Connecting Optimization and Generalization via Gradient Flow Path Length

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Abstract

Optimization and generalization are two essential aspects of machine learning. In this paper, we propose a framework to connect optimization with generalization by analyzing the generalization error based on the length of optimization trajectory under the gradient flow algorithm after convergence. Through our approach, we show that, with a proper initialization, gradient flow converges following a short path with an explicit length estimate. Such an estimate induces a length-based generalization bound, showing that short optimization paths after convergence are associated with good generalization, which also matches our numerical results. Our framework can be applied to broad settings. For example, we use it to obtain generalization estimates on three distinct machine learning models: underdetermined $\ell_p$ linear regression, kernel regression, and overparameterized two-layer ReLU neural networks.

1 Introduction

From the perspective of statistical learning theory, the goal of machine learning is to find a predictive function that can give accurate predictions on new data. For supervised learning problems, empirical risk minimization (ERM) is a common practice to achieve this goal. The idea of ERM is to minimize a cost function on observed data using an optimization algorithm. Therefore, a fundamental question is: \emph{given a training algorithm, does it produce a solution with good generalization?}
This question has been the subject of a substantial body of literature. One line of works considered the case where gradient methods converge to minimal norm solutions on kernel regression [Bartlett et al., 2020, Tsigler and Bartlett, 2020, Liang and Rakhlin, 2020, Liang et al., 2020], and then analyzed the generalization properties of those minimal norm solutions. However, the phenomenon of norm minimization has only been proven to occur with the quadratic loss with an appropriate initialization scheme. Another line of works focused on overparameterized models, e.g., neural networks under the Neural Tangent Kernel (NTK) regime [Allen-Zhu et al., 2019, Arora et al., 2019, Cao and Gu, 2020, Ji and Telgarsky, 2020, Chen et al., 2021], proving that overparameterized neural networks trained by (stochastic) gradient descent ((S)GD) have good generalization properties on certain target functions, e.g. polynomial functions. All of these works have made significant progress on the interplay of optimization and generalization. However, they focused on studying specific settings, such as the NTK and models possessing minimal norm solutions. In this paper, we propose to study general loss function conditions that induce direct connections between optimization and generalization.

We start with the simple observation - as illustrated in Figure [1] - that under a generic random initialization, the generalization error for both linear models and neural networks is positively correlated with the length of the optimization path\(^1\) after convergence. More precisely, short optimization paths are associated with low generalization error. Here, by length we refer to the trajectory or path length of the parameter evolution during training\(^2\). These empirical findings suggest that the trajectory length could be used to connect optimization and generalization. Intuitively, the length of the optimization path can be viewed as a kind of capacity control, and a short path indicates low “complexity”. In other words, a general condition that guarantees a short optimization path can be used to induce good generalization properties, provided that the training error is low. For this purpose, inspired by the theory in Bolte et al. [2007] that Lojasiewicz gradient inequality (LGI) induces an explicit bound for the gradient flow path, we consider Uniform-LGI (Definition \[3.3\]) which is a modified version of LGI and plays a critical role in obtaining a length estimate for the gradient flow trajectory. We use this estimate to derive length-based generalization bounds for loss functions satisfying the Uniform-LGI.

**Contributions.** Our contributions are three-fold:

- We focus on the gradient flow algorithm and propose a framework for combining optimization and generalization. This framework is based on the length of the gradient flow trajectory, and its key component is the Uniform-LGI.

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\(^1\)For discrete iterations, we use the sum of the distance between every two consecutive iterations to represent the length of the optimization path (See details in Appendix A.1).

\(^2\)This differs from the notion of “length of time” used in early-stopping type of algorithms.
Figure 1: Illustrations of the relationship between optimization path lengths and generalization gaps. (a) Linear regression model and random feature model. (b) Fully connected neural networks. (c) Convolution neural networks. We train all the models by GD/Adam under Gaussian initialization \( \mathcal{N}(\mu, \sigma^2) \) with varied \( \mu \) and \( \sigma \), and record the trajectory lengths \( \text{len}(w(0), \infty) \) from initialization until convergence. We observe that the short optimization path is associated with good generalization. See experiment settings and more numerical results in Appendix A.1.

- We first give a length-based generalization bound (Theorem 3.1) for a common initialization method. Then we provide an explicit length-estimate for the gradient flow trajectory (Theorem 3.4) under the Uniform-LGI.

- We further show applications of Theorems 3.4 and 3.1 to obtain generalization bounds on underdetermined \( \ell_p \) linear regression (Theorem 4.2), kernel regression (Theorem 4.4), and overparameterized 2-layer ReLU neural networks (Theorem 4.5). These bounds match existing results derived for individual cases and expand upon the scenarios where we can rigorously establish the phenomenon of benign overfitting.

2 Related Works

**Generalization.** Traditional VC dimension-based generalization bounds depend on the number of parameters and are vacuous for huge models such as overparameterized neural networks. To overcome this limitation, several non-vacuous generalization bounds are proposed. For example, the norm/margin-based generalization bounds [Neyshabur et al., 2015, Bartlett et al., 2017, Golowich et al., 2018, Neyshabur et al., 2019], and the PAC-Bayes-based bounds [Dziugaite and Roy, 2017, Neyshabur et al., 2018, Zhou et al., 2019, Rivasplata et al., 2020]. However, these bounds tend to focus less on optimization, e.g., norm-based generalization bounds may
not discuss how small-norm solutions are obtained through practical training. In this paper, we connect the optimization and generalization by deriving generalization bounds based on the optimization path length.

**Optimization.** Theoretically analyzing the training process of most machine learning models is a challenging problem as the loss landscapes are highly non-convex. One approach to studying non-convex optimization problems is to use the Polyak-Lojasiewicz (PL) condition [Polyak, 1963], which characterizes the local geometry of loss landscapes and ensures the existence of global minima. It is shown in [Karimi et al., 2016] that GD admits linear convergence for a class of optimization objective functions under the PL condition. In this paper, we modify the original LGI to get length estimates of the optimization paths, which will be used to derive length-based generalization bounds.

**Interface between optimization and generalization.** Implicit bias builds the bridge between optimization and generalization, which has been widely studied to explain the generalization ability of machine learning models. Recent works [Soudry et al., 2018a,b, Nacson et al., 2019a,b, Lyu and Li, 2020] showed that linear classifiers or deep neural networks trained by GD/SGD maximizes the margin of the separating hyperplanes and therefore generalizes well. Other works [Arora et al., 2019, Zou and Gu, 2019, Cao and Gu, 2020, Ji and Telgarsky, 2020, Chen et al., 2021] considered overparameterized neural networks in the lazy training regime where the minimizer has good generalization due to the low “complexity” of the parameter space. In this work, we focus on specific conditions on loss functions under which we can connect optimization and generalization based on the lengths of optimization paths.

### 3 Main results

We introduce the notations and the problem setting in Section 3.1. We then derive a length-based generalization bound in Section 3.2. To validate our theoretical findings, we numerically evaluate the correlation between the path length and the generalization gap in Section 3.3. Lastly, we give an explicit length estimate for the gradient flow trajectory in Section 3.4 under the Uniform-LGI property.

#### 3.1 Setup and Notations

Consider a supervised learning problem on a hypothesis space \( \mathcal{F} = \{ f(w, \cdot) : \mathbb{R}^d \to \mathbb{R} \mid w \in W \} \), where \( W \) is a parameter set in Euclidean space. Given a loss function \( \ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R} \), and a training set \( S = \{(x_i, y_i)\}_{i=1}^n \subseteq \mathbb{R}^d \times \mathbb{R} \) with \( n \) independent and identically distributed (i.i.d.) samples from a joint distribution \( D \), the goal of ERM is to optimize the empirical loss function
\[ \mathcal{L}_n(w) \] on \( S \):

\[
\arg\min_w \mathcal{L}_n(w) := \frac{1}{n} \sum_{i=1}^n \ell(f(w,x_i),y_i).
\]

We assume that, for any \((x,y) \sim \mathcal{D}\), we have \( \|x\| = 1, |y| \leq 1 \). This can be achieved by data normalization. To simplify the analysis, we optimize the empirical loss by gradient flow\(^3\)

\[
\frac{dw(t)}{dt} = -\nabla \mathcal{L}_n(w(t)), \quad t \in [0, +\infty),
\]

where \( w(t) \) is the parameter value at time \( t \), \( w(0) \) is the value of the parameters at initialization, and \( \nabla \mathcal{L}_n(w) \) is the gradient of \( \mathcal{L}_n(w) \) with respect to \( w \). We define the length of the gradient flow curve from \( w(0) \) to \( w(t) \) as

\[
\text{len}(w(0), t) := \int_0^t \left\| \frac{dw(s)}{ds} \right\| \, ds.
\]

**Notations.** We use \( \|\cdot\| \) to denote the \( \ell_2 \) norm of a vector or the spectral norm of a matrix, and use \( \|\cdot\|_F \) to denote the Frobenius norm of a matrix. For a set \( S \in \mathbb{R}^n \), we use \( \partial S \) to denote its boundary. We use \( d(S_1, S_2) \) to represent the Euclidean distance between two sets \( S_1, S_2 \), which is defined as \( d(S_1, S_2) = \{ \inf \|s_1 - s_2\| : s_1 \in S_1, s_2 \in S_2 \} \). For two vectors, we use \( \langle \cdot, \cdot \rangle \) to denote their inner product. Let \( \lambda_{\min}(A) \) and \( \lambda_{\max}(A) \) be the smallest and largest eigenvalues of a symmetric matrix \( A \). For any positive integer \( n \), we denote \( [n] = \{1, 2, \ldots, n\} \). We use \( O(\cdot) \) to stand for Big-O notation.

### 3.2 How does the path length affect generalization?

Throughout this subsection, we assume that there exists an almost everywhere differentiable function \( \Psi : \mathbb{R}^{p+q} \to \mathbb{R} \) such that \( f(w, \cdot) \) can be represented in the following form,

\[
\forall x \in \mathbb{R}^d, \ f(w, x) = \Psi \left( \alpha_1^\top x, \ldots, \alpha_p^\top x, \beta_1, \ldots, \beta_q \right)
\]

with \( \alpha_1, \ldots, \alpha_p \in \mathbb{R}^d, \beta_1, \ldots, \beta_q \in \mathbb{R} \), and \( w = \text{vec} \{ \alpha_1, \ldots, \alpha_p, \beta_1, \ldots, \beta_q \} \in \mathbb{R}^{pd+q} \). Here \( \text{vec} \) is the vectorization operator that concatenates all elements into a column vector. A wide class of functions can be represented in the form (2). Examples include linear functions \( f(w, x) = w^\top x \) and two-layer neural networks \( f(w, x) = a^\top \phi(Wx) \) with \( a \in \mathbb{R}^m, W \in \mathbb{R}^{m \times d} \).

**Additional notations.** For the loss function \( \ell \), we use \( L_\ell(S) \) to denote its Lipschitz constant (the maximal gradient norm) on \( S \) with respect to its first argument. For \( \Psi \) in (2), we define \( L_\Psi(S) := (L^{(1)}_\Psi(S), \ldots, L^{(p)}_\Psi(S), L^{(p+1)}_\Psi(S), \ldots, L^{(p+q)}_\Psi(S)) \top \), where \( L^{(i)}_\Psi(S) \) is the Lipschitz constant of \( \Psi \) on \( S \) with respect to the \( i \)-th variable. Let \( w^{(0)} := \text{vec} \{ \alpha_1^{(0)}, \ldots, \alpha_p^{(0)}, \beta_1^{(0)}, \ldots, \beta_q^{(0)} \} \) and use \( \mathcal{L}_D(w) \) to denote the expected loss \( \mathbb{E}_{(x,y) \sim \mathcal{D}} [\ell(f(w,x),y)] \). For \( a = (a_1, \ldots, a_p) \top \)

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\(^3\)Here we assume the existence of the gradient flow and the limit \( \lim_{t \to \infty} w(t) \).
and \( b = (b_1, \ldots, b_q)^\top \), we define \( S_{a,b} = \{ w : \forall i \in [p], j \in [q], \| \alpha_i \| \leq a_i, \| \beta_j \| \leq b_j \} \), and \( M_{a,b} = \sup_{w \in S_{a,b}, \| x \| \leq 1, \| y \| \leq 1} \ell (f(w, x), y) \).

In the next theorem, we provide a generalization bound based on a magnitude control of the gradient flow path length \( \text{len}(w(0), \infty) \).

**Theorem 3.1.** Consider an initialization scheme such that \( w(0) \) is independent of the training samples and suppose that for any \( \delta \in (0, 1) \), there exist \( M_\delta, R_{n,\delta} > 0 \) such that \( \| w(0) \| \leq M_\delta \), \( \text{len}(w(0), \infty) \leq R_{n,\delta} \) with probability at least \( 1 - \delta \) over the initialization and the training samples.

Then, we have with probability at least \( 1 - \delta \) over initialization and the training samples, the generalization error of the global minimum \( w(\infty) \) is bounded as:

\[
L_D(w(\infty)) \leq \min_w L_n(w) + \sup_{\| a \|^2 + \| b \|^2 \leq R^2} \frac{2RL_\ell(S_{a,b}) \| L_\Psi(S_{a,b}) \|}{\sqrt{n}} + 3M_{a,b} \sqrt{\frac{3(p + q) + \log(2/\delta)}{2n}},
\]

where \( R = \sqrt{2(M_\delta + R_{n,\delta})} \).

The proof of Theorem 3.1 is detailed in Appendix B. There are five key terms in (3):

- **\( M_\delta \):** This is a high probability upper bound for the \( \ell_2 \) norm of the initialized vector \( \| w(0) \| \).
  
  In practice, for commonly used initialization schemes, such as Xavier initialization \cite{Glorot2010} and Kaiming initialization \cite{He2015}, the norm \( \| w(0) \| \) is uniformly bounded with high probability.

- **\( R_{n,\delta} \):** This is an high probability upper bound for the optimization path length over the initialization and training samples. In theorem 3.1, we assume that such a bound exists, and show that it immediately yields a generalization estimate based on this bound. In theorem 3.4, we give a sufficient condition to obtain such path estimate. The asymptotic analysis of \( R_{n,\delta} \) is problem-dependent, and we provide several examples in Section 4.

- **\( L_\ell(S_{a,b}) \) and \( M_{a,b} \):** These quantities are directly related to the loss function \( \ell \). For instance, given a loss function \( \ell : \mathbb{R} \times \mathbb{R} \to [0, 1] \) that is 1-Lipschitz in the first argument, we have that \( L_\ell(S_{a,b}) = M_{a,b} = 1 \).

