} \right)
\]
and note that we wish to bound the terms $\rho_i^* - \hat{\rho}_i = \cos(\theta_i^*) - \cos(\hat{\theta}_i)$. We have
\[
\cos(\theta_i^*) - \cos(\hat{\theta}_i) = \left( \frac{Y_i^* - \hat{Y}_i}{\|Y_i^*\|_2 \|\hat{Y}_i\|_2} \right)^\top \left( \frac{W_i}{\|W_i\|_2} \right) \\
\leq \left\| \frac{Y_i^* - \hat{Y}_i}{\|Y_i^*\|_2 \|\hat{Y}_i\|_2} \right\|_2 \\
\leq \sqrt{2 \left( 1 - \cos \left( \Theta(Y_i^*, \hat{Y}_i) \right) \right)}
\]
where we applied Cauchy-Schwarz and the definition of cosine. Plugging in this upper bound yields the theorem. \qed

Lemma 8.21 (Perturbation Bound III). Suppose we learn $\hat{W} = W + E$ and $\hat{K}_{\text{ReLU}} = K_{\text{ReLU}} + H$ from samples, and $VV^\top = \hat{V} \hat{V}^\top + F$ where $V$ and $\hat{V}$ are the eigenvectors of $K_{\text{ReLU}}$ and $\hat{K}_{\text{ReLU}}$ respectively. Then, we bound the perturbation error
\[
1 - \cos \left( \Theta(Y_i^*, \hat{Y}_i) \right) \leq (1 + \pi + \|F_i\|_2) (\|F_i\|_2 \|W\|_2 + \|E\|_F)
\]
in terms of properties of $E, F, W, \text{ and } K_{\text{ReLU}}$, where $\hat{Y}$ is the optimum reconstruction for $\hat{W}, \hat{K}_{\text{ReLU}}$, noting that as $\|E\|_F, \|F_i\|_2 \to 0$, the upper bound tends to 0.

Proof. Define $K_{\text{ReLU}} = V \Sigma V^\top$ and $\hat{K}_{\text{ReLU}} = \hat{V} \hat{\Sigma} \hat{V}^\top$ since the kernel matrix is real symmetric. Let $VV^\top = VV^\top + F$. We will use $V_i$ to denote the $i^{\text{th}}$ column of $V^\top$. First note we have by Algorithm 1
\[
Y^* = WWV^\top \\
\hat{Y} = W\hat{V} \hat{V}^\top
\]
Then we need to lower bound \( \cos \left( \Theta(Y_i^*, \hat{Y}_i) \right) \).

\[
\cos \left( \Theta(Y_i^*, \hat{Y}_i) \right) = \frac{(WVV_i) \mathbf{V} \mathbf{V}_i^T (W + E) \hat{V}_i}{\|WVV_i\|_2 \cdot \|(W + E) \hat{V}_i\|_2}
\]

\[
= \frac{\langle W(VV_i + F_i), WVV_i \rangle}{\|WVV_i\|_2 \cdot \|(W + E)(VV_i + F_i)\|_2}
\]

where we applied Cauchy-Schwarz and since we know that \( \|\hat{Y}_i\|_2 = \sqrt{\rho_i} \geq 1/\pi \) from Theorem 4.2. Here we define

\[
s_i = \frac{\|WVV_i\|_2}{\|WVV_i\|_2 + \|W\|_2 \|F_i\|_2 + \|E\|_F + \|E\|_F \|F_i\|_2}
\]

Note \( s_i \in [0, 1] \). Now we handle the second term:

\[
\frac{\langle E(VV_i + F_i), WVV_i \rangle}{\|WVV_i\|_2 \cdot \|(W + E)(VV_i + F_i)\|_2}
\]

\[
\geq -\pi \|E\|_F \|\hat{V}_i\|_2
\]

Putting it all together, we get

\[
1 - \cos \left( \Theta(Y_i^*, \hat{Y}_i) \right) \leq 1 - s_i + \pi (\|F_i\|_2 \|W\|_2 + \|E\|_F)
\]

Finally, we can bound \( 1 - s_i \):

\[
1 - s_i = \frac{\|W\|_2 \|F_i\|_2 + \|E\|_F + \|E\|_F \|F_i\|_2}{\|WVV_i\|_2 + \|W\|_2 \|F_i\|_2 + \|E\|_F + \|E\|_F \|F_i\|_2}
\]

\[
\leq \frac{\|W\|_2 \|F_i\|_2 + \|E\|_F + \|E\|_F \|F_i\|_2}{\|W\|_2 \|F_i\|_2 + \|E\|_F + \|E\|_F \|F_i\|_2}
\]

\[
\leq \frac{\|W\|_2 \|F_i\|_2 + \|E\|_F + \|E\|_F \|F_i\|_2}{\|W\|_2 \|F_i\|_2 + \|E\|_F + \|E\|_F \|F_i\|_2}
\]

\[
\frac{\|W\|_2 \|F_i\|_2 + \|E\|_F + \|E\|_F \|F_i\|_2}{\|W\|_2 \|F_i\|_2 + \|E\|_F + \|E\|_F \|F_i\|_2}
\]

\[\square\]

### 8.4 Proofs for Section 4

We recall the useful definition:

**Definition 4.1** (ReLU Kernel: 1st-Order Arc-Cosine Kernel). For the ReLU activation, the associated non-linearity kernel (Definition 2.5) is known as the first-order arc-cosine kernel [Cho and Saul, 2009], defined by \( k(x, y) := \|x\|_2 \|y\|_2 \cdot \sqrt{h}(\rho_{xy}) \), where \( \rho_{xy} := \frac{x^T y}{\|x\|_2 \|y\|_2} \) and \( \sqrt{h}(\rho_{xy}) = \sqrt{1 - \rho_{xy}^2 + (\pi - \cos^{-1}(\rho_{xy})) \rho_{xy}} / \pi \).