- **\( L_\Psi(S_{a,b}) \):** This term is related to the properties of \( f \). For example, when \( f \) is linear, \( \Psi(x, y) = x + y \), then \( L_\Psi(S_{a,b}) = \sqrt{2} \).

**Remark 3.2.** Theorem 3.1 shows that a short optimization path length implies a good generalization bound. Note that our generalization bound is stated for the model after convergence \( (w(\infty)) \). Nevertheless, one can also get generalization estimates during training if a path length
estimate can be obtained (see an example in Appendix C.1). The generalization bound in Theorem 3.1 relies essentially on the path length estimate. We provide in Theorem 3.4 a sufficient condition that ensures the existence of such estimate. Consequently, as long as one can obtain path length estimates (say from stochastic analysis of SGD), one can still apply Theorem 3.1 to obtain generalization estimates. Path length estimates for other types of training algorithms is an interesting future direction.

### 3.3 Evaluation of the correlation between the path length measure and the generalization gap

For a Lipschitz loss function $\ell$, the key term in the complexity measure given in in theorem 3.1 is

$$\sup_{\|a\|^2 + \|b\|^2 \leq R^2} \frac{R \|L(R(S_{a,b}))\|}{\sqrt{n}}$$

up to some universal constant. In this subsection, we aim to demonstrate the association between the length-based complexity measure (4) and the generalization gap. To show this, we follow Jiang et al. [2020], Dziugaite et al. [2020] to compare the length-based measure with another 18 complexity measures (including norm-based, flatness-based and margin-based measures, see details in Appendix A.2) by calculating the Kendall’s rank coefficient [Kendall, 1938]. Specifically, for a set of training processes $P = \{p_1, p_2, \ldots, p_k\}$ where each $p_i$ corresponds to one particular training process that contains all the information of the model during training, then the Kendall’s rank coefficient $\tau_P$ of a complexity measure $\mu$ and the generalization gap $g$ is given by

$$\tau_P = \frac{\sum_{i,j \in [k], i \neq j} \text{sgn}(\mu(p_i) - \mu(p_j)) \text{sgn}(g(p_i) - g(p_j))}{k(k-1)},$$

where $\text{sgn}$ is the sign function. From the expression of $\tau_P$, we can see that $\tau_P \in [-1, 1]$, and the larger is $\tau_P$, the more close is the complexity measure $\mu$ to the generalization gap.

Note that our length-based complexity measure (4) is monotonically increasing with respect to $R$ provided everything else is fixed. In that case, the Kendall’s rank coefficient between (4) and the generalization gap is equivalent to that between $R/\sqrt{n}$ (here $R = M_\delta + R_{n,\delta}$, specified in equation (3)) and the generalization gap. Therefore, we may consider the length-based measure $\mu_{\text{Length}}$ to be

$$\mu_{\text{Length}} = \frac{\|w(0)\| + \text{len}(w(0), \infty)}{\sqrt{n}}.$$ (5)

In our experiments, we train 2-layer and 5-layer Multi-layer Perceptron (MLP) on MNIST [LeCun et al., 1998]; VGG16 and VGG19 [Simonyan and Zisserman, 2015] models on CIFAR10.
Krizhevsky et al., 2009. All the models are trained by Adam optimizer with learning rate 0.001, and the training process is stopped once the number of epochs is 1000 or the cross entropy loss firstly reaches at 0.01. For each model, we use random initialization and only vary the initialization scheme to produce 15 groups of experiments (see more experiment details in Appendix A.1). After finishing the training, we calculate all the selected complexity measures and record the generalization gap (based on 0-1 classification error)

\[ g := \text{Training accuracy} - \text{Test accuracy}. \]

Finally, we can obtain the Kendall’s rank coefficient \( \tau_P \) for each complexity measure \( \mu \) and \( g \). The results are shown in Table 1. We observe that, among all the selected complexity measures, the length-based measure (5) has strong positive correlation with the generalization gap over the four models.

| Complexity Measure            | 2-layer MLP | 5-layer MLP | VGG16  | VGG19  | Average score |
|-------------------------------|------------|------------|--------|--------|--------------|
| Length                        | 0.536      | 0.581      | 0.5    | 0.385  | 0.500        |
| Pacbayes mag flatness         | 0.256      | 0.610      | 0.481  | 0.307  | 0.413        |
| Pacbayes flatness             | 0.367      | 0.568      | 0.511  | -0.046 | 0.350        |
| Pacbayes init                 | 0.631      | 0.619      | 0.083  | -0.297 | 0.259        |
| Log prod of fro               | 0.402      | 0.314      | 0.2    | 0.099  | 0.254        |
| Log prod of fro over margin   | 0.383      | 0.295      | 0.15   | 0.121  | 0.237        |
| Path norm                     | 0.383      | 0.219      | 0.283  | 0.033  | 0.230        |
| Pacbayes orig                 | 0.440      | 0.162      | 0.35   | -0.121 | 0.208        |
| Path norm over margin         | 0.345      | 0.181      | 0.233  | 0.033  | 0.197        |
| Fro over spec                 | -0.096     | 0.581      | 0.15   | 0.077  | 0.178        |
| Dist spec init                | 0.478      | 0.543      | 0.0    | -0.407 | 0.154        |
| Fro dist                      | 0.478      | 0.619      | -0.1   | -0.473 | 0.131        |
| Log spec init main            | 0.459      | 0.295      | -0.017 | -0.231 | 0.127        |
| Param norm                    | 0.536      | 0.048      | 0.117  | -0.209 | 0.123        |
| Pacbayes mag init             | 0.019      | -0.067     | -0.1   | -0.011 | -0.040       |
| Log prod of spec              | 0.345      | -0.276     | -0.017 | -0.253 | -0.05        |
| Log spec orig main            | 0.268      | -0.276     | 0.0    | -0.231 | -0.060       |
| Log prod of spec over margin  | 0.287      | -0.295     | -0.05  | -0.253 | -0.078       |
| Inverse margin                | -0.402     | -0.124     | -0.2   | -0.055 | -0.195       |

Table 1: Kendall’s rank coefficient for selected complexity measures on various models given different random initialization (all the other hyperparameters remain the same). The explicit expressions for all the listed complexity measures are provided in Appendix A.2.

Comparison. It was shown in Jiang et al. 2020, Dziugaite et al. 2020 that PACBayes-sharpness-based measures outperform norm-based measures in terms of the Kendall’s rank coefficient and distributional robustness, which is consistent with our findings. It is worth noting

\footnote{We use Adam instead of SGD is to obtain faster convergence. The learning rate is set as PyTorch default.}
that, however, our experiment settings are different from theirs. In particular, we only change the initialization scheme and keep the other hyperparameters (e.g. batch size, network architecture, learning rate) the same. This is important in the sense that some of the generalization bounds highly depend on the hyperparameters, but the expressions of the corresponding complexity measures do not reflect such dependencies. For example, the distance-based generalization bounds in Neyshabur et al. [2019], Nagarajan and Kolter [2019] rely on the depth of the neural networks, while the distance-based measure (equation (23) in Dziugaite et al. [2020]) is barely the Frobenius distance without a depth-dependent factor. Another example is the length-based measure (4), where the term $L_{\Psi}$ depends on the network architecture. Thus, to make the complexity measure consistent with the generalization bound, we only vary the initialization scheme and do not compare the Kendall’s rank coefficient across the models. We are therefore not proposing (5) as a universal generalization gap predictor.

3.4 Explicit path length estimate via Uniform-LGI

In this subsection, we introduce Uniform-LGI, a condition on the loss function that guarantees the gradient flow path length can be estimated. Then, together with Theorem 3.1, we connect optimization and generalization.

The classic LGI gives a lower bound on the gradient of a differentiable function based on its value above its minimum. Many functions, e.g., real analytic functions and subanalytic functions, satisfy this property, at least locally [Bolte et al., 2007]. Here, we require a global version of this inequality as a condition to control the gradient flow trajectory. Let us define this notion below.

**Definition 3.3 (Uniform-LGI).** A function $L(w)$ satisfies Uniform-LGI on a set $S$ with constants $c > 0$ and $\theta \in [\frac{1}{2}, 1)$, if $\|\nabla L(w)\| \geq c (L(w) - \min_{v \in W} L(v))^\theta$, $\forall w \in S$.

In the special case when $\theta = 1/2$ and $c = \sqrt{2\mu}$, the Uniform-LGI corresponds to the $\mu$-PL condition [Karimi et al., 2016]. Here we give examples of functions satisfying the Uniform-LGI but not the PL condition: $L(w) = w^{2k}, k \in \mathbb{Z}^+$. When $k \geq 2$, $L(w)$ satisfies the Uniform-LGI on $\mathbb{R}$ with $c = 2k$ and $\theta = 1 - 1/2k$.

The next result shows that under the uniform-LGI condition, gradient flow returns a global minimum with an explicit estimate of the gradient flow trajectory length as in the following theorem.

**Theorem 3.4.** For any initialization $w^{(0)}$, if $L_n(w)$ satisfies Uniform-LGI on a closed set $S_n$
with constants $c_n, \theta_n$ such that $S_n \supseteq B\left(w^{(0)}, r_n(w^{(0)})\right)$, where

$$r_n(w^{(0)}) = \frac{(\mathcal{L}_n(w^{(0)}) - \min_w \mathcal{L}_n(w))^{1-\theta_n}}{c_n(1-\theta_n)},$$  \hspace{1cm} (6)$$

then $w^{(t)}$ converges to a global minimum $w^{(\infty)}$ with the trajectory length upper bounded by $\text{len}(w^{(0)}, \infty) \leq r_n(w^{(0)})$. The convergence rate is given by:

$$\theta_n = \frac{1}{2} : \quad g_n(t) \leq e^{-c_2^2 t} g_n(0),$$

$$\frac{1}{2} < \theta_n < 1 : \quad g_n(t) \leq (1 + M_n t)^{-1/(2\theta_n - 1)} g_n(0),$$

where $g_n(t) = \mathcal{L}_n(w^{(t)}) - \min_w \mathcal{L}_n(w), M_n = c_n^2 (2\theta_n - 1) (\mathcal{L}_n(w^{(0)}) - \min_w \mathcal{L}_n(w))^{2\theta_n - 1}.$

The proof of Theorem 3.4 is given in Appendix C. This theorem yields that once the loss function satisfies the Uniform-LGI around the initialization, gradient flow returns a global minimum with an explicit trajectory length estimate. Moreover, for any fixed $n$, $\text{len}(w^{(0)}, \infty)$ decreases as the initial loss value decreases. The calculation of $c_n, \theta_n$ for different $n$ should be analyzed case by case based on the loss landscape, as shown in Section 4.

As a corollary, one can also derive generalization estimates that evolve according to the training time (early stopping). See Appendix C.1 for additional results.

4 Applications

In this section, we apply the framework to three models. To obtain clean expressions of the generalization bound in terms of the sample size $n$, it is helpful to consider a range of $n$ relating to the dimension $d$. In particular, we consider underdetermined systems where the ratio $n/d$ remains finite unless stated otherwise:

$$\exists \gamma_0, \gamma_1 \in (0, \infty), \text{ s.t. } \forall d, \gamma_0 d \leq n = n(d) \leq \gamma_1 d.$$  

Note that this setting is non-asymptotic since we do not require $d$ to be infinite. For each application, we evaluate the test error on a loss function $\tilde{\ell} : \mathbb{R} \times \mathbb{R} \to [0, 1]$ is 1-Lipschitz (on the first argument) with $\tilde{\ell}(y, y) = 0$. The following steps are taken in our framework:

**Step 1.** Establish the Uniform-LGI property and find the Uniform-LGI constants $c_n$ and $\theta_n$.

**Step 2.** Apply Theorem 3.4 to get an estimate of the path length.

**Step 3.** Apply Theorem 3.1 to get generalization results from the path length estimates.
4.1 Underdetermined $\ell_p$ linear regression

We begin with an underdetermined linear regression model $f(w, x) = w^\top x$ with an $\ell_p$ loss function ($p \geq 2$ is an even positive integer):

$$\arg\min_{w \in \mathbb{R}^d} \mathcal{L}_n(w) := \frac{1}{pn} \sum_{i=1}^{n} (w^\top x_i - y_i)^p,$$  \hspace{1cm} (7)

where the input data matrix $X = (x_1, \ldots, x_n)^\top \in \mathbb{R}^{n \times d}$ has full row rank. Then the above regression model has at least one global minimum with zero loss.

**Target function.** Suppose the training data is generated from an underlying function $g : \mathbb{R}^d \rightarrow \mathbb{R}$ with $y_i = g(x_i), \forall i \in [n]$. Let $Y = (y_1, \cdots, y_n)^\top$, and assume that there exits $c^* > 0$ such that

$$\|Y\| \leq c^* \sqrt{\lambda_{\max}(XX^\top)}. \hspace{1cm} (8)$$

The inequality (8) actually indicates that $g$ is Lipschitz with a dimension independent Lipschitz constant. Functions satisfying (8) include linear/non-linear functions. For example, $g(x) = \phi(x^\top w^*)$, where $w^* \in \mathbb{R}^d$ with $\|w^*\|_2 \leq c^*$ for some constant $c^*$, and $\phi(\cdot)$ is Lipschitz with $\phi(0) = 0$.

**Assumption 4.1.** The entries of $X$ are i.i.d. subgaussian random variables with zero mean, unit variance, and subgaussian moments[7] bounded by 1.

This assumption allows us to study the spectral properties of the sample matrix using some tools from random matrix theory. Especially, when $n(d)/d$ converges to some constant $\gamma \in (0, 1)$, the Marchenko–Pastur law [Marčenko and Pastur, 1967] shows that $\lambda_{\min}(XX^\top)/n$ converges to $(1 - \sqrt{\gamma})^2$ almost surely. The non-asymptotic results are provided in Rudelson and Vershynin [2010].

Performing our three-step analysis, we get the following results:

**Theorem 4.2.** Consider the underdetermined $\ell_p$ linear regression model [7]. Suppose that there exists a universal constant $c_0 \geq 1$ such that $\forall d, \|w^{(0)}\|_2 \leq c_0$.

**Step 1.** $\mathcal{L}_n(w)$ satisfies Uniform-LGI globally on $\mathbb{R}^d$ with

$$c_n = p^{1-1/p} \sqrt{\frac{\lambda_{\min}(XX^\top)}{n}}, \hspace{0.5cm} \theta_n = 1 - 1/p.$$

[7]The subgaussian moment of $X$ is defined as $\inf \left\{ \mathcal{M} \geq 0 \mid \text{E} e^{tX} \leq e^{\mathcal{M} t^2/2}, \forall t \in \mathbb{R} \right\}$.  

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**Step 2.** $\mathcal{L}_n(w^{(t)})$ converges to zero linearly for $p = 2$ and sublinearly for $p \geq 4$, i.e.,

$$p = 2, \quad \mathcal{L}_n(w^{(t)}) \leq \exp\left(-2\lambda_{\min}(XX^\top)t/n\right)\mathcal{L}_n(w^{(0)}) ;$$

$$p \geq 4, \quad \mathcal{L}_n(w^{(t)}) \leq (1 + Mt)^{-\frac{p}{p-2}}\mathcal{L}_n(w^{(0)}),$$

where $M = p^{1-\frac{2}{p}}(p - 2)\frac{\lambda_{\min}(XX^\top)}{n}$. 

**Step 3.** Under Assumption 4.1, for any target function that satisfies (8), we have with probability at least $1 - \delta - \tau d - n + 1 - \tau d$ over the samples,

$$\mathbb{E}_{(x,y) \sim D} \left[ \hat{\ell} \left( f(w^{(\infty)}, x), y \right) \right] \leq O \left( n^{-\frac{1}{p}} + \frac{\log(\frac{1}{\delta})}{n} \right),$$

where $\tau \in (0,1)$ depends only on the subgaussian moment of the entries.

The proof of Theorem 4.2 is given in Appendix D.1. This theorem shows that compared to the PL condition that corresponds to $p = 2$, the uniform-LGI is more general and can be applied to more cases.

**Comparison.** This result is related to Bartlett et al. [2020] that studied the phenomenon of benign overfitting in high-dimensional $\ell_2$ linear regression. Our result coincides with theirs as both results uncover some scenarios for benign overfitting in linear regression. In particular, Bartlett et al. [2020] focused on the minimum $\ell_2$ norm estimator. They showed that, if the eigenvalue sequence of the covariance operator $\Sigma := \mathbb{E}[xx^\top]$ have suitable decay rates, then the generalization error will decrease to zero as $n$ increases. In contrast, our result differs from theirs in the problem settings. Specifically, we do not assume the minimum norm property and consider the optimization process that was omitted in Bartlett et al. [2020]. Also, we evaluate the generalization error of the convergence point on a globally Lipschitz loss function. In our setting, entries of each input $x$ are i.i.d. random variables, meaning that $\Sigma = I_{d \times d}$ without decaying eigenvalues. The requirement of i.i.d. entries for each input is a limitation due to the lack of non-asymptotic results of the spectral properties for random matrices with non-i.i.d. entries. However, this limitation can be overcome if one considers the asymptotic results (Livshyts [2018], Bose et al. [2021]). Moreover, our result works for $\ell_p$ loss functions with any even positive integer $p$. This expands the understanding of benign overfitting in the high-dimensional setting.

### 4.2 Kernel Regression

Consider a positive definite kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ with its corresponding feature map $\varphi : \mathbb{R}^d \to \mathcal{F}$ satisfying $\langle \varphi(x), \varphi(y) \rangle_{\mathcal{F}} = k(x, y)$. We assume that $|k(x, x)| \leq 1, \forall x \in \mathcal{X}$. Let $\mathcal{H}$ be the
reproducing kernel Hilbert space (RKHS) with respect to \( k \). If \( \mathcal{F} = \mathbb{R}^s \), then the kernel regression model with \( \ell_p \) loss is to solve the following problem

\[
\arg\min_{w \in \mathbb{R}^s} \mathcal{L}_n(w) := \frac{1}{2n} \sum_{i=1}^n (w^\top \varphi(x_i) - y_i)^p,
\]

where \( p \geq 2 \) is an even integer. Similar to the \( \ell_p \) linear regression case, we consider the following target function:

**Target function.** Suppose the training data is generated by an underlying function \( g : \mathbb{R}^d \to \mathbb{R} \) with \( y_i = g(x_i), \forall i \in [n] \). We further assume that there exists \( c^* > 0 \) such that

\[
\|Y\| \leq c^* \cdot \sqrt{\lambda_{\max}(k(\mathcal{X}, \mathcal{X}))},
\]

where \( k(\mathcal{X}, \mathcal{X}) \) is the \( n \times n \) kernel matrix with \( k(\mathcal{X}, \mathcal{X})_{ij} = k(x_i, x_j) \).

Here, we list an example of class of functions that satisfies (10): \( g(x) = \phi(\varphi(x)^\top w^*) \) where \( w^* \in \mathbb{R}^s \) with \( (\forall s) \|w^\|_2 \leq c^* \) for some constant \( c^* \), and \( \phi(\cdot) \) is Lipschitz with \( \phi(0) = 0 \). To get the generalization results of kernel regression, we will discuss two types of kernels separately: radial basis function (RBF) kernel and inner product kernel.

**RBF kernel.** We study the RBF kernel of the form \( k(x, y) = \varrho(\|y - x\|) \) for a certain RBF \( \varrho \).

For the input data, we define the separation distance of \( \mathcal{X} \) as \( \text{SD} := \frac{1}{2} \min_{i \neq j} \|x_i - x_j\|, \forall i, j \in [n] \).

**Inner product kernel.** For the inner product kernel, we consider \( k(x, y) = \varrho(x^\top y_d) \).

Following El Karoui et al. [2010], we make the following assumption on the function \( \varrho \):

**Assumption 4.3.** \( \varrho \) is \( C^3 \) in a neighborhood of 0 with \( \varrho(0) = 0, \varrho(1) > \varrho'(0) \geq 0, \varrho''(0) \geq 0 \).

We now apply our three-step machinery to get optimization and generalization results. For the RBF kernel, the generalization bound depends on the separation distance of the samples. For the inner product kernel, we study the high-dimensional random kernel matrix.

**Theorem 4.4.** Consider the kernel regression model (9). Suppose that there exists a universal constant \( c_0 \geq 1 \) such that \( (\forall s) \|w^{(0)}\|_2 \leq c_0 \).

**Step 1.** \( \mathcal{L}_n(w) \) satisfies Uniform-LGI globally on \( \mathbb{R}^s \) with

\[
c_n = p^{1-1/p} \sqrt{\frac{\lambda_{\min}(k(\mathcal{X}, \mathcal{X}))}{n}}, \quad \theta_n = 1 - 1/p,
\]

where \( c_n \) is controlled by the kernel and input samples.
Step 2. \( \mathcal{L}_n(w^{(t)}) \) converges to zero linearly for \( p = 2 \) and sublinearly for \( p \geq 4 \), i.e.,

\[
\begin{align*}
  p = 2, & \quad \mathcal{L}_n(w^{(t)}) \leq \exp\left(-2\lambda_{\min}(k(X, X))t/n\right) \mathcal{L}_n(w^{(0)}); \\
  p \geq 4, & \quad \mathcal{L}_n(w^{(t)}) \leq (1 + Mt)^{-\frac{p}{p-2}} \mathcal{L}_n(w^{(0)}),
\end{align*}
\]

where \( M = p^{-\frac{2}{p}}(p - 2)^{\lambda_{\min}(k(X, X))} \mathcal{L}_n(w^{(0)})^{-\frac{2}{p}} \).

Step 3. For any target function that satisfies (10) we have:

- For the RBF kernel, suppose that \( \varphi : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}_{\geq 0} \) is a decreasing function and \( \varphi(||x||) \in L^1(\mathbb{R}^d) \). If there exists two positive constants \( q_{\min} \) and \( q_{\max} \) such that \( SD \in [q_{\min}, q_{\max}] \) for all \( n \), then with probability at least \( 1 - \delta \) over the samples,

\[
\mathbb{E}_{(x, y) \sim D}\left[ \hat{\ell}\left(f(w^{(\infty)}, x), y\right) \right] \leq O\left(n^{-\frac{1}{p}} + \sqrt{\frac{\log(\frac{1}{\delta})}{n}}\right).
\]

- For the inner product kernel, under Assumption 4.1 and Assumption 4.3, if \( d \) is large enough and \( \delta > 0 \) is small enough such that \( d^{-1/2} \left(\sqrt{3}\delta^{-1/2} + \log^{0.51} d\right) \leq 0.5(\varphi(1) - \varphi'(0)) \), then with probability at least \( 1 - \delta - d^{-2} \) over the samples, we have

\[
\mathbb{E}_{(x, y) \sim D}\left[ \hat{\ell}\left(f(w^{(\infty)}, x), y\right) \right] \leq O\left(n^{-\frac{1}{p}} + \sqrt{\frac{\log(\frac{1}{\delta})}{n}}\right).
\]

The proof of Theorem 4.4 is given in Appendix D.2.

Example 1. Kernels satisfying the conditions and assumptions in Theorem 4.4 include (1) (RBF) Gaussian: \( \varphi(r) = e^{-\rho r^2}, \rho > 0 \); (2) (RBF) Multiquadrics: \( \varphi(r) = (\rho + r^2)^{\beta/2}, \rho > 0, \beta \in \mathbb{R}\backslash 2\mathbb{N}, \beta < -d \). (3) (Inner product) Polynomial kernel: \( \varphi(r) = r^\beta, \beta \in \mathbb{Z}^+, \beta \geq 2 \); (4) (Inner product) NTK corresponding to Two-layer ReLU neural networks on \( S^{d-1}(\sqrt{d}) \): \( \varphi(r) = \frac{r(\pi - \arccos(r))}{2\pi} \).

Comparison. The \( p = 2 \) result of the inner product kernel is related to [Liang and Rakhlin 2020] who derived generalization bounds for the minimum RKHS norm estimator. They showed that when the data covariance matrix and the kernel matrix enjoy certain decay of the eigenvalues, the generalization bound vanishes as \( n \) goes to infinity. For example, for exponential kernel and the covariance matrix \( \Sigma := \mathbb{E}[xx^\top] \) with the \( j \)-th eigenvalue \( \lambda_j(\Sigma) = j^{-\alpha} \), the \( \ell_2 \) generalization bound becomes \( O(n^{-\frac{2\alpha}{2\alpha+1}}) \) when \( \alpha \in (0, 1) \) and \( n > d \). In comparison, we get an optimal generalization bound \( O\left(n^{-1/2}\right) \) for identity covariance matrix on a globally Lipschitz

\[\text{Here } d \text{ is fixed and } n \text{ is varied.}\]
loss function. Again, we emphasize that the i.i.d. assumption can be relaxed if more new results of random matrix theory are available. Further, we extend the works in Liang and Rakhlin [2020] by proving a new result of the RBF kernel. Note that the result of the RBF kernel is not under the high-dimensional setting; thus it is not a direct adaptation of Liang and Rakhlin [2020], and the proof itself is of independent interest.

4.3 Overparameterized two-layer Neural Networks

In this section, we show that our framework can be applied to neural network models. More specifically, we obtain generalization bounds for shallow neural networks in the overparameterized regime (large width).

First, define a two-layer ReLU neural network under the NTK parameterization [Lee et al., 2019]:

\[ f(w, x) = \frac{1}{\sqrt{m}} w_2^\top \phi(W_1 x), \]

where \( \phi(x) = \max\{0, x\}, x \in \mathbb{R}^d \) is the input, \( W_1 \in \mathbb{R}^{m \times d}, w_2 \in \mathbb{R}^m \) are parameters, \( w = \text{vec} (\{W_1, w_2\}) \in \mathbb{R}^{m(d+1)} \), and \( m \) is the width (number of hidden units).

We consider minimizing the quadratic loss by gradient flow:

\[ \arg\min_w L_n(w) := \frac{1}{2n} \sum_{i=1}^n (f(w, x_i) - y_i)^2. \] (11)

**Random initialization.** \( W_1^{(0)} \) is drawn from Gaussian \( \mathcal{N}(0, \frac{1}{d} I_{m \times d}) \) and \( w_2^{(0)} \) are drawn i.i.d. from uniform distribution \( U\{-1, 1\}, \forall i \in [m] \).

Following the setting in Du et al. [2019], we only train the hidden layer \( W_1 \) and leave the output layer \( w_2 \) as random initialization to simplify the analysis.

**NTK matrix.** The NTK matrix \( \Theta(t) \) is defined as:

\[ \Theta_{ij}(t) = \langle \nabla_{W_1} f(w(t), x_i), \nabla_{W_1} f(w(t), x_j) \rangle, \]

and denote \( \hat{\Theta} \) by the limiting matrix:

\[ \hat{\Theta}_{ij} = x_i^\top x_j \mathbb{E}_{w \sim \mathcal{N}(0, \frac{1}{d} I_d)} [\phi'(w^\top x_i) \phi'(w^\top x_j)], \forall i, j \in [n]. \]

Similarly, we apply our three-step analysis to derive the following results.

**Theorem 4.5.** Consider the two-layer ReLU neural network [11]. For any \( \delta \in (0, 1) \), if \( m \geq \text{poly}\left(n, \lambda_{\min}(\hat{\Theta}), \delta^{-1}\right) \), then

**Step 1.** With probability at least \( 1 - \delta \) over training samples and random initialization, \( L_n(w^{(t)}) \) satisfies the Uniform-LGI on \( \{w(t) : t \geq 0\} \) with

\[ c_n = \sqrt{\lambda_{\min}(\hat{\Theta})/n}, \quad \theta_n = 1/2. \]

\footnote{Here \( \lambda_{\min}(\hat{\Theta}) \) changes with \( n \).}
Step 2. $\mathcal{L}_n(w^{(t)})$ converges to zero linearly:

$$\mathcal{L}_n(w^{(t)}) \leq \exp\left(-\lambda_{\min}(\hat{\Theta}) t/n\right) \mathcal{L}_n(w^{(0)}).$$

Step 3. Under Assumption 4.1 for any target function that satisfies (8), if $\gamma_1 \in (0,1)$, then with probability at least $1 - \delta - \tau d - n^{-1} - \tau^d$ over the samples and random initialization,

$$\mathbb{E}_{(x,y) \sim \mathcal{D}} \left[ \ell\left(f(w^{(\infty)}, x), y\right) \right] \leq O\left(\sqrt{\log(\frac{n}{\delta})} \frac{n}{n}\right),$$

where $\tau \in (0,1)$ depends only on the subgaussian moment of the entries.