We provide an accompanying Hermite expansion of \( \sqrt{h} \) in Lemma 8.6.
8.4.1 Alternate Characterization of ReLU SVD

In the following theorem, we take advantage of specific properties of the ReLU activation and its associated kernel to come to another understanding of the objective in Problem 2.1.

**Theorem 4.2 (ReLU SVD).** Consider the goal of finding the optimal rank-$r$ solution to the objective $\mathcal{R}(Y)$ in Problem 2.1 with known $W \in \mathbb{R}^{d \times m}$. Suppose we solve the following problem:

$$
\Lambda^* = \arg \max_{\Lambda \in (0,1)^d; \|\Lambda\|_1 = r} \sum_{i=1}^m \|W_i\|_2^2 \cdot h \left( \frac{\|\Sigma \text{ diag}(\Lambda) V_i\|_2}{\|\Sigma V_i\|_2} \right)
$$

where $W = U \Sigma V^T$ with $U \in \mathbb{R}^{d \times d}$, $\Sigma \in \mathbb{R}^{d \times d}$ is diagonal, and $V \in \mathbb{R}^{m \times d}$, with $U^T U = I_{d \times d}$, $V^T V = I_{d \times d}$ and $V_i \in \mathbb{R}^d$ is the $i$th column of $V^T$, and where $h$ is defined in Definition 2. Then, the optimal rank-$r$ matrix $Y^* \in \mathbb{R}^{d \times m}$ minimizing the initial objective Eq. (1) is given by $Y^* = U \text{ gnorm}(\text{ diag}(\Lambda^*) \Sigma V^T)$, where $\text{gnorm}(A)_i := A_i \cdot \sqrt{\|A_i\|_2}$ for the $i$th column of $A$.

**Proof.** First, we expand

$$
E_{x \sim N(0, I)} \left[ \|\sigma(x^T Y) - \sigma(x^T W)\|_2^2 \right] = E_{x \sim N(0, I)} \left[ \|\sigma(x^T Y)\|_2^2 \right] + E_{x \sim N(0, I)} \left[ \|\sigma(x^T W)\|_2^2 \right] - 2E_{x \sim N(0, I)} \left[ \langle \sigma(x^T Y), \sigma(x^T W) \rangle \right]
$$

$$
= C + \frac{1}{2} \|Y\|_F^2 - 2E_{x \sim N(0, I)} \left[ \langle \sigma(x^T Y), \sigma(x^T W) \rangle \right] = C + \frac{1}{2} \|Y\|_F^2 - \sum_{i=1}^m \|W_i\|_2 \cdot Y_i : V_i = \sqrt{h} \left( \frac{Y_i^T W_i}{\|W_i\|_2 \|Y_i\|_2} \right)
$$

where $C = \frac{1}{2} \|W\|_F^2$ is a constant independent of choice of $Y$, and letting $\rho_i = \frac{Y_i^T W_i}{\|Y_i\|_2 \|W_i\|_2}$ and $\beta_i = \|Y_i\|_2$, where $Y_i$ and $W_i$ are column $i$ of $Y, W$ respectively. In the above display, we used Lemma 8.23 and Lemma 8.6.

Now, we can re-write the minimization problem as a maximization problem:

$$
\max_{\rho, \beta: Y \in \mathbb{R}^{d \times m} \text{ is rank } r} \sum_{i=1}^m \left[ \|W_i\|_2 \sqrt{h}(\rho_i) \right] \beta_i - \frac{1}{2} \beta_i^2
$$

Note we can write this as an optimization problem over just $\rho \in \mathbb{R}^m$, since the choice of norm $\beta_i = \|Y_i\|_2$ is independent of the value of $\rho_i$. Since the objective as a function of $\beta_i$ is separable and concave in each term of the sum, we can easily solve the maximization problem by setting the derivative to 0:

$$
\beta_i^* = \|W_i\|_2 \sqrt{h}(\rho_i)
$$

Plugging in this optimal choice of $\beta_i$ for any choice of $\rho$ (and remembering that we must correctly re-normalize later), we get the new objective:

$$
\max_{\rho: Y \in \mathbb{R}^{d \times m} \text{ is rank } r} \frac{1}{2} \sum_{i=1}^m \|W_i\|_2^2 \cdot h(\rho_i)
$$

(45)

Now, all that remains is to parameterize low-rank $Y$ as a function of $\rho$. Let us write $W = U \Sigma V^T$ and $Y = D \Lambda B^T$ via singular value decomposition, understanding that $\Sigma \in \mathbb{R}^{d \times d}$ is a full-rank diagonal matrix and $\Lambda \in \mathbb{R}^{d \times d}$ is a rank-$r$ diagonal matrix (with only $r$ non-zero terms on the diagonal), and...
$U^TU = I, V^TV = I, D^TD = I, B^TB = I$ are orthonormal matrices. Now we can see how to choose $D, B,$ and $\Lambda$ to maximize the objective. We have

$$\rho_i = \frac{B_i^T \Lambda D^T U \Sigma V_i}{\|B_i^T \Lambda\|_2 \|W_i\|_2}$$

where $B_i \in \mathbb{R}^d$ is the $i^{th}$ column of $B^T$ and $V_i \in \mathbb{R}^d$ is the $i^{th}$ column of $V^T$, noting that $\|B_i^T \Lambda D^T\|_2 = \|B_i^T \Lambda\|_2$ since $D$ is orthonormal.