The proof of Theorem 4.5 is deferred to Appendix D.3.

Comparison. Our result is related to Arora et al. [2019], which gave an NTK-based generalization bound for overparameterized two-layer ReLU neural networks. This result matches with theirs in the sense that we discover some underlying functions that are provably learnable. Examples of learnable target functions in Arora et al. [2019] include polynomials $y = (\beta^T x)^p$, non-linear activations $y = \cos(\beta^T x) - 1$, $y = \tilde{\phi}(\beta^T x)$ with $\tilde{\phi}(z) = z \cdot \arctan(z/2)$, $\|\beta\| \leq 1$. Our result, furthermore, expands the target function class that is provably learnable since we only require $\tilde{\phi}$ to be Lipschitz. In addition, they set the standard deviation of the initialization to be at most $O(1/n)$, whereas we use a different initialization with order $O(1/\sqrt{d})$ that is more often applied in practice. Our result is also related to Liu et al. [2020], which proved that overparameterized deep neural networks satisfy the PL condition. Further, we extend this work by analyzing the generalization based on the length of optimization trajectories.

5 Conclusion

In this work, we connect optimization path lengths to generalization. For this purpose, we propose a framework to bridge the gap between optimization and generalization based on the trajectory length. The pivotal component is the Uniform-LGI property: a condition on the loss function, by which we show that gradient flow returns a global minimum with an explicit length estimate. Further, we derive a length-based generalization bound given such a length estimate. Finally, we apply the framework to three machine learning models with certain target functions. By estimating the trajectory lengths, we get non-vacuous generalization bounds that do not suffer from the curse of dimensionality. This framework is not a direct variant of the NTK method, and the results show that our framework is favorable for inducing connections between optimization and generalization.
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A Experiments

A.1 Experiments settings

In this subsection, we describe the details of our experiments for Figure 1 and Table 1.

Linear Regression model. The model that we use is underdetermined $\ell_2$ linear regression without regularization. The data set contains 130 data points $\{(x_i, y_i)\}^{130}_{i=1} \subseteq \mathbb{R}^{200} \times \mathbb{R}$. The inputs $x_i (\forall i \in [130])$ are uniformly drawn from the 200-dimensional unit sphere. Labels $y_i (\forall i \in [130])$ are generated by a linear target function $y_i = \beta^T x_i$ with some $\beta \in \mathbb{R}^{200}$ that satisfies $\|\beta\| = 1$. We train this model by gradient descent $w^{(k+1)} = w^{(k)} - \eta \nabla L_n(w^{(k)})$ with step size $\eta = 0.05$ on the mean square loss (MSE). Entries of $w^{(0)}$ are initialized i.i.d. from Gaussian distribution $\mathcal{N}(\mu, \sigma^2)$ with $\mu = 2^{-5}, 2^{-2}, 2^{1}, 2^{4}$ and $\sigma = 2^{-5}, 2^{-2}, 2^{1}, 2^{4}$ respectively. We stop the training once the difference of loss between two consecutive steps $|L_n(w^{(K+1)}) - L_n(w^{(K)})| < 10^{-8}$. Then $\text{len}(w^{(0)}, \infty)$ is approximated by $\sum_{k=1}^{K} \|w^{(k)} - w^{(k-1)}\|$. For each pair of $\mu$ and $\sigma$, we record the length $\text{len}(w^{(0)}, \infty)$, the training error and the test error on the convergence point.

Random feature model. In this experiment, the model that we consider is a two-layer ReLU neural network $w_2^T \phi(W_1 x)$. Here $\phi$ is the ReLU function, $W_1 \in \mathbb{R}^{200 \times 200}$, $w_2 \in \mathbb{R}^{200}$. We only train the last layer $w_2$, and thus this can be viewed as a random feature model with features extracted by $\phi(W_1 x)$. The data set consists of 130 data points $\{(x_i, y_i)\}^{130}_{i=1} \subseteq \mathbb{R}^{200} \times \mathbb{R}$. The inputs $x_i (\forall i \in [130])$ are uniformly drawn from the 200-dimensional unit sphere. All labels $y_i (\forall i \in [130])$ are generated by a teacher network $\hat{\omega}_2^T \phi(\hat{W}_1 x_i)$ with the same architecture for some $\hat{w}_2, \hat{W}_1$. We train only the top layer by gradient descent with momentum 0.9 and step seize 0.05 under the mean square loss (MSE). Entries of $w_2^{(0)}$ are initialized i.i.d. from $\mathcal{N}(\mu, \sigma^2)$ with $\mu = -5, -2, 1, 4$ and $\sigma = 2^{-5}, 2^{-2}, 2^{1}, 2^{4}$ respectively. We stop the training once the difference of loss between two consecutive steps is less than $10^{-8}$. For each pair of $\mu$ and $\sigma$, we use the same method as on linear regression to approximate the trajectory length. Then we record the training error and the test error on the convergence point.

Neural Network model. For MNIST dataset, the models that we use are 3 and 5 layer MLP with batch normalization. The activation function is ReLU and the number of hidden units in each layer is 100. For CIFAR10 dataset, we use the classic VGG16 and VGG19 models. For all the models, we initialize each parameter by Gaussian $\mathcal{N}(\mu, \sigma^2)$, and we vary $(\mu, \sigma)$ for each linear and convolution layer to produce 15 groups of experiments. Specifically, for each linear layer, if this is the last layer, then $(\mu, \sigma)$ are independently sampled from $\mathcal{N}(0, 1)$; if this is the hidden layer, then $\mu = 0$ and $\sigma \sim \mathcal{N}(0, 1)$. For each convolution layer, $\mu$ is set to be zero and $\sigma$ is sampled from $\mathcal{N}(0, 1)$ (then take an absolute value of $\sigma$). All the models are trained by Adam optimizer with batch size 64, learning rate 0.001, and the training process is stopped once the
number of training epochs is 1000 or the cross entropy loss first reaches at 0.01. Finally, we record the generalization gap (difference between training accuracy and test accuracy) and the length $\text{len}(w^{(0)}, \infty)$.

**Varied learning rate.** For the linear regression and random feature model, we provide additional results by only changing the learning rate. Figure 2, 3 and 4 correspond to step size $\eta = 0.01, 0.1, 0.5$ respectively. We observe that the optimization path lengths are nearly the same for both small learning rate and moderate learning rate, and the numerical results are associate with our theory.

![Figure 2: learning rate = 0.01](image2.png)

![Figure 3: learning rate = 0.1](image3.png)

![Figure 4: learning rate = 0.5](image4.png)
A.2 Selected complexity measures

In this subsection, we provide the details for the selected complexity measures in Table 1. All the measures except the length-based measure are directly quoted from Dziugaite et al. [2020]. For easier reference, we list the terms on the following table.

| Complexity measure                  | Position in Dziugaite et al. [2020] |
|-------------------------------------|-------------------------------------|
| Pacbayes mag flatness               | equation (33)                       |
| Pacbayes flatness                   | equation (30)                       |
| Pacbayes init                       | equation (28)                       |
| Log prod of fro                     | equation (20)                       |
| Log prod of fro over margin         | equation (19)                       |
| Path norm                           | equation (27)                       |
| Pacbayes orig                       | equation (29)                       |
| Path norm over margin               | equation (26)                       |
| Fro over spec                       | equation (16)                       |
| Dist spec init                      | equation (24)                       |
| Fro dist                            | equation (23)                       |
| Log spec init main                  | equation (12)                       |
| Param norm                          | equation (25)                       |
| Pacbayes mag init                   | equation (31)                       |
| Log prod of spec                    | equation (15)                       |
| Log spec orig main                  | equation (13)                       |
| Log prod of spec over margin        | equation (14)                       |
| Inverse margin                      | equation (11)                       |

Table 2: Positions of the selected complexity measures in Dziugaite et al. [2020]

B Proof of Theorem 3.1

In this section, we will prove Theorem 3.1. This proof is based on the Rademacher complexity theory and the covering number of $\ell_2$ balls. Now we introduce some known technical lemmas that are used to build our proof.

The first lemma gives a generalization bound of a function class based on the Rademacher complexity, which is proved in Mohri et al. [2018].

**Lemma B.1.** Consider a family of functions $\mathcal{F}$ mapping from $\mathcal{Z}$ to $[a, b]$. Let $\mathcal{D}$ denote the distribution according to which samples are drawn. Then for any $\delta > 0$, with probability at least $1 - \delta$ over the draw of an i.i.d. sample $S = \{z_1, \ldots, z_n\}$ of size $n$, the following holds for all $f \in \mathcal{F}$:

$$
\mathbb{E}_{z \sim \mathcal{D}}[f(z)] - \frac{1}{n}\sum_{i=1}^{n} f(z_i) \leq 2\mathcal{R}_S(\mathcal{F}) + 3(b - a)\sqrt{\frac{\log(2/\delta)}{2n}},
$$
where $\mathcal{R}_S(\mathcal{F})$ is the empirical Rademacher complexity with respect to the sample $S$, defined as:

$$
\mathcal{R}_S(\mathcal{F}) = \mathbb{E}_\sigma \left[ \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i f(z_i) \right].
$$

Here $\{\sigma_i\}_{i=1}^{n}$ are i.i.d. random variables drawn from $U\{-1, 1\}$.

In the next lemma, we prove a shifted version of the Ledoux-Talagrand contraction inequality [Ledoux and Talagrand, 2013], which is useful to bound the length-based Rademacher complexity.

**Lemma B.2.** Let $g : \mathbb{R} \to \mathbb{R}$ be a convex and increasing function. Let $\phi_i : \mathbb{R} \to \mathbb{R}$ be $L$-Lipschitz functions, then for any bounded set $T \subset \mathbb{R}$ and any $t^{(0)} \in \mathbb{R}$, we have

$$
\mathbb{E}_\sigma \left[ g \left( \sup_{(t-t^{(0)}) \in T} \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t_i^{(0)} \right) \right) \right) \right] \leq \mathbb{E}_\sigma \left[ g \left( L \sup_{(t-t^{(0)}) \in T} \sum_{i=1}^{n} \sigma_i \left( t_i - t_i^{(0)} \right) \right) \right],
$$

and

$$
\mathbb{E}_\sigma \left[ \sup_{(t-t^{(0)}) \in T} \left| \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t_i^{(0)} \right) \right) \right| \right] \leq 2L \mathbb{E}_\sigma \left[ \sup_{(t-t^{(0)}) \in T} \left| \sum_{i=1}^{n} \sigma_i \left( t_i - t_i^{(0)} \right) \right| \right].
$$

The special case for $t^{(0)} = 0$ corresponds to the original Ledoux-Talagrand contraction inequality. Here we prove a shifted version.

**Proof.** First notice that

$$
\mathbb{E}_\sigma \left[ g \left( \sup_{(t-t^{(0)}) \in T} \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t_i^{(0)} \right) \right) \right) \right] = \mathbb{E}_{\sigma_1, \ldots, \sigma_{n-1}} \left[ \mathbb{E}_{\sigma_n} \left[ g \left( \sup_{(t-t^{(0)}) \in T} \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t_i^{(0)} \right) \right) \right) \right] \right].
$$

Let $u_{n-1}(t) = \sum_{i=1}^{n-1} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t_i^{(0)} \right) \right)$, then

$$
\mathbb{E}_{\sigma_n} \left[ g \left( \sup_{(t-t^{(0)}) \in T} \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t_i^{(0)} \right) \right) \right) \right] = \frac{1}{2} g \left( \sup_{(t-t^{(0)}) \in T} u_{n-1}(t) + \left( \phi_n(t_n) - \phi_n \left( t_n^{(0)} \right) \right) \right) + \frac{1}{2} g \left( \sup_{(t-t^{(0)}) \in T} u_{n-1}(t) - \left( \phi_n(t_n) - \phi_n \left( t_n^{(0)} \right) \right) \right).
$$
Suppose that the above two suprema can be reached at $t'$ and $\tilde{t}$ respectively, i.e.,

$$
\sup_{(t-t(0))\in T} u_{n-1}(t) + \left( \phi_n(t_n) - \phi_n(t_n(0)) \right) = u_{n-1}(t') + \left( \phi_n(t_n') - \phi_n(t_n(0)) \right);
$$

$$
\sup_{(t-t(0))\in T} u_{n-1}(t) - \left( \phi_n(t_n) - \phi_n(t_n(0)) \right) = u_{n-1}(\tilde{t}) - \left( \phi_n(\tilde{t}_n) - \phi_n(t_n(0)) \right).
$$

Otherwise we add an arbitrary positive number $\varepsilon$ in the above equations. Therefore,

$$
\mathbb{E}_{\sigma_n} \left[ g \left( \sup_{(t-t(0))\in T} \sum_{i=1}^n \sigma_i \left( \phi_i(t_i) - \phi_i(t_i(0)) \right) \right) \right] = \frac{1}{2} \left[ g \left( u_{n-1}(t') + \left( \phi_n(t_n') - \phi_n(t_n(0)) \right) \right) \right] + \frac{1}{2} \left[ g \left( u_{n-1}(\tilde{t}) - \left( \phi_n(\tilde{t}_n) - \phi_n(t_n(0)) \right) \right) \right].
$$

Without loss of generality, we assume

$$
\begin{align*}
\sup_{(t-t(0))\in T} u_{n-1}(t') + \left( \phi_n(t_n') - \phi_n(t_n(0)) \right) &\geq u_{n-1}(\tilde{t}) + \left( \phi_n(\tilde{t}_n) - \phi_n(t_n(0)) \right); \\
\sup_{(t-t(0))\in T} u_{n-1}(\tilde{t}) - \left( \phi_n(\tilde{t}_n) - \phi_n(t_n(0)) \right) &\geq u_{n-1}(t') - \left( \phi_n(t_n') - \phi_n(t_n(0)) \right),
\end{align*}
$$

(12)

For the other cases, the method remains the same. We set

$$
\begin{align*}
a &= u_{n-1}(\tilde{t}) - \left( \phi_n(\tilde{t}_n) - \phi_n(t_n(0)) \right), \\
b &= u_{n-1}(\tilde{t}) - L(\tilde{t}_n - t_n(0)), \\
a' &= u_{n-1}(t') + L(t_n' - t_n(0)), \\
b' &= u_{n-1}(t') + \left( \phi_n(t_n') - \phi_n(t_n(0)) \right),
\end{align*}
$$

Now our goal is to prove:

$$
g(a) - g(b) \leq g(a') - g(b').
$$

(13)

Considering the following four cases:

1. $t_n' \geq t_n(0)$ and $\tilde{t}_n \geq \tilde{t}_n(0)$. By the Lipschitzness of $\phi_n$ and equation (12) we know $a \geq b, b' \geq b$, and

$$
(a - b) - (a' - b') = \phi_n(t_n') - \phi_n(\tilde{t}_n) - L(t_n' - \tilde{t}_n).
$$

If $t_n' \geq \tilde{t}_n$, we can get $a - b \leq a' - b'$. By the fact that $g$ is convex and increasing, we have $g(y + x) - g(x)$ is increasing in $y$ for every $x \geq 0$. Hence for $x = a - b$,

$$
g(a) - g(b) = g(b + x) - g(b) \leq g(b' + x) - g(b') \leq g(a') - g(b').
$$
If \( t'_n < \tilde{t}_n \), we change \( \phi_n \) into \( -\phi_n \) and switch \( t' \) and \( \tilde{t} \), and the proof is similar.