Since $h$ is convex and monotone-increasing, we want to maximize the value of $\rho_i$ subject to the low-rank constraint whenever it is the case that the parameter choices made for $\rho_i$ do not affect the other $\rho_i$ (since overall we want to maximize $\sum_{i=1}^n \|W_i\|^2 \cdot h(\rho_i)$). We proceed by identifying the optimal choice of parameters for each of $B, D,$ and $\Lambda$. For any choice of $B, \Lambda$, the optimal choice of $D$ is $U$ since $D$ is constrained to be orthonormal. Now fix any choice of diagonal rank-$r$ $\Lambda^*$. We wish to maximize the following over $B_i$:

$$\max_{\|\Lambda^*B_i\|_2 = 1} \frac{B_i^T \Lambda^* \Sigma V_i}{\|B_i^T \Lambda^*\|_2 \|W_i\|_2}$$

Choosing $w = \Lambda^* B_i$ (and now working with the versions of $B_i, V_i \in \mathbb{R}^r$, where the $r$ dimensions correspond to the dimensions which are non-zero on the diagonal for $\Lambda^* \in \mathbb{R}^{d\times d}$), we get the problem

$$\max_{\|w\|_2 = 1} \frac{w^T \Sigma V_i}{\|w\|_2 \cdot \|W_i\|_2}$$

for which the solution is $w = \Sigma V_i$ (by Cauchy-Schwarz). Then, we get

$$B_i = \Lambda^{*^{-1}} \Sigma V_i$$

and plugging it in, we get that with this choice of $B_i$, the correlations are

$$\rho_i = \frac{B_i^T \Lambda^* \Sigma V_i}{\|B_i^T \Lambda^*\|_2 \|W_i\|_2} = \frac{V_i^T \Sigma_{r\times r}^2 V_i}{\|\Sigma_{r\times r} V_i\|_2 \|W_i\|_2}$$

$$= \frac{\|\Sigma_{r\times r} V_i\|_2}{\|W_i\|_2} = \frac{\|\Sigma_{d\times d} \Lambda^* V_i\|_2}{\|\Sigma_{d\times d} V_i\|_2}$$  \hspace{1cm} (46)

since we note $\|W_i\|_2 = \|U \Sigma V_i\|_2 = \|\Sigma V_i\|_2$ and where we now restrict $\Lambda^* \in \mathbb{R}^{d\times d}$ to be a diagonal matrix with $r$ ones on the diagonal and the rest of the entries zero. At the end we also interchanged between $V_i \in \mathbb{R}^r$ (with $r$ coordinates chosen by $\Lambda^*$) and $V_i \in \mathbb{R}^d$.

\[\square\]

**Lemma 8.22** (ReLU Decomposition). Let ReLU be defined by $\sigma(x) = \max(0, x)$.

$$\sigma(x) = \frac{x + |x|}{2}$$ \hspace{1cm} (47)

**Proof.** Observe that if $x \leq 0$, $\sigma(x) = 0$. Otherwise, it equals $x$. \[\square\]

**Lemma 8.23** (ReLU Norm).

$$\mathbb{E}_{x \sim \mathcal{N}(0, I)} \left[ \|\sigma(x^T Y)\|_2^2 \right] = \frac{1}{2} \|Y\|_F^2$$ \hspace{1cm} (48)

\[This\ minor\ step\ is\ important\ since\ it\ defines\ the\ inverse\ $\Lambda^{*\^{-1}} \in \mathbb{R}^{r\times r}$. We switch between the $r$-dimensional version and the $d$-dimensional version freely, where the version being used depends on context.\]
Proof. We have

\[
\|\sigma(Y^\top x)\|_2^2 = \sum_{i=1}^m \sigma(Y_i^\top x)^2
\]
\[
= \frac{1}{4} \sum_{i=1}^m (Y_i^\top x + |Y_i^\top x|)^2
\]
\[
= \frac{1}{4} \sum_{i=1}^m (2(Y_i^\top x)^2 + 2\langle Y_i^\top x, Y_i^\top x \rangle)
\]
\[
= \frac{1}{2} \|Y^\top x\|_2^2 + \frac{1}{2} \sum_{i=1}^m (Y_i^\top x)^2 \text{sgn}(Y_i^\top x)
\]

Now we take expectation over \(x \sim \mathcal{N}(0, I)\).

\[
E_{x \sim \mathcal{N}(0, I)} \left[ \|Y^\top x\|_2^2 \right] = E_{x \sim \mathcal{N}(0, I)} \left[ \text{Tr} \left( x^\top Y Y^\top x \right) \right]
\]
\[
= \text{Tr} \left( Y^\top E_{x \sim \mathcal{N}(0, I)} \left[ xx^\top \right] Y \right)
\]
\[
= \text{Tr} \left( Y^\top Y \right)
\]
\[
= \|Y\|_F^2
\]

(49)

For the second term, apply linearity of expectation and condition on the events that \(Y_i^\top x > 0\) and \(Y_i^\top x < 0\). Since \(Y_i\) is fixed and \(x\) is an isotropic Gaussian (which is spherically symmetric), the probability that \(Y_i^\top x > 0\) is equal to the probability that \(Y_i^\top x < 0\). Thus, letting \(q_i = P(Y_i^\top x > 0)\),

\[
q_i \sum_{i=1}^m E_{x \sim \mathcal{N}(0, I)} \left[ (Y_i^\top x)^2 \text{sgn}(Y_i^\top x) \right] I(Y_i^\top x > 0) + (1 - q_i) \sum_{i=1}^m E_{x \sim \mathcal{N}(0, I)} \left[ (Y_i^\top x)^2 \text{sgn}(Y_i^\top x) \right] I(Y_i^\top x < 0)
\]

(50)

and we get the desired result. \(\square\)

Lemma 8.24 (Reduction to 1-Dimensional Correlation). Consider \(W, Y \in \mathbb{R}^{d \times m}\), and ReLU nonlinearity \(\sigma\), which is applied elementwise. Then,

\[
E_{x \sim \mathcal{N}(0, I)} \left[ \langle \sigma(x^\top Y), \sigma(x^\top W) \rangle \right]
\]
\[
= \sum_{i=1}^m ||W_i||_2 ||Y_i||_2 \cdot E_{g_1^1, g_2^2} [\sigma(g_1^1) \sigma(g_2^2)]
\]

(51)

where \(g_1^1, g_2^2\) are univariate standard Gaussians with correlation \(E_{g_1^1, g_2^2} [g_1^1 g_2^2] = \rho_i\) and \(\rho_i = \frac{W_i^\top Y_i}{||W_i||_2 ||Y_i||_2} \in [0, 1]\). \(W_i, Y_i\) are the columns of \(W, Y\) respectively.

Proof. First apply linearity of expectation to get a sum over \(m\) correlations corresponding to column vectors \(Y_i, W_i\). Then, using the positive homogeneous property of ReLU \((\sigma(c \cdot x) = c \cdot \sigma(x)\) for \(c \geq 0\)), we can normalize \(Y_i, W_i\) and pull out their \(\ell_2\) norms. Then using joint Gaussianity, we can replace \(Y_i^\top x\) and \(W_i^\top x\) with \(g_1^1, g_2^2\). Finally, observe

\[
E_{x \sim \mathcal{N}(0, I)} \left[ \text{Tr} \left( Y_i^\top x x^\top W_i \right) \right] \cdot \frac{1}{||Y_i||_2 ||W_i||_2} = \frac{\text{Tr} \left( Y_i^\top I W_i \right)}{||Y_i||_2 ||W_i||_2} = \frac{Y_i^\top W_i}{||Y_i||_2 ||W_i||_2}
\]

(52)

(53)

(54)
8.4.2 Lower Bounding the Gap

**Lemma 4.3** (Relationship between SVD and ReLU SVD). Suppose \( W = U \Sigma V^T \in \mathbb{R}^{d \times m} \). Consider the solution for rank-\( r \) ReLU SVD (given by \( Y^* \)) as described in Theorem 4.2. If \( h(\rho) \) is replaced with \( \rho^2 \), and we always choose \( \Lambda^* \) to correspond to the top \( r \) singular values of \( \Sigma \), then \( Y^* \) is the standard SVD solution. Denote \( \rho \) as shorthand, denote \( Y \) as defined in Problem 2.1; \( Y \) suboptimality of the SVD solution

\[
\|Y\|_2^2 - \sum_{i=1}^{m} \left( \|W_i\|_2^2 \sqrt{h(\rho_i)} \beta_i - \frac{1}{2} \beta_i^2 \right)
\]

as computed in Theorem 4.2. We know that choosing \( \Lambda^* \) to correspond to the top \( r \) singular values is not necessarily optimal, and so if we bound the difference between the SVD solution and the choice of \( \rho^*_\text{SVD} \) with correct scaling, we are also lower bounding the difference between the SVD solution and the optimal choice of \( \rho^*_\text{SVD} \). If we choose \( \Lambda^* \) to correspond to the top \( r \) singular values (sub-optimally) and then set \( \beta_i = \|W_i\|_2 \cdot \sqrt{h(\rho^*_\text{SVD}(i))} \) optimally, we get that the value of the objective is

\[
\|W\|_2^2 - \frac{1}{2} \sum_{i=1}^{m} \|W_i\|_2^2 \cdot h(\rho^*_\text{SVD}(i))
\]

On the other hand, if we do the SVD solution, we can note that since we pick the same \( \Lambda^* \), the SVD solution only differs in that we plug in \( \beta_i = \rho^*_\text{SVD}(i) \) to the objective instead (Lemma 4.3): Thus, the resulting value of that objective is

\[
\|W\|_2^2 - \frac{1}{2} \sum_{i=1}^{m} \left( \|W_i\|_2 \cdot \sqrt{h(\rho^*_\text{SVD}(i))} \rho^*_\text{SVD}(i) - \frac{1}{2} \rho^*_\text{SVD}(i)^2 \right)
\]

Therefore, computing the absolute difference to get the suboptimality gap, we get

\[
\sum_{i=1}^{m} \left( \|W_i\|_2 \cdot \sqrt{h(\rho^*_\text{SVD}(i))} \rho^*_\text{SVD}(i) - \frac{1}{2} \rho^*_\text{SVD}(i)^2 \right)
\]

which after normalizing by \( d \) proves the result. \( \square \)

Using the lower bound in Theorem 4.4, we can now characterize the conditions on the full-rank matrix \( W \in \mathbb{R}^{d \times m} \) where the optimum of \( \mathcal{R}(Y) \) from Problem 2.1 and the SVD solution are significantly different.

**Corollary 8.25.** Consider \( W \in \mathbb{R}^{d \times m} \) and the problem of finding the best nonlinear approximation low-rank \( Y \in \mathbb{R}^{d \times m} \), as described in Theorem 4.2. Then, cases where more correlation terms \( \rho^*_\text{SVD}(i) \) are smaller result in the SVD solution having larger sub-optimality gaps (measured with respect to \( \mathcal{R}(Y) \) defined in Problem 2.1).
Proof. From the proofs of Theorem 4.2 and Theorem 4.4, we only need to consider the difference between \( \sqrt{h}(\rho^*_{\text{SVD}}(i)) \) and \( \rho^*_{\text{SVD}}(i) \). Note that the gap between \( \sqrt{h}(\rho^*_{\text{SVD}}(i)) \) and \( \rho^*_{\text{SVD}}(i) \) increases as \( \rho^*_{\text{SVD}}(i) \) decreases (since \( \sqrt{h}(\rho^*_{\text{SVD}}(i)) \) is a convex and monotone increasing upper bound to \( \rho^*_{\text{SVD}}(i) \) which converges at \( \rho^*_{\text{SVD}}(i) = 1 \), see Lemma 8.7 and Corollary 2).