2. \( t'_n \leq t^{(0)}_n \) and \( \tilde{t}_n \leq t^{(0)}_n \). Similarly, by changing the signs we can get the same result.

3. \( t'_n \geq t^{(0)}_n \) and \( \tilde{t}_n \leq t^{(0)}_n \). For this case we have \( a \leq b \) and \( b' \leq a' \), so \( g(a) + g(b') \leq g(b) + g(a') \).

4. \( t'_n \leq t^{(0)}_n \) and \( \tilde{t}_n \geq t^{(0)}_n \). For this case we can change \( \phi_n \) to \( -\phi_n \), then we have \( a \geq b \) and \( a' \leq b' \), and finally we get \( g(a) + g(b') \leq g(b) + g(a') \).

Thus equation (13) yields that

\[
\mathbb{E}_{\sigma_n} \left[ g \left( \sum_{(t-t^{(0)}) \in T} \sup_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t^{(0)}_i \right) \right) \right) \right] \\
\leq \frac{1}{2} \left[ g \left( u_{n-1} (t') + \left( \phi_n (t'_n) - \phi_n \left( t^{(0)}_n \right) \right) \right) \right] + \frac{1}{2} \left[ g \left( u_{n-1} (\tilde{t}) - \left( \phi_n (\tilde{t}_n) - \phi_n \left( t^{(0)}_n \right) \right) \right) \right] \\
\leq \frac{1}{2} \left[ g \left( u_{n-1} (t') + L \left( t'_n - t^{(0)}_n \right) \right) \right] + \frac{1}{2} \left[ g \left( u_{n-1} (\tilde{t}) - L \left( \tilde{t}_n - t^{(0)}_n \right) \right) \right] \\
\leq \frac{1}{2} \left[ g \left( \sup_{(t-t^{(0)}) \in T} u_{n-1} \left( t \right) + L \left( t_n - t^{(0)}_n \right) \right) \right] + \frac{1}{2} \left[ g \left( \sup_{(t-t^{(0)}) \in T} u_{n-1} \left( t \right) - L \left( t_n - t^{(0)}_n \right) \right) \right] \\
= \mathbb{E}_{\sigma} \left[ g \left( \sum_{(t-t^{(0)}) \in T} \sup_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t^{(0)}_i \right) \right) \right) \right].
\]

Applying the same method to \( \sigma_{n-1}, \ldots, \sigma_1 \) successively, we obtain the first inequality

\[
\mathbb{E}_{\sigma} \left[ g \left( \sum_{(t-t^{(0)}) \in T} \sup_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t^{(0)}_i \right) \right) \right) \right] \leq \mathbb{E}_{\sigma} \left[ g \left( L \sum_{(t-t^{(0)}) \in T} \sup_{i=1}^{n} \sigma_i \left( t_i - t^{(0)}_i \right) \right) \right].
\]

For the second inequality, since \( |x| = [x]_+ + [x]_- \) with \( [x]_+ = \max(0, x) \) and \( [x]_- = \max(0, -x) \),

\[
\mathbb{E}_{\sigma} \left[ \sup_{(t-t^{(0)}) \in T} \left| \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t^{(0)}_i \right) \right) \right| \right] \\
\leq \mathbb{E}_{\sigma} \left[ \sup_{(t-t^{(0)}) \in T} \left| \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t^{(0)}_i \right) \right) \right| \right] + \mathbb{E}_{\sigma} \left[ \sup_{(t-t^{(0)}) \in T} \left| \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t^{(0)}_i \right) \right) \right| \right] \\
= 2 \mathbb{E}_{\sigma} \left[ \sup_{(t-t^{(0)}) \in T} \left| \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t^{(0)}_i \right) \right) \right| \right],
\]

where the last equality is by \( [-x]_- = [x]_+ \) and \( \sigma \) has the same distribution with \( -\sigma \).

A simple fact is that

\[
\sup_{(t-t^{(0)}) \in T} \left| \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t^{(0)}_i \right) \right) \right| = \left[ \sup_{(t-t^{(0)}) \in T} \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t^{(0)}_i \right) \right) \right]_+.
\]
Since $\max(0, x)$ is convex and increasing, then by the first inequality we have

$$
\mathbb{E}_\sigma \left[ \sup_{(t-t(0)) \in T} \left[ \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t_i^{(0)} \right) \right) \right] \right] = \mathbb{E}_\sigma \left[ \sup_{(t-t(0)) \in T} \left[ \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t_i^{(0)} \right) \right) \right] \right] + \mathbb{E}_\sigma \left[ \left( \sup_{(t-t(0)) \in T} \left[ \sum_{i=1}^{n} \sigma_i \left( \phi_i(t_i) - \phi_i \left( t_i^{(0)} \right) \right) \right] \right) \right] \\
\leq \mathbb{E}_\sigma \left[ L \sup_{(t-t(0)) \in T} \sum_{i=1}^{n} \sigma_i \left( t_i - t_i^{(0)} \right) \right] \\
\leq L \mathbb{E}_\sigma \left[ \sup_{(t-t(0)) \in T} \left| \sum_{i=1}^{n} \sigma_i \left( t_i - t_i^{(0)} \right) \right| \right] 
$$

This completes the proof.

Now we apply Lemma B.2 to bound the empirical Rademacher complexity of an element-wise distance constrained function class. In the following lemma, all the notations are consistent with Theorem 3.1 unless stated otherwise.

**Lemma B.3.** Given a function class $F_{a,b} := \{ x \mapsto f(w, x) : w \in S_{a,b} \}$ and sample $S = \{ x_1, \ldots, x_n \}$ with $\| x_i \| = 1$ for all $i \in [n]$, then we have

$$
R_S(F_{a,b}) \leq \sqrt{\frac{\| a \|^2 + \| b \|^2}{n}} \| L \Psi \| (S_{a,b}) kr
$$

**Proof.** By definition,

$$
n R_S(F_{a,b}) = \mathbb{E}_\sigma \left[ \sup_{w \in S_{a,b}} \sum_{i=1}^{n} \sigma_i f(w, x_i) \right] \\
= \mathbb{E}_\sigma \left[ \sup_{w \in S_{a,b}} \sum_{i=1}^{n} \sigma_i f(w, x_i) \right] - \mathbb{E}_\sigma \left[ \sum_{i=1}^{n} \sigma_i f(0, x_i) \right] \\
= \mathbb{E}_\sigma \left[ \sup_{w \in S_{a,b}} \sum_{i=1}^{n} \sigma_i (f(w, x_i) - f(0, x_i)) \right].
$$

Now we decompose the term $f(w, x_i) - f(0, x_i)$ as:

$$
f(w, x_i) - f(0, x_i) \\
= \Psi \left( x_i^\top \alpha_1, \ldots, x_i^\top \alpha_p, \beta_1, \ldots, \beta_q \right) - \Psi \left( 0, \ldots, 0, 0, \ldots, 0 \right) \\
= \left( \Psi \left( x_i^\top \alpha_1, \ldots, x_i^\top \alpha_p, \beta_1, \ldots, \beta_q \right) - \Psi \left( 0, \ldots, 0, 0, \ldots, 0 \right) \right) + \cdots + \left( \Psi \left( 0, \ldots, 0, 0, \ldots, 0, \beta_q \right) - \Psi \left( 0, \ldots, 0, 0, \ldots, 0 \right) \right).
$$
Then by the above decomposition and Lemma B.2, we have

\[
E_{\sigma} \left[ \sup_{w \in S_{a,b}} \sum_{i=1}^{n} \sigma_i (f(w, x_i) - f(0, x_i)) \right] 
\leq L^{(1)}_\Psi (S_{a,b}) E_{\sigma} \left[ \sup_{w \in S_{a,b}} \sum_{i=1}^{n} \sigma_i x_i^\top \alpha_1 \right] + \cdots + L^{(p+q)}_\Psi (S_{a,b}) E_{\sigma} \left[ \sup_{w \in S_{a,b}} \sum_{i=1}^{n} \sigma_i \beta_q \right].
\]

Notice that

\[
E_{\sigma} \left[ \sup_{w \in S_{a,b}} \sum_{i=1}^{n} \sigma_i x_i^\top \alpha_1 \right] = E_{\sigma} \left[ \sup_{\|\alpha_1\| \leq a_1} \sum_{i=1}^{n} \sigma_i x_i \right] 
\leq a_1 E_{\sigma} \left[ \sum_{i=1}^{n} \sigma_i x_i \right] 
\leq a_1 \sqrt{n}.
\]

And

\[
E_{\sigma} \left[ \sup_{w \in S_{a,b}} \sum_{i=1}^{n} \sigma_i \beta_q \right] = E_{\sigma} \left[ \sup_{|\beta_q| \leq b_q} \sum_{i=1}^{n} \sigma_i \beta_q \right] 
\leq b_q E_{\sigma} \left[ \sum_{i=1}^{n} \sigma_i \right] 
\leq b_q \sqrt{n}.
\]

Therefore, by the Cauchy-Schwarz inequality, we can get

\[
E_{\sigma} \left[ \sup_{w \in S_{a,b}} \sum_{i=1}^{n} \sigma_i (f(w, x_i) - f(0, x_i)) \right] \leq L^{(1)}_\Psi (S_{a,b}) a_1 \sqrt{n} + \cdots + L^{(p+q)}_\Psi (S_{a,b}) b_q \sqrt{n} 
\leq \sqrt{n} \left( \|a\|^2 + \|b\|^2 \right) \|L_\Psi (S_{a,b})\|.
\]

Finally, we have

\[
R_S(\mathcal{F}_{a,b}) \leq \sqrt{\frac{\|a\|^2 + \|b\|^2}{n}} \|L_\Psi (S_{a,b})\|.
\]
Lemma B.3 gives an upper bound of the Rademacher complexity based on the element-wise distance. Notice that \( \|w(\infty)\| \leq \|w(0)\| + \text{len}(w(0), \infty) \). To obtain a length-based generalization bound, we consider to use \( S_{a,b} \) to cover the length-constrained space \( \{w : \|w\| \leq R\} \), and then taking a union bound. For the \( \ell_2 \) ball covering number, we use the following result from [Neyshabur et al., 2019, Lemma 11].

**Lemma B.4.** Given any \( \epsilon, D, \beta > 0 \), consider the set \( S_{D}^{\beta} = \{ x \in \mathbb{R}^{D} : \|x\| \leq \beta \} \). Then there exist \( N \) sets \( \{T_{i}\}_{i=1}^{N} \) of the form \( \{ x \in \mathbb{R}^{D} : |x_j| \leq \alpha_i^j, \forall j \in [D]\} \) such that \( S_{D}^{\beta} \subseteq \bigcup_{i=1}^{N} T_{i} \) and \( \|\alpha^i\| \leq \beta(1 + \epsilon), \forall i \in [N] \) where \( N = \left( \frac{K+D-1}{D-1} \right) \) and \( K = \left\lceil \frac{D}{(1+\epsilon)^2} \right\rceil \).

**Lemma B.5.** For any two positive integers \( n, k \) with \( n \geq k \), we have

\[
\binom{n}{k} \leq \left( \frac{en}{k} \right)^k.
\]

**Proof.** Note that

\[
\binom{n}{k} = \frac{n!}{k!(n-k)!} \leq \frac{n^k}{k^k} \leq e^k \left( \frac{n}{k} \right)^k.
\]

The last step is by

\[
e^k = \sum_{i=0}^{\infty} \frac{k^i}{i!} \geq \frac{k^k}{k!}.
\]

Now combining Lemma B.1, B.3, B.4 and B.5, we are ready to prove Theorem 3.1.

**Proof of Theorem 3.1.** First we apply Lemma B.4 with \( \epsilon = \sqrt{2} - 1 \), \( D = p+q \), and \( \beta = M_\delta + R_{n,\delta} \), then there exist \( N \) sets \( S_{a^k,b^k} \) such that \( S_{D}^{\beta} \subseteq \bigcup_{k=1}^{N} S_{a^k,b^k} \) and \( \sqrt{\|a^k\|^2 + \|b^k\|^2} \leq \sqrt{2}\beta \), with \( N = \left( \frac{2^{D-1}}{D-1} \right) \).

Therefore, for each parameter space \( S_{a^k,b^k} \), by Lemma B.3 we have

\[
\mathcal{R}_s(F_{a^k,b^k}) \leq \sqrt{\frac{2}{n}} \beta \|L\psi(S_{a^k,b^k})\|.
\]

Notice that the local Lipschitz constant of \( \ell \) in \( S_{a^k,b^k} \) is \( L_\ell(S_{a^k,b^k}) \). Hence, by Lemma B.1 and the Ledoux-Talagrand contraction inequality, for any \( \delta > 0 \), with probability at least \( 1 - \delta/N \) over the training sample, the following holds for all \( w \in S_{a^k,b^k}: \)

\[
\mathcal{L}_D(w) \leq \mathcal{L}_n(w) + \frac{2\sqrt{2}\beta L_\ell(S_{a^k,b^k}) \|L\psi(S_{a^k,b^k})\|}{\sqrt{n}} + 3M_\beta \sqrt{\frac{\log(2N/\delta)}{2n}},
\]

30
where \( M_\beta = \sup_{a^k, b^k} \|a_k\|^2 + \|b_k\|^2 \leq 2\beta^2 \sup_{w \in S_{a^k, b^k}} \|x\| \leq 1, |y| \leq 1 \ell (f(w, x), y) \).

Since \( w^{(\infty)} \in S^D_\beta \subseteq \bigcup_{k=1}^N S_{a^k, b^k} \), by taking the union bound over all sets \( S_{a^k, b^k} \), we can get with probability at least \( 1 - \delta \) over the initialization \( I \) the training sample,

\[
L_D(w^{(\infty)}) \leq L_n(w^{(\infty)}) + \sup_{\|a\|^2 + \|b\|^2 \leq 2\beta^2} \frac{2\sqrt{2}\beta L_n(S_{a, b}) \| L_\psi(S_{a, b}) \|}{\sqrt{n}} + 3M_{a, b} \sqrt{\frac{\log(2N/\delta)}{2n}}.
\]

Theorem 3.4 already showed that \( L_n(w^{(\infty)}) = \min_w L_n(w) \). Thus it remains to bound the term \( \log N \). For \( D = 1, N = 1 \). For \( D \geq 2 \), by Lemma B.5,

\[
\log N \leq (D - 1) \log \left( \frac{e(2D - 1)}{D - 1} \right) < 2.1(D - 1) < 3D = 3(p + q).
\]

Finally, let \( R = \sqrt{2} \beta \), we complete the proof of Theorem 3.1.

\[\square\]

C Proof of Theorem 3.4

In this section we will prove Theorem 3.4, our proof is based on the next lemma, showing that the gradient flow trajectory is always inside \( S_n \).

**Lemma C.1.** For any initialization \( w^{(0)} \), if \( L_n(w) \) satisfies Uniform-LGI on a closed set \( S_n \supseteq B \left( w^{(0)}, r_n(w^{(0)}) \right) \) with constants \( c_n, \theta_n \), where \( r_n(w^{(0)}) = \frac{(L_n(w^{(0)}) - \min_w L_n(w))^{1 - \theta_n}}{c_n(1 - \theta_n)} \), then

\[ w(t) \in S_n, \ \forall t \in [0, \infty). \]

**Proof.** Let

\[ T = \inf \{ t \geq 0, w(t) \notin S_n \}, \]

then it is sufficient to prove that \( T = \infty \). Otherwise, if \( T < \infty \), then by the continuity of the curve \( \{w(t)\}_{t \geq 0} \), we know that \( w(T) \) is in the boundary of \( S_n \), therefore

\[ \text{len}(w^{(0)}, T) \geq d(w^{(0)}, \partial S_n) \geq r_n(w^{(0)}). \] (14)

Now we consider the following two cases.

**Case (i).** \( L_n(w(T)) = \min_w L_n(w) \). Since \( L_n(w(t)) \) is non-increasing, we have \( L_n(w(t)) \) = \( \min_w L_n(w) \) and \( w(t) = w(T) \) for \( t \geq T \). Notice that \( S_n \) is a closed set, thus \( w(t) \in S_n \) for \( t \in [0, T] \), meaning that \( T = \infty \), which contradicts with \( T < \infty \).
Case (ii). $L_n(w^{(T)}) > \min_w L_n(w)$. By chain rule, we have for all $t \in [0, T],$

$$\frac{dL_n(w(t))}{dt} = \left\langle \nabla L_n(w(t)), \frac{dw(t)}{dt} \right\rangle$$

$$= - \left\| \nabla L_n(w(t)) \right\| \frac{dw(t)}{dt}$$

$$\leq -c_n \left( L_n(w(t)) - \min_w L(w) \right) \theta_n \frac{dw(t)}{dt}.$$

Then we can bound the trajectory length $\text{len}(w(0), T)$ as

$$\text{len}(w(0), T) = \int_0^T \left\| \frac{dw(t)}{dt} \right\| dt$$

$$\leq \int_0^T -\frac{1}{c_n} \left( L_n(w(t)) - \min_w L(w) \right)^{-\theta_n} dL_n(w(t))$$

$$= \frac{1}{c_n(1 - \theta_n)} \left[ \left( L_n(w(0)) - \min_w L(w) \right)^{1-\theta_n} - \left( L_n(w(T)) - \min_w L(w) \right)^{1-\theta_n} \right]$$

$$< r_n(w(0)),$$

which contradicts with (14).

Now we begin to prove Theorem 3.4.

**Proof.** By Lemma C.1, we know that $L_n(w(t))$ satisfies Uniform-LGI for all $t \in [0, \infty)$. Then by the proof of Lemma C.1, we have $\forall t \in [0, \infty)$,

$$\text{len}(w(0), t) \leq \frac{1}{c_n(1 - \theta_n)} \left[ \left( L_n(w(0)) - \min_w L(w) \right)^{1-\theta_n} - \left( L_n(w(t)) - \min_w L(w) \right)^{1-\theta_n} \right].$$

(16)

For the convergence rate, note that

$$\frac{d \left( L_n(w(t)) - \min_w L(w) \right)}{dt} = \left\langle \nabla L_n(w(t)), \frac{dw(t)}{dt} \right\rangle$$

$$= - \left\| \nabla L_n(w(t)) \right\|^2$$

$$\leq -c_n^2 \left( L_n(w(t)) - \min_w L(w) \right)^{2\theta_n}.$$

(17)

Therefore

$$\left( L_n(w(t)) - \min_w L(w) \right)^{-2\theta_n} d \left( L_n(w(t)) - \min_w L(w) \right) \leq -c_n^2 dt.$$

Integrating on both sides of the equation, we can get $\forall t \in [0, \infty),

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when $\theta_n = \frac{1}{2}$,

$$
\mathcal{L}_n(w^{(t)}) - \min_w \mathcal{L}_n(w) \leq e^{-c_n^2 t} \left( \mathcal{L}_n(w^{(0)}) - \min_w \mathcal{L}_n(w) \right);
$$

(18)

when $\frac{1}{2} < \theta_n < 1$,

$$
\mathcal{L}_n(w^{(t)}) - \min_w \mathcal{L}_n(w) \leq (1 + M t)^{-1/(2\theta_n - 1)} \left( \mathcal{L}_n(w^{(0)}) - \min_w \mathcal{L}_n(w) \right),
$$

(19)

where $M = c_n^2 (2\theta_n - 1) \left( \mathcal{L}_n(w^{(0)}) - \min_w \mathcal{L}_n(w) \right)^{2\theta_n - 1}$.

Taking the limit on both sides of (18) and (19), since $w(\infty)$ is the limit of $w^{(t)}$, we have

$$
\mathcal{L}_n(w^{(\infty)}) = \min_w \mathcal{L}_n(w).
$$

Hence $w^{(\infty)}$ is a global minimum. Taking the limit on both sides of (16), we get

$$
\text{len}(w^{(0)}, \infty) \leq r_n(w^{(0)}).
$$

This completes the proof.

\[\square\]

C.1 Additional of results for the generalization during training the model

Theorem 3.1 gives a length-based generalization bound for the final model. In this subsection, we apply our framework to derive generalization estimates that evolves according to the length of time (number of epochs) of training by combining the length estimate obtained in Theorem 3.4.

The approach is to give a generalization bound for early stopping when the loss value first reaches $\varepsilon \geq 0$. The idea is that, when there exists $T > 0$ such that $\mathcal{L}_n(w^T) = \varepsilon$, then by the inequality (15) in the proof of Lemma C.1, we can get an upper bound for the length $\text{len}(w^{(0)}, T)$ in terms of $\mathcal{L}_n(w^{(0)}), \min_w \mathcal{L}(w), \varepsilon, c_n, \theta_n$. Finally, we can get a generalization bound by our new length estimate.

To get a clean expression for the generalization bound, we assume the optimal value of the empirical loss function $\mathcal{L}_n(w)$ is zero. Then the rigorous statement is stated as follows:

**Corollary C.2.** Consider a training criterion of early stopping that the training is stopped once the empirical loss value first reaches $\varepsilon \geq 0$. Then for any given $\varepsilon \geq 0$, under the notations and conditions in Theorem 3.4, suppose that for any $\delta \in (0, 1)$, there exists $r_{n, \delta}$ such that $r_n(w^{(0)}) \leq r_{n, \delta}$ with probability at least $1 - \delta$ over the initialization and the training samples.

Then, we have with probability at least $1 - \delta$ over initialization and the training samples, the
generalization error for the stopping parameter $w$ is given by:

$$L_D(w) \leq \varepsilon + \sup_{\|a\|^2 + \|b\|^2 \leq r_{\varepsilon,n,\delta}} \frac{2r_{\varepsilon,n,\delta}L_\delta(S_{a,b}) \|L_\Psi(S_{a,b})\|}{\sqrt{n}} + 3M_{a,b} \sqrt{\frac{3(p + q + \log(2/\delta))}{2n}}, \quad (20)$$

where $r_{\varepsilon,n,\delta} = \sqrt{2(M_{\delta} + r_{n,\delta} - \frac{\varepsilon^{1-\theta n}}{c_n(1-\theta n)})}$.

**Remark C.3.** Corollary C.2 shows a trade-off between $\varepsilon$ and the term $r_{\varepsilon,n,\delta}$. The case for $\varepsilon = 0$ corresponds to the combining results of Theorem 3.1 and Theorem 3.4.

**Proof.** The proof is straightforward. Notice that by the inequality (15), we can bound the length $\text{len}(w(0), w)$ as

$$\text{len}(w(0), w) \leq r_n(w(0)) - \frac{\varepsilon^{1-\theta n}}{c_n(1-\theta_n)},$$

where $r_n(w(0))$ is specified in equation (6). Then by the same argument in the proof of Theorem 3.1, we may directly replace $r_n(w(0))$ with $r_n(w(0)) - \frac{\varepsilon^{1-\theta n}}{c_n(1-\theta_n)}$ to get the desired bound. \qed

### D Proofs for Section 4

In this section, our goal is to prove all the theorems in Section 4. A crucial part of the proofs is the spectral analysis of the random matrix $X$. Therefore, we start with introducing the non-asymptotic results of $\lambda_{\max}(XX^\top)$ and $\lambda_{\min}(XX^\top)$ from [Rudelson and Vershynin, 2010].

The first result is from [Rudelson and Vershynin, 2010, Proposition 2.4], characterizing the non-asymptotic behavior of the largest singular value of subgaussian matrices.

**Lemma D.1.** Let $A$ be an $N \times n$ random matrix whose entries are independent mean zero subgaussian random variables whose subgaussian moments are bounded by 1. Then for every $t \geq 0$, with probability at least $1 - 2e^{-ct^2}$ over the randomness of the entries,

$$\sqrt{\lambda_{\max}(AA^\top)} \leq C(\sqrt{N} + \sqrt{n}) + t,$$

where $c$ and $C$ are two positive constants that depend only on the subgaussian moment of the entries.

The second result is from [Rudelson and Vershynin, 2009, Theorem 1.1], characterizing the non-asymptotic behavior of the smallest singular value of subgaussian matrices.

**Lemma D.2.** Let $A$ be an $N \times n$ random matrix whose entries are independent and identically distributed subgaussian random variables with zero mean and unit variance. If $N > n$, then for
every \( \varepsilon > 0 \), with probability at least \( 1 - (C_1\varepsilon)^{N-n+1} - c_1^N \) over the randomness of the entries,

\[
\sqrt{\lambda_{\min}(A^\top A)} \geq \varepsilon(\sqrt{N} - \sqrt{n-1}),
\]

where \( C_1 > 0 \) and \( c_1 \in (0, 1) \) depend only on the subgaussian moment of the entries.

**D.1 Proof of Theorem 4.2**

In this section, we will prove Theorem 4.2 based on the three steps in our framework. All the notations are consistent with Theorem 4.2 unless stated otherwise.

**Proof of Theorem 4.2** First, we prove the result for Step 1. For a vector \( a = (a_1, \ldots, a_n)^\top \in \mathbb{R}^n \), we use \( a^\odot m \) to denote the element-wise power, i.e., \( a^\odot m = (a_1^m, \ldots, a_n^m)^\top \). For the \( \ell_p \) linear regression loss function \( L_n(w) \), notice that

\[
\nabla L_n(w) = \frac{1}{n} \sum_{i=1}^n (w^\top x_i - y_i)^{p-1} x_i = \frac{1}{n} (X^\top (Xw - Y)^{\odot (p-1)}).
\]

Then since \( X \) has full row rank, we have \( \forall w \in \mathbb{R}^d, \)

\[
\|\nabla L_n(w)\| = \frac{1}{n} \|X^\top (Xw - Y)^{\odot (p-1)}\| \\
\geq \frac{\sqrt{\lambda_{\min}(XX^\top)}}{n} \| (Xw - Y)^{\odot (p-1)} \| \\
= \frac{\sqrt{\lambda_{\min}(XX^\top)}}{n} \|Xw - Y\|_{2p-2}^{p-1} \\
\geq \frac{\sqrt{\lambda_{\min}(XX^\top)}}{n} \|Xw - Y\|_p^{p-1} \cdot n^{1/p - 1/2} \\
= p^{1-1/p} \sqrt{\frac{\lambda_{\min}(XX^\top)}{n}} L_n(w)^{1-1/p}.
\]

Therefore,

\[
c_n = p^{1-1/p} \sqrt{\frac{\lambda_{\min}(XX^\top)}{n}}, \quad \theta_n = 1 - 1/p.
\]

For Step 2, note that \( \min_w L_n(w) = 0 \), then the result can be proved by directly plugging \( c_n \) and \( \theta_n \) into Theorem 3.4.

Next, we prove the result for Step 3. By Theorem 3.4 and the property of the target function,
we have for any \(w^{(0)}\) that satisfies \(\|w^{(0)}\|_2 \leq c_0\),

\[
\begin{align*}
    r_n(w^{(0)}) &= \frac{\sqrt{n} (p \mathcal{L}_n(w^{(0)}))^{1/p}}{\sqrt{\lambda_{\text{min}}(XX^\top)}} \\
    &= n^{1/2-1/p} \frac{\|Xw^{(0)} - Y\|_p}{\sqrt{\lambda_{\text{min}}(XX^\top)}} \\
    &\leq n^{1/2-1/p} \frac{\|Xw^{(0)} - Y\|_2}{\sqrt{\lambda_{\text{min}}(XX^\top)}} \\
    &\leq n^{1/2-1/p} \sqrt{\frac{\lambda_{\text{max}}(XX^\top)}{\lambda_{\text{min}}(XX^\top)}} (c_0 + c^*) .
\end{align*}
\]

Now we apply Lemma \textbf{D.1} with \(A = X\) and \(t = \sqrt{\frac{\log(4/\delta)}{c}}\), then we have with probability at least \(1 - \delta/2\) over the samples,

\[
\sqrt{\lambda_{\text{max}}(XX^\top)} \leq C(\sqrt{n} + \sqrt{d}) + \sqrt{\frac{\log(4/\delta)}{c}},
\]

where \(c\) and \(C\) are two positive constants that depend only on the subgaussian moment of the entries.