\[ \text{Remark 8.26 (Orthogonality Intuition for Corollary 8.25). Corollary 8.25 roughly translates to a statement about the approximate orthogonality of the columns of } W - \text{ if the columns of } W \text{ are all mostly orthogonal, it is hard to achieve large correlations } \rho_i = \left( \frac{W_i}{\|W_i\|_2}, \frac{Y_i}{\|Y_i\|_2} \right) \text{ with a low-rank } Y \in \mathbb{R}^{d \times m} \text{ since we can only select } Y_i \text{ which span a certain subspace} - \text{ if the columns are approximately orthogonal, they do not live in a degenerate subspace and if for instance they are chosen uniformly randomly on the sphere, they will typically be near orthogonal to the vectors of the low-rank subspace spanned by the columns of } Y. \text{ Therefore, since the } \rho_i \text{ will be typically small in this setting, by Corollary 8.25, there will be a larger sub-optimality gap for the SVD.} \]

When \( \max_i \rho^*_{\text{SVD}}(i) < 1 \) (larger \( \rho^*_{\text{SVD}}(i) \) correspond to smaller gaps), we can prove a stronger result:

**Corollary 8.27.** Suppose the columns of \( W \in \mathbb{R}^{d \times m} \) satisfy \( \|W_i\|_2 = 1 \) for all \( i \in [m] \). Then, the suboptimality of SVD is lower bounded in terms of the growth rates of \( m,d \), if \( d = \Theta(n), m = \Omega(n^{1+\delta}) \) for any \( \delta > 0 \), and we have that \( \max_{i \in [m]} \rho^*_{\text{SVD}}(i) < \rho_{\text{max}} < 1 \), then the sub-optimality gap grows as \( d \) increases. Furthermore, the sub-optimality gap is monotone non-decreasing as \( r \) decreases.

**Proof.** Using Theorem 4.4 and the fact that \( \|W_i\|_2 = 1 \) for all \( i \in [m] \), we have

\[
\frac{1}{2d} \left\| \sqrt{h}(\rho^*_{\text{SVD}}) - \rho^*_{\text{SVD}} \right\|_2^2 = \frac{1}{2d} \sum_{i=1}^{m} \left( \sqrt{h}(\rho^*_{\text{SVD}}(i)) - \rho^*_{\text{SVD}}(i) \right)^2 \\
\geq \frac{m}{2d} \cdot \left( \sqrt{h}(\rho_{\text{max}}) - \rho_{\text{max}} \right)^2 \\
\geq \frac{c_1 \cdot n^{1+\delta}}{c_2 \cdot n} \cdot \left( \sqrt{h}(\rho_{\text{max}}) - \rho_{\text{max}} \right)^2 \\
\geq \Omega \left( d^{\delta} \cdot \left( \sqrt{h}(\rho_{\text{max}}) - \rho_{\text{max}} \right)^2 \right)
\]

where we used the fact that \( \sqrt{h}(\rho^*_{\text{SVD}}(i)) - \rho^*_{\text{SVD}}(i) \) decreases as \( \rho^*_{\text{SVD}}(i) \) increases. Then note that the maximum correlation attainable by the low-rank SVD approximation, \( \rho_{\text{max}} \), is a monotone non-decreasing function of the rank \( r \). This fact follows because by reducing the rank, we only further restrict the choice of subspace which the columns \( Y_i \in \mathbb{R}^r \) can live in. Applying this fact, we have that as \( r \) decreases, by Corollary 8.25, \( \left( \sqrt{h}(\rho_{\text{max}}) - \rho_{\text{max}} \right)^2 \) does not decrease. \( \square \)

**Corollary 4.5 (Spherical Weights).** Suppose the columns of \( W \in \mathbb{R}^{d \times m} \) are drawn from the uniform distribution over the surface of the unit sphere\(^4\). Consider target rank \( r \leq d \). Assume that \( r \gg \Theta(\log(m)) \). Then with probability at least constant, \( \rho_{\text{max}} \leq \sqrt{\frac{d}{\pi}} \), and thus \( \frac{1}{2} (\mathcal{R}(Y_{\text{SVD}})) - \mathcal{R}(Y(\rho^*_{\text{SVD}})) \geq \Omega \left( d^{\delta} \cdot \left( \frac{1}{2} - \frac{1}{2} \sqrt{\frac{d}{\pi}} \right)^2 \right) \), assuming that \( m = d^{1+\delta} \) for some \( \delta > 0 \) and that \( \sqrt{\frac{d}{\pi}} < \frac{2}{\pi} \).

\(^4\)This assumption is reasonable, given the many similar init distributions used in practice (e.g., He and Glorot inits [He et al., 2015, Glorot and Bengio, 2010]).
All that remains is to bound $E$ where $g$ where $m$ distribution for the max over these $t$ more than $ρ$ using the lower bound from Corollary 8.27. Thus, the key step in this proof is to upper bound $ρ_{max}$ with high probability by $\sqrt{r}$.

\[
\rho_{SVD}(i) = \|ΣE_rV_i\|_2/\|W_i\|_2
\]

where $W = UΣV^T$ with $V_i ∈ R^d$ being a column of $V^T$ and $E_r = \text{diag}(Λ^*)$, where $Λ^* ∈ \{0, 1\}^d$ is a binary vector with $r$ non-zero entries chosen does not matter by spherical symmetry (we can multiply by a permutation matrix, which is a rotation matrix, and not affect the distribution). Thus, we find that $Σ$ is diagonal.

Now, treating $W$ and its SVD as random variables, note that $W = UΣV^T$, whose columns are uniformly distributed on the surface of the sphere, can be written as a matrix of $m$ i.i.d. Gaussian vectors drawn from $N(0, I_{d×d})$ with normalized columns, and that $U ∈ R^{d×d}$ is an orthogonal matrix. By the fact that the Gaussian is rotationally symmetric, multiplying by $U^T$ does not change the distribution. Thus we find that $ΣV^T ∈ R^{d×m}$ is also a matrix of $m$ independent Gaussians distributed according to $N(0, I_{d×d})$. Note that the specific $r$ non-zero entries chosen does not matter by spherical symmetry (we can multiply by a permutation matrix, which is a rotation matrix, and not affect the distribution). Thus, we can write

\[
ρ_{max} = \max_{i ∈ [m]} \left\|ΣV_i\right\|_2 = \max_{i ∈ [m]} \left\{ \sum_{j=1}^{r} \frac{g_{ij}^2}{∥g_i∥_2^2} \right\}
\]

where $g_i ∼ N(0, I_{d×d})$ for $i ∈ [m]$ are i.i.d. standard Gaussians. Now we apply Talagrand’s concentration inequality (as stated in Theorem 4.20 in Van Handel [2016]).

We can easily check that the max over the $m$ values of $ρ_{SVD}(i)$ is a convex, 1-Lipschitz function, and therefore Talagrand’s inequality applies:

\[
P(|ρ_{max} − E[ρ_{max}]| > t) ≤ C \cdot \exp \left(−c \cdot t^2\right)
\]

where $c, C$ are universal constants (we will abuse the notation $c, C$ throughout to denote universal constants). All that remains is to bound $E[ρ_{max}]$ above; then probability that $ρ_{max}$ deviates above this upper bound by more than $t$ is also still bounded by $C \cdot \exp \left(−c \cdot t^2\right)$.

Thus, we have

\[
E[ρ_{max}] = E \left[ \max_{i ∈ [m]} \left\{ \sum_{j=1}^{r} \frac{g_{ij}^2}{∥g_i∥_2^2} \right\} \right]
\]

Then, since $z_i := \sqrt{\sum_{j=1}^{r} \frac{g_{ij}^2}{∥g_i∥_2^2}} ∈ [0, 1]$ are independent and identically distributed, we get that the distribution for the max over these $m$ variables is given by

\[
P(ρ_{max} > t) = 1 - (1 - P(z > t))^m
\]
for $z = z_1$.

Now we seek a better understanding of $\mathbb{P}(z > t)$ so we can compute an upper bound on $\mathbb{E}[\rho_{\max}]$. First we have

$$\mathbb{P}\left(\|g_i\|_2 \not\in (1 + \epsilon) \cdot d\right) \leq \exp(-c \cdot d \cdot \min(\epsilon, \epsilon^2))$$

by standard Gaussian norm concentration (Theorem 3.1.1 in Vershynin [2018]).

Then consider the vector $h_i = [g_{i1}, \cdots, g_{ir}]$ while also conditioning on the previous bound holding (e.g., conditioning on $\|h_i\|_2^2 \leq (1 + \epsilon) \cdot d$). Denote this event by $F$.

After conditioning, these random variables also still satisfy the concentration of Gaussian norm condition since the event $F$ only decreases the probability that $\|h_i\|_2$ does not lie within the band, and we have

$$\mathbb{P}\left(\|h_i\|_2 \not\in (1 + \epsilon) \cdot r \mid F\right) \leq \exp(-c \cdot r \cdot \min(\epsilon, \epsilon^2))$$

Then union bounding over both events gives us that

$$\mathbb{P}\left(\|h_i\|_2 \not\in \left[\sqrt{1 - \epsilon} \cdot r, \sqrt{1 + \epsilon} \cdot r\right]\right) \leq 2 \exp(-c \cdot r \cdot \min(\epsilon, \epsilon^2))$$

(59)

We can use this fact about $\mathbb{P}(z > t)$ to upper bound the expectation. We have

$$\mathbb{E}[\rho_{\max}] = \mathbb{E}[\max_{i \in [m]} z_i]$$

$$= \int_{0}^{\infty} (1 - (1 - \mathbb{P}(z > t))^m) \, dt$$

$$= \int_{0}^{1} (1 - (1 - \mathbb{P}(z > t))^m) \, dt$$

$$\leq \int_{0}^{\sqrt{\frac{1}{\epsilon} - 1}} \frac{1}{d} \, dt$$

$$+ \int_{\sqrt{\frac{1}{\epsilon} - 1}}^{1} \left(1 - (1 - \exp(-c \cdot r \cdot \epsilon^2))^m\right) \, dt$$

$$\leq \sqrt{\frac{1 + \epsilon}{1 - \epsilon}} \cdot \frac{r}{d} + \left(1 - \sqrt{\frac{1 + \epsilon}{1 - \epsilon}} \cdot \frac{r}{d}\right) \cdot v(m, r)$$

(60)

where we used the fact that $z \in [0, 1]$ and we upper bounded the probabilities by partitioning on some fixed small choice of $\epsilon < 1$ (say, 0.000001). Here, we define

$$v(m, r) := 1 - \exp(-m \cdot \exp(-\Theta(r \cdot \epsilon^2)))$$

where we think of $\epsilon$ as constant. Therefore, $v(m, r) \in [0, 1]$ and $v(m, r) \rightarrow 1$ if $\log(m)/r \rightarrow \infty$, and $v(m, r) \rightarrow 0$ if $\log(m)/r \rightarrow 0$. If $v(m, r) \rightarrow 1$, then we see that $\rho_{\max} \rightarrow 1$, and if $v(m, r) \rightarrow 0$ (and $\epsilon \rightarrow 0$), $\rho_{\max} \rightarrow \sqrt{r/d}$.

Therefore, applying the Talagrand concentration result to the upper bound on $\mathbb{E}[\rho_{\max}]$, for $r \gg \log(m)$, we have that with high probability, $\rho_{\max} = \Theta(\sqrt{\frac{1}{d}})$.