Similarly, let \(\tau = c_1 \in (0,1), \varepsilon = \tau/C_1 > 0\), then Lemma \textbf{D.2} implies that with probability at least \(1 - \tau^{d-n+1} - \tau^d\) over the samples,

\[
\sqrt{\lambda_{\text{min}}(XX^\top)} \geq \frac{\tau}{C_1} (\sqrt{d} - \sqrt{n-1}),
\]

where \(C_1 > 0\) and \(\tau \in (0,1)\) depend only on the subgaussian moment of the entries.

Taking the union bound, we have with probability at least \(1 - \delta/2 - \tau^{d-n+1} - \tau^d\) over the initialization and the training samples,

\[
\begin{align*}
    \frac{r_n(w^{(0)})}{\sqrt{n}} &\leq n^{-1/p} (c_0 + c^*) \frac{C(\sqrt{n} + \sqrt{d}) + \sqrt{\frac{\log(4/\delta)}{c}}}{\tau/C_1 (\sqrt{d} - \sqrt{n-1})} \\
    &\leq n^{-1/p} (c_0 + c^*) \frac{C(\sqrt{n} + \sqrt{d}) + \sqrt{\frac{\log(4/\delta)}{cd}}}{\tau/C_1 (1 - \sqrt{\frac{n-1}{d}})} \\
    &\leq n^{-1/p} (c_0 + c^*) \frac{CC_1(\sqrt{n_1} + 1)}{\tau (1 - \sqrt{n_1})} + C_1 \frac{\gamma_1 \log(4/\delta)}{cn} \\
    &\leq O \left( n^{-1/p} + n^{-1/p} \sqrt{\frac{\log(1/\delta)}{n}} \right).
\end{align*}
\]

Recall for the linear regression model \(\textbf{[7]}\), \(f(w, x) = w^\top x\). Thus \(\Psi(x) = x\) is an identity function.
with \( p = 1, q = 0 \), and \( \| L_\Psi(S_{a,b}) \| = 1 \) for any \( a, b \). Since the loss function \( \tilde{\ell} \) is bounded by 1 and 1-Lipschitz, we know that \( L_\ell(S_{a,b}) = M_R = 1 \) for any \( a \) and \( b \). Finally by Theorem 3.1 and \( \tilde{\ell}(y, y) = 0 \), we have with probability at least \( 1 - \delta/2 \) over the samples,

\[
\mathbb{E}_{(x,y) \sim D} \left[ \tilde{\ell} \left( f(w^{(\infty)}, x), y \right) \right] \leq \frac{2\sqrt{2}(r_n(w^{(0)}) + c_0)}{\sqrt{n}} + 3\sqrt{\frac{3 + \log(4/\delta)}{2n}}.
\]

Combining the inequality (23), we have with probability at least \( 1 - \delta - \tau d/n + 1 - \tau d \) over training samples,

\[
\mathbb{E}_{(x,y) \sim D} \left[ \tilde{\ell} \left( f(w^{(\infty)}, x), y \right) \right] \leq O \left( n^{-1/p} \right) + O \left( \sqrt{\frac{\log(1/\delta)}{n}} \right).
\]

This completes the proof of Theorem 4.2.

D.2 Proof of Theorem 4.4

In this section, we will prove Theorem 4.4. First, we present some useful lemmas for proving our results, and then we give the proofs of Theorem 4.4 for the RBF kernel and the inner product kernel separately.

For the RBF kernel \( k(x, y) = \varrho(\|y - x\|) \), the following two lemmas give non-asymptotic bounds for \( \lambda_{\text{max}}(k(\mathcal{X}, \mathcal{X})) \) and \( \lambda_{\text{min}}(k(\mathcal{X}, \mathcal{X})) \) based on the separation distance \( \text{SD} \) of \( \mathcal{X} \).

The first lemma is from [Diederichs and Iske, 2019, Lemma 3.1], providing an upper bound for \( \lambda_{\text{max}}(k(\mathcal{X}, \mathcal{X})) \).

**Lemma D.3.** For the RBF kernel, if \( \varrho : \mathbb{R} \geq 0 \to \mathbb{R} \geq 0 \) is a decreasing function, then

\[
\lambda_{\text{max}}(k(\mathcal{X}, \mathcal{X})) \leq \varrho(0) + 3d \sum_{t=1}^{\infty} \left( t + 2 \right)^{d-1} \varrho(t \cdot \text{SD}),
\]

and the sum of the infinite series in equation (24) is finite if and only if \( \varrho(\|x\|) \in L^1(\mathbb{R}^d) \).

The next lemma is adapted from [Wendland, 2004, Theorem 12.3], giving a lower bound for \( \lambda_{\text{min}}(k(\mathcal{X}, \mathcal{X})) \).

**Lemma D.4.** Suppose that \( k \) is a positive-definite RBF kernel. If \( \varrho(\|x\|) \in L^1(\mathbb{R}^d) \), one can define the Fourier transform of \( \varrho \) as \( \hat{\varrho}(\omega) := (2\pi)^{-d/2} \int_{\mathbb{R}^d} \varrho(\omega)e^{-ix^\top \omega}d\omega \). With a decreasing function \( \varrho_0(M) \) and two constants \( M_d, C_d \) defined as

\[
\varrho_0(M) := \inf_{\|x\| \leq 2M} \hat{\varrho}(x), \quad M_d = 6.38d, \quad C_d = \frac{1}{2\Gamma(d/2 + 1)} \left( \frac{M_d}{2^{3/2}} \right)^d,
\]

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where $\Gamma$ is the gamma function. Then a lower bound on $\lambda_{\text{min}}(k(\mathcal{X}, \mathcal{X}))$ is given by

$$\lambda_{\text{min}}(k(\mathcal{X}, \mathcal{X})) \geq C_d \cdot \varrho_0 (M_d/SD) \cdot SD^{-d}.$$ 

For the inner product kernel $k(x, y) = \varrho \left( \frac{x^\top y}{d} \right)$, it is shown in [El Karoui et al., 2010] that the kernel matrix $k(\mathcal{X}, \mathcal{X})$ can be approximated by the linear combination of all-ones matrix $11^\top$, sample covariance matrix $\mathcal{X}\mathcal{X}^\top$ and identity matrix. To obtain non-asymptotic results on the spectra of the kernel matrix $k(\mathcal{X}, \mathcal{X})$, we borrow the technique from [Liang and Rakhlin, 2020, Proposition A.2], and show the result for subgaussian entries in the next lemma.

**Lemma D.5.** For the inner product kernel, suppose that the entries of $\mathcal{X}$ are i.i.d. subgaussian random variables with zero mean and unit variance, then with probability at least $1 - \delta - d^{-2}$ over the entries,

$$\left\| k(\mathcal{X}, \mathcal{X}) - k^{\text{lin}}(\mathcal{X}, \mathcal{X}) \right\| \leq d^{-1/2} \left( \delta^{-1/2} + \log^{0.51} d \right),$$

where $k^{\text{lin}}(\mathcal{X}, \mathcal{X})$ is defined as

$$k^{\text{lin}}(\mathcal{X}, \mathcal{X}) := \left( \varrho(0) + \frac{\varrho''(0)}{d} \right) 11^\top + \frac{\varrho'(0)}{d} \mathcal{X}\mathcal{X}^\top + \left( \varrho(1) - \varrho(0) - \varrho'(0) \right) I_{n \times n}.$$

**Proof.** Note that the sample covariance matrix $\Sigma_d = I_{d \times d}$, then by applying [Liang and Rakhlin, 2020 Proposition A.2] with subgaussian random entries we can prove this lemma.

**Lemma D.6.** Suppose that $A, B \in \mathbb{R}^{n \times n}$ are two symmetric matrices, then we have

$$\lambda_{\text{min}}(A + B) \geq \lambda_{\text{min}}(A) + \lambda_{\text{min}}(B).$$

**Proof.** Note that for any $x \in \mathbb{R}^n$ with $\|x\| = 1$,

$$x^\top (A + B)x = x^\top Ax + x^\top Bx \geq \lambda_{\text{min}}(A) + \lambda_{\text{min}}(B).$$

By definition, we have

$$\lambda_{\text{min}}(A + B) = \inf_{\|x\| = 1} x^\top (A + B)x \geq \lambda_{\text{min}}(A) + \lambda_{\text{min}}(B),$$

which completes the proof. 

Now we are ready to prove Theorem 4.4.
Proof of Theorem 4.4. For Step 1. Notice that \( \forall w \in \mathbb{R}^s \),

\[
\| \nabla \mathcal{L}_n(w) \| = \frac{1}{n} \left\| \varphi(X)^\top (\varphi(X)w - \mathcal{Y})^{p-1} \right\|
\geq \frac{\sqrt{\lambda_{\min}(\varphi(X)^\top \varphi(X))}}{n} \left\| (\varphi(X)w - \mathcal{Y})^{p-1} \right\|
= \frac{\sqrt{\lambda_{\min}(k(X,X))}}{n} \| \varphi(X)w - \mathcal{Y} \|_{2p-2}^{p-1}
\geq \frac{\sqrt{\lambda_{\min}(k(X,X))}}{n} \| \varphi(X)w - \mathcal{Y} \|_{p}^{p-1} \cdot n^{1/p-1/2}
= p^{1-1/p} \sqrt{\frac{\lambda_{\min}(k(X,X))}{n}} \mathcal{L}_n(w)^{1-1/p}.
\]

Therefore, \( \mathcal{L}_n(w) \) satisfies the Uniform-LGI globally on \( \mathbb{R}^s \) with

\[
c_n = p^{1-1/p} \sqrt{\frac{\lambda_{\min}(k(X,X))}{n}}, \quad \theta_n = 1 - 1/p.
\]

For Step 2. Since \( k \) is a positive-definite kernel, and \( \theta_n = 1 - 1/p \), then \( \min_w \mathcal{L}_n(w) = 0 \), thus by Theorem 3.4 we can directly get the result.

The proof of Step 3 is two-sided. First, since \( \forall x \in \mathcal{X}, \| \varphi(x) \| = \sqrt{k(x,x)} \leq 1 \), then the kernel regression model (9) can be viewed as \( \ell_p \) linear regression on inputs \( \varphi(X) \). Hence, \( \Psi \) is an identity function with \( p = 1, q = 0 \), and \( \| L_{\Psi}(S_{a,b}) \| = L_{\ell}(S_{a,b}) = M_R = 1 \) for any \( a, b \). This means that we only need to bound the term \( r_n(w^{(0)})/\sqrt{n} \).

By Theorem 3.4 and the property of the target function, for any \( w^{(0)} \) that satisfies \( \| w^{(0)} \|_2 \leq c_0 \), we have

\[
r_n(w^{(0)}) = \sqrt{n} \left( p \mathcal{L}_n(w^{(0)}) \right)^{1/p} \sqrt{\lambda_{\min}(k(X,X))}
= n^{1/2-1/p} \left( \frac{\| \varphi(X)w^{(0)} - \mathcal{Y} \|_p}{\sqrt{\lambda_{\min}(k(X,X))}} \right)
\leq n^{1/2-1/p} \left( \frac{\| \varphi(X)w^{(0)} - \mathcal{Y} \|_2}{\sqrt{\lambda_{\min}(k(X,X))}} \right)
\leq n^{1/2-1/p} \left( \frac{\| \varphi(X)w^{(0)} \| + \| \mathcal{Y} \|}{\sqrt{\lambda_{\min}(k(X,X))}} \right)
\leq n^{1/2-1/p} \sqrt{\frac{\lambda_{\max}(k(X,X))}{\lambda_{\min}(k(X,X))}} (c_0 + c^*).
\]

Then for the RBF kernel, Lemma D.3 and Lemma D.4 indicate that there exists a positive constant \( C(\varrho, d, q_{\min}, q_{\max}) \) that only depends on \( \varrho, d, q_{\min}, q_{\max} \) such that

\[
\frac{\lambda_{\max}(k(X,X))}{\lambda_{\min}(k(X,X))} \leq C(\varrho, d, q_{\min}, q_{\max}), \quad \forall n \geq 1,
\]

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which implies that for all initialization \( w^{(0)} \),

\[
\frac{r_n(w^{(0)})}{\sqrt{n}} \leq O \left( n^{-1/p} \right).
\]  

(26)

Therefore, by Theorem 3.1 and Lemma 3.1 we have with probability at least \( 1 - \delta \) over training samples,

\[
\mathbb{E}_{(x,y) \sim D} \left[ \tilde{\ell} \left( f(w^{(\infty)}, x), y \right) \right] \leq O \left( n^{-1/p} \right) + O \left( \sqrt{\frac{\log(1/\delta)}{n}} \right),
\]

which completes the proof for the RBF kernel.