Now we can use the argument of Corollary 8.27 and plug in our upper bound on $\rho_{\max}$ to get a lower bound on $\left(\sqrt{h}(\rho_{\max}) - \rho_{\max}\right)^2$ with probability at least $1 - \exp(-\Theta(t^2)) - \exp(-\Theta(r \cdot \epsilon^2))$:

$$\left(\sqrt{h}(\rho_{\max}) - \rho_{\max}\right)^2$$

$$\geq \left(\sqrt{h} \left[t + \sqrt{\frac{1 + \epsilon}{1 - \epsilon}} \cdot \frac{r}{d}\right] - \left(t + \sqrt{\frac{1 + \epsilon}{1 - \epsilon}} \cdot \frac{r}{d}\right)\right)^2$$

$$= \left(\frac{1}{\pi} - \frac{1}{2} \left(t + \sqrt{\frac{1 + \epsilon}{1 - \epsilon}} \cdot \frac{r}{d}\right)\right)^2$$

(61)
assuming that \( t + \sqrt{\frac{1 + r}{1 - r}} \cdot \frac{\pi}{2} \) < \( \frac{2}{\pi} \), where we plugged in the approximation

\[
\left( \sqrt{h}(\rho) - \rho \right)^2 = \left( \frac{\sqrt{1 - \rho^2} + (\pi - \arccos(\rho))\rho}{\pi} - \rho \right)^2
\]

\[
= \left( \frac{\sqrt{1 - \rho^2}}{\pi} + \left( \frac{\pi - \arccos(\rho)}{\pi} - 1 \right) \rho \right)^2
\]

\[
\geq \left( \frac{1}{\pi} \left( \sqrt{1 - \rho^2 + \rho^2} - \frac{\rho}{2} \right) \right)^2
\]

\[
\geq \left( \frac{1}{\pi} - \frac{1}{2} \rho \right)^2
\]

where we used the upper bound \( \arccos(\rho) \leq \frac{\pi}{2} - \rho \) for \( \rho \in [0, 1] \). This bound is only valid when \( \rho < 2/\pi \) since otherwise the term inside the square is not positive (and it needs to be since \( \sqrt{h}(\rho) \) is an upper bound on \( \rho \)).

More generally, we can just plug in the formula for \( \sqrt{h} \) given in Definition 4.1 to be precise.

\[\Box\]

Remark 8.28 (What if \( \rho_{\max} = 1 ? \)). It is possible for the upper bound \( \rho_{\max} = 1 \), even for low-rank \( r \) – consider a case where most of the columns of \( W \) are highly correlated and point in the same direction. It is not difficult to see that one can compute a new column of \( W \) which corresponds to one of the columns of \( Y_{\text{SVD}} \) for some choice of rank \( r \), and to then add that new column to \( W \). The resulting \( W \) will have an SVD such that one of the columns of \( Y \) is identical to this new column of \( W \), and thus \( \rho_{\max} = 1 \). Indeed, in the current proof for Corollary 4.5, we see that if the rank \( r \) does not grow sufficiently compared to \( m \), the network width, \( \rho_{\max} \to 1 \) with high probability.

However, this issue is mostly an artefact of our analysis method: In reality, to get an optimal bound for a given \( W \), instead of upper bounding \( \rho_{\max} \), we should integrate across all the values of \( \rho_{\text{SVD}} \) to get our lower bound (e.g. compute the actual \( \ell_2 \) norm). In the Gaussian case, it turns out that most \( \rho_{\text{SVD}}(i) \approx \sqrt{\frac{1}{2}} \) (see Figure 4), and so to get a rough sense of what the bound looks like, we can simply plug in \( \rho_{\text{SVD}}(i) = \sqrt{\frac{1}{2}} \). Note that for constant \( r \), as \( r \) gets very small, \( \sqrt{h}(\rho) - \rho \approx 1/\pi \), and plugging in to Corollary 8.27, we get a lower bound on the gap between SVD and the optimum solution to be order \( \Omega(d^4) \). Since this precise control is not essential to our point, we leave out the detailed proof.
Figure 4: Here we plot the mean values of $\rho^*_\text{SVD}$ for different choices of $m, d,$ and $r$. The standard deviations range between 0.08 and 0 (from smallest $r/d = 0.1$ to largest $r/d = 1$). The x-axis is the rank scale $r/d$. We can see that for $m/d$ large enough, the mean corresponds to $\sqrt{r/d}$.

## 9 Appendix: More Experiment Results

Table 3: Comparison of WS-NKP Across Rank Scales for EfficientNet-b9. We show by how many percent points the best performing method, WS-NKP, beats the other methods, for the Weight Decay regularization.

| Rank Scale | Top-1 Accuracy for WS-NKP |
|------------|---------------------------|
| 0.05       | 66.90 ± 0.11 (best by 0.36) |
| 0.1        | 72.28 ± 0.04 (best by 0.21) |
| 0.15       | 73.31 ± 0.04 (sub-optimal) |
| 0.2        | 74.01 ± 0.11 (overlaps w/best) |
| Full-Rank  | 79.62 ± 0.05 |

50
Table 4: Comparison of WS-NKP Across Rank Scales for EfficientNet-b7. We show by how many percent points the best performing method, WS-NKP, beats the other methods, for the Weight Decay regularization.

| Rank Scale | Top-1 Accuracy for WS-NKP |
|------------|---------------------------|
| 0.05       | 59.63 ± 0.37 (best by 0.63) |
| 0.1        | 69.09 ± 0.16 (best by 0.20) |
| 0.15       | 71.74 ± 0.02 (best by 0.07) |
| 0.2        | 72.72 ± 0.03 (best by 0.27) |
| Full-Rank  | 78.70 ± 0.02 |

Table 5: Comparison of NKP Across Rank Scales for EfficientNet-b3. We show by how many percent points the best performing method, NKP, beats the other methods, for the Weight Decay regularization.

| Rank Scale | Top-1 Accuracy for NKP |
|------------|------------------------|
| 0.05       | 38.22 ± 0.28 (overlaps w/best) |
| 0.1        | 56.96 ± 0.19 (overlaps w/best) |
| 0.15       | 63.55 ± 0.16 (best by 0.53) |
| 0.2        | 66.32 ± 0.02 (best by 0.27) |
| Full-Rank  | 76.63 ± 0.19 |

Table 6: Comparison of NKP and WS-NKP Across Rank Scales for EfficientNet-b0. We show by how many percent points WS-NKP compares against the other methods, for the Weight Decay regularization.

| Rank Scale | Top-1 Accuracy for NKP or WS-NKP |
|------------|----------------------------------|
| 0.05       | 32.39 ± 0.26 (best by 1.17) |
| 0.1        | 47.84 ± 0.24 (suboptimal) |
| 0.15       | 55.19 ± 0.10 (best by 0.20) |
| 0.2        | 59.38 ± 0.18 (suboptimal) |
| Full-Rank  | 74.50 ± 0.13 |

Table 7: Comparison of WS-NKP Across Rank Scales for ResNet-50. We show by how many percent points the best performing method, WS-NKP, beats the other methods, for the Weight Decay regularization.

| Rank Scale | Top-1 Accuracy for WS-NKP |
|------------|---------------------------|
| 0.05       | 57.37 ± 0.08 (best by 0.45) |
| 0.1        | 64.74 ± 0.04 (best by 0.65) |
| 0.15       | 67.74 ± 0.03 (best by 0.16) |
| 0.2        | 69.37 ± 0.07 (best by 0.33) |
| 0.25       | 70.37 ± 0.06 (best by 0.25) |
| Full-Rank  | 78.1 |

Table 8: Comparison of WS-NKP Across Rank Scales for ResNet-50. We show by how many percent points the best performing method, WS-NKP, beats the other methods, for the Frobenius Decay regularization.

| Rank Scale | Top-1 Accuracy for WS-NKP |
|------------|---------------------------|
| 0.05       | 58.22 ± 0.31 (best by 0.49) |
| 0.1        | 65.93 ± 0.05 (best by 0.24) |
| 0.15       | 67.83 ± 0.42 (sub-optimal) |
| 0.2        | 69.47 ± 0.09 (best by 0.25) |
| 0.25       | 70.16 ± 0.09 (best by 0.19) |
| Full-Rank  | 78.1 |
10 Appendix: Beyond Low-Rank Approximation

The general idea of function approximation at initialization applies to other efficient approximation techniques beyond low-rank deep networks. In particular, we outline how it can be used in the case of general structured matrices via a straightforward extension, as well as in a case where other approximations of a network’s weights are baked in (as in Choromanski et al. [2020]).

**Definition 10.1** (Performer Approximation from Choromanski et al. [2020]). For $Q, K, V \in \mathbb{R}^{L \times d}$, let the standard attention layer be defined

$$\text{Att}_{Q,K}(V) = D^{-1}AV$$

where we define the attention matrix to be

$$A = \exp \left( \frac{QK^T}{\sqrt{d}} \right)$$

and the diagonal normalization matrix

$$D = \text{diag} (A1_L)$$

Then, the Performer approximation to the attention is given by a random feature map approximation:

$$\hat{\text{Att}}_{Q,K}(V) = \hat{D}^{-1}\hat{A}V$$

where

$$\hat{A} = \hat{Q}\hat{K}^T; \quad \hat{D} = \text{diag} \left( \hat{Q}\hat{K}^T1_L \right)$$

and

$$\hat{Q} = \phi(Q); \quad \hat{K} = \phi(K)$$

where low-rank (likely randomized) feature map $\phi: \mathbb{R}^d \to \mathbb{R}^r$ is applied to the row vectors. There is a specific family of feature maps that defines the Performer approximation, but our method applies regardless of the choice of $\phi$. The Performer is more efficient to compute since we can break down the matrix multiplications into an $r \times L$ by $L \times d$ matmul and an $L \times r$ by $r \times d$ matmul, resulting in time complexity $O(Lrd)$ instead of $O(L^2 + Ld)$, and with space complexity $O(Lr + Ld + rd)$.

For the Performer objective of Choromanski et al. [2020] (and any other approximation of Transformer), layerwise function approximation at initialization yields the following objective:

**Definition 10.2** (Layerwise Function Approximation at Initialization for Performer). Suppose we have a neural net with Transformer blocks with substructure

$$f_\theta(V) = g_w(\text{Att}_{Q,K}(V))$$

defined by $g: \mathbb{R}^{L \times d} \to \mathbb{R}^n$. The Performer version of the network is instead

$$\hat{f}_\theta(V) = g_w(\hat{\text{Att}}_{Q,K}(V))$$

where $w \in \mathbb{R}^D$ and $\theta = (w, Q, K)$. Then, our procedure is as follows:

1. Sample $\theta \sim \mathcal{D}$;

2. Solve $\min_{\nu \in \mathbb{R}^{D \times 2(L \times d)}} \mathbb{E}_{V \sim N(0,1/\sqrt{Ld})} \left[ \left\| f_\theta(V) - \hat{f}_\nu(V) \right\|_2^2 \right]$

3. Use $\nu^*$ as the initialization.

As one can see, this general strategy can be applied to any layer approximation method, given an original initialization scheme $\mathcal{D}$ and the ability to optimize the weights to match the original initialization weights. The key element in our approach is taking more of the function into account compared to simply trying to match parameters.