For the inner product kernel, to obtain an upper bound for \( \lambda_{\text{max}}(k(\mathcal{X}, \mathcal{X})) \), first notice that

\[
\lambda_{\text{max}}(k(\mathcal{X}, \mathcal{X})) = \| k(\mathcal{X}, \mathcal{X}) \| \leq \| k^{\text{lin}}(\mathcal{X}, \mathcal{X}) \| + \| k(\mathcal{X}, \mathcal{X}) - k^{\text{lin}}(\mathcal{X}, \mathcal{X}) \|.  
\]  

(27)

By Lemma D.6 we can get

\[
\lambda_{\text{min}}(k(\mathcal{X}, \mathcal{X})) \geq \lambda_{\text{min}}(k^{\text{lin}}(\mathcal{X}, \mathcal{X})) + \lambda_{\text{min}}(k(\mathcal{X}, \mathcal{X}) - k^{\text{lin}}(\mathcal{X}, \mathcal{X})) 
\]

\[
\geq \lambda_{\text{min}}(k^{\text{lin}}(\mathcal{X}, \mathcal{X})) - \| k(\mathcal{X}, \mathcal{X}) - k^{\text{lin}}(\mathcal{X}, \mathcal{X}) \|.  
\]  

(28)

Under Assumption 4.3 Lemma D.5 implies that

\[
\left\| k^{\text{lin}}(\mathcal{X}, \mathcal{X}) \right\| \leq \frac{\varrho''(0)}{d} \left\| 11^T \right\| + \frac{\varrho'(0)}{d} \left\| \mathcal{X} \mathcal{X}^T \right\| + \left( \varrho(1) - \varrho'(0) \right)
\]

\[
\leq \frac{n \varrho''(0)}{d} + \varrho'(0) \lambda_{\text{max}}(\mathcal{X} \mathcal{X}^T) + \left( \varrho(1) - \varrho'(0) \right)
\]

\[
\leq \gamma_1 \varrho''(0) + \varrho'(0) \lambda_{\text{max}}(\mathcal{X} \mathcal{X}^T) + \left( \varrho(1) - \varrho'(0) \right),
\]

and

\[
\lambda_{\text{min}}(k^{\text{lin}}(\mathcal{X}, \mathcal{X})) \geq \varrho(1) - \varrho'(0) > 0.
\]

Thus, by equation (28) we have

\[
\lambda_{\text{min}}(k(\mathcal{X}, \mathcal{X})) \geq \left( \varrho(1) - \varrho'(0) \right) - \left\| k(\mathcal{X}, \mathcal{X}) - k^{\text{lin}}(\mathcal{X}, \mathcal{X}) \right\|.  
\]  

(29)

Under Assumption 4.1 by equation (21), we have with probability at least \( 1 - \delta/3 \) over the
\[
\frac{\lambda_{\text{max}}(XX^\top)}{d} \leq \left(C \sqrt{\frac{n}{d}} + 1 + \sqrt{\frac{\log(6/\delta)}{cd}}\right)^2 \leq \left(C(\sqrt{\gamma_1} + 1) + \sqrt{\frac{\gamma_1 \log(6/\delta)}{cn}}\right)^2.
\]

Therefore, by equation (27), with probability at least \(1 - \delta/3\) over the samples,

\[
\lambda_{\text{max}}(k(X, X)) \leq \gamma_1 \varphi''(0) + \varphi'(0) \left(C(\sqrt{\gamma_1} + 1) + \sqrt{\frac{\gamma_1 \log(4/\delta)}{cn}}\right)^2 + N(1) + \|k(X, X) - k_{\text{lin}}(X, X)\|.
\]

By Lemma \ref{lemma:D.5} for large \(d\) and small \(\delta\) such that \(d^{-1/2} \left(\sqrt{3}d^{-1/2} + \log^{0.51} d\right) \leq 0.5(\varphi(1) - \varphi'(0))\), we have with probability at least \(1 - \delta/3 - d^{-2}\) over the entries,

\[
\|k(X, X) - k_{\text{lin}}(X, X)\| \leq 0.5(\varphi(1) - \varphi'(0)).
\]

Then equation (29) and (30) yields that with probability at least \(1 - 2\delta/3 - d^{-2}\) over the samples,

\[
\lambda_{\text{min}}(k(X, X)) \geq 0.5(\varphi(1) - \varphi'(0)),
\]

\[
\lambda_{\text{max}}(k(X, X)) \leq \gamma_1 \varphi''(0) + \varphi'(0) \left(C(\sqrt{\gamma_1} + 1) + \sqrt{\frac{\gamma_1 \log(4/\delta)}{cn}}\right)^2 + 1.5(\varphi(1) - \varphi'(0)).
\]

Hence, by equation (25), with probability at least \(1 - \delta - d^{-2}\) over the samples, we have

\[
\frac{r_n(w(0))}{\sqrt{n}} \leq O \left(n^{-1/p} + \sqrt{\frac{\log(1/\delta)}{n^{1/2 + 1/p}}}\right).
\]

Combining Theorem \ref{thm:3.1}, we get with probability at least \(1 - \delta - d^{-2}\) over the samples,

\[
\mathbb{E}_{(x, y) \sim D} \left[\hat{\ell} \left(f(w^{(\infty)}, x), y\right)\right] \leq O \left(n^{-1/p}\right) + O \left(\sqrt{\frac{\log(1/\delta)}{n}}\right),
\]

which completes the proof.

\begin{flushright}
\Box
\end{flushright}

**D.3 Proof of Theorem 4.5**

In this section, we will prove Theorem 4.5. We first introduce some important lemmas for proving our final results. Lemma \ref{lemma:D.7} shows that the smallest eigenvalue of the NTK matrix \(\Theta(t)\) has a lower bounded given the overparameterization, by which we can prove the optimization result. In
Lemma D.8, we show that the eigenvalues of the NTK matrix are related to the data covariance matrix. Then by combining Lemma D.11 and Lemma D.9 we can prove the generalization result.

**Lemma D.7.** For any \( \delta \in (0, 1) \), if \( m \geq \text{poly}(n, \lambda_{\min}(\hat{\Theta}), \delta^{-1}) \), then with probability at least \( 1 - \delta \) over the random initialization,

\[
\lambda_{\min}(\Theta(t)) \geq \frac{1}{2} \lambda_{\min}(\hat{\Theta}), \quad \forall t \geq 0.
\]

**Proof.** The proof is the same as the proof of [Du et al., 2019, Lemma 3.4]. \( \square \)

**Lemma D.8.**

\[
\lambda_{\min}(\hat{\Theta}) \geq \lambda_{\min}(XX^\top) / 4.
\]

**Proof.** Notice that for ReLU activation \( \phi \), a simple fact is that \( \phi'(ax) = \phi'(x) \) holds for any \( x \in \mathbb{R} \) given that \( a > 0 \). Therefore,

\[
\hat{\Theta}_{ij} = x_i^\top x_j \mathbb{E}_{w \sim \mathcal{N}(0, \frac{1}{d}I)} \left[ \phi'(w^\top x_i) \phi'(w^\top x_j) \right] \\
= x_i^\top x_j \mathbb{E}_{w \sim \mathcal{N}(0, \frac{1}{d}I)} \left[ \phi'(w^\top x_i) \phi'(w^\top x_j) \right] \\
= \frac{x_i^\top x_j (\pi - \arccos(x_i^\top x_j))}{2\pi} \\
= \frac{x_i^\top x_j}{4} + \frac{x_i^\top x_j}{2\pi} \arcsin(x_i^\top x_j) \\
= \frac{x_i^\top x_j}{4} + \frac{1}{2\pi} \sum_{k=0}^{\infty} \frac{(2k)!}{4^k (k!)^2 (2k+1)} (x_i^\top x_j)^{2k+2}.
\]

Then

\[
\hat{\Theta} = \frac{XX^\top}{4} + \frac{1}{2\pi} \sum_{k=0}^{\infty} \frac{(2k)!}{4^k (k!)^2 (2k+1)} (XX^\top)^{\circ(2k+2)} \\
= \frac{XX^\top}{4} + \frac{1}{2\pi} \sum_{k=0}^{\infty} \frac{(2k)!}{4^k (k!)^2 (2k+1)} ((XX^\top)^{\circ(2k+2)})^\top (XX^\top)^{\circ(2k+2)},
\]

where \( \circ \) is the element-wise product, and \( \circ \) is the Khatri-Rao product\(^8\).

Since \((XX^\top)^{\circ(2k+2)})^\top (XX^\top)^{\circ(2k+2)}\) is positive semidefinite, we have

\[
\lambda_{\min}(\hat{\Theta}) \geq \lambda_{\min}(XX^\top) / 4,
\]

which completes the proof.

\(^8\)For \( A = (a_1, \ldots, a_n) \in \mathbb{R}^{m \times n}, B = (b_1, \ldots, b_n) \in \mathbb{R}^{p \times n} \), then \( A \circ B = [a_1 \circ b_1, \ldots, a_n \circ b_n] \), where \( \circ \) is the Kronecker product.
In the next lemma, we adopt an inequality from [Montgomery-Smith, 1990].

**Lemma D.9.** If \( \{\sigma_i\}_{i=1}^n \) are i.i.d. drawn from \( U\{-1,1\} \), then for any \( x = (x_1, \ldots, x_n)^\top \in \mathbb{R}^n \), with probability at least \( 1 - \delta \) over \( \sigma \),
\[
\left| \sum_{i=1}^n \sigma_i x_i \right| \leq \sqrt{2 \log(2/\delta)} \|x\|.
\]

The following lemma gives a sharp bound for a Chi-square variable, which is from [Laurent and Massart, 2000, Lemma 1].

**Lemma D.10.** Let \((Y_1, \ldots, Y_D)\) be i.i.d. Gaussian variables, with mean 0 and variance 1. Then with probability at least \( 1 - \delta \) over \( Y \),
\[
\sum_{i=1}^D Y_i^2 \leq D + 2 \sqrt{D \log \left( \frac{1}{\delta} \right)} + 2 \log \left( \frac{1}{\delta} \right).
\]

The next lemma is quoted from [Arora et al., 2019, Lemma 5.4], giving an upper bound for the empirical Rademacher complexity if one has an accurate estimate for the distance with respect to each hidden unit.

**Lemma D.11.** Given \( R > 0 \), consider the following function class
\[
\mathcal{F} = \left\{ x \mapsto f(w, x) : \|W_{i,r} - W_{i,r}^{(0)}\| \leq R (\forall r \in [m]), \|W_1 - W_1^{(0)}\|_F \leq B \right\}
\]
with \( W_{1,r} \in \mathbb{R}^d \) the \( r \)-th row of \( W_1 \). Then for an i.i.d. sample \( S = \{x_1, \ldots, x_n\} \) and every \( B > 0 \), with probability at least \( 1 - \delta \) over the random initialization, the empirical Rademacher complexity is bounded as:
\[
\mathcal{R}_S(\mathcal{F}) \leq \frac{B}{\sqrt{2n}} \left( 1 + \left( \frac{2 \log(2/\delta)}{m} \right)^{1/4} \right) + 2R^2 \sqrt{md} + R \sqrt{2 \log(2/\delta)}.
\]

Now we are ready to prove Theorem 4.5.

**Proof of Theorem 4.5.** For Step 1. By Lemma D.7 if \( m \geq \text{poly} \left( n, \lambda_{\min}^{-1}(\hat{\Theta}), \delta^{-1} \right) \), then with
probability at least $1 - \delta$ over the random initialization,

\[
\| \nabla \mathcal{L}_n(w^{(t)}) \| = \frac{1}{n} \left\| \sum_{i=1}^{n} (f(w, x_i) - y_i) \nabla f(w^{(t)}, x_i) \right\|
\]

\[
= \frac{1}{n} \left\| \nabla f(w^{(t)}, \mathcal{X})^\top \left( f(w^{(t)}, \mathcal{X}) - \mathcal{Y} \right) \right\|
\]

\[
\geq \frac{2 \lambda_{\min}(\Theta(t))}{n} \sqrt{\mathcal{L}_n(w^{(t)})}
\]

\[
\geq \frac{\lambda_{\min}(\hat{\Theta})}{n} \sqrt{\mathcal{L}_n(w^{(t)})}
\]

holds for any $t \geq 0$, which means that $\mathcal{L}_n(w^{(t)})$ satisfies the Uniform-LGI for any $t \geq 0$ with

\[
c_n = \sqrt{\frac{\lambda_{\min}(\hat{\Theta})}{n}}, \quad \theta_n = 1/2.
\]

For Step 2. By equation (17), we can directly get $\mathcal{L}_n(w^{(t)})$ converges to zero with a linear convergence rate:

\[
\mathcal{L}_n(w^{(t)}) \leq \exp \left( -\lambda_{\min}(\hat{\Theta}) t/n \right) \mathcal{L}_n(w^{(0)}).
\]

For Step 3. By equation (16) and Lemma D.8, the length $\text{len}(w^{(0)}, \infty)$ can be bounded as

\[
\text{len}(w^{(0)}, \infty) \leq r_n(w^{(0)}) = 2 \sqrt{\frac{n\mathcal{L}_n(w^{(0)})}{\lambda_{\min}(\Theta)}} \leq 4 \sqrt{\frac{n\mathcal{L}_n(w^{(0)})}{\lambda_{\min}(\mathcal{X}\mathcal{X}^\top)}}.
\]

By the property of the target function, we have

\[
\sqrt{n\mathcal{L}_n(w^{(0)})} = \sqrt{\frac{1}{2} \sum_{i=1}^{n} \left( \frac{1}{\sqrt{m}} w_2^\top \phi(W_1^{(0)} x_i) - y_i \right)^2}
\]

\[
\leq \sum_{i=1}^{n} \left( \frac{1}{\sqrt{m}} w_2^\top \phi(W_1^{(0)} x_i) \right)^2 + y_i^2
\]

\[
\leq \sum_{i=1}^{n} \left( \frac{1}{\sqrt{m}} w_2^\top \phi(W_1^{(0)} x_i) \right)^2 + \sum_{i=1}^{n} y_i^2
\]

\[
\leq \frac{1}{m} \sum_{i=1}^{n} \left( w_2^\top \phi(W_1^{(0)} x_i) \right)^2 + c^* \sqrt{\lambda_{\max}(\mathcal{X}\mathcal{X}^\top)}.
\]

Since the entries of $w_2$ are drawn i.i.d. from $U\{-1,1\}$, then by Lemma D.9 for each $i \in [n]$,
with probability at least $1 - \delta/6n$ over $w_2$,

$$
\left( w_2^\top \phi(W_1^{(0)} x_i) \right)^2 \leq 2 \log \left( \frac{12n}{\delta} \right) \left\| \phi(W_1^{(0)} x_i) \right\|^2.
$$

Taking the union bound over all $i = 1, 2, \ldots, n$, we have with probability at least $1 - \delta$ over the random initialization,

$$
\sqrt{\frac{1}{m} \sum_{i=1}^n \left( w_2^\top \phi(W_1^{(0)} x_i) \right)^2} \leq \sqrt{\frac{2 \log(12n/\delta)}{m} \sum_{i=1}^n \left\| \phi(W_1^{(0)} x_i) \right\|^2}
= \sqrt{\frac{2 \log(12n/\delta)}{m} \left\| \phi \left( W_1^{(0)} X^\top \right) \right\|_F}
\leq \sqrt{\frac{2 \log(12n/\delta)}{m} \left\| W_1^{(0)} X^\top \right\|_F}
\leq \sqrt{\frac{2 \log(12n/\delta)}{m} \left\| W_1^{(0)} \right\|_F \| X \|}
= \sqrt{\frac{2 \log(12n/\delta)}{m} \left\| W_1^{(0)} \right\|_F \sqrt{\lambda_{\text{max}}(X X^\top)}}.
\quad (32)
$$

For the Gaussian random matrix $W_1^{(0)} \sim \mathcal{N}(0, \frac{1}{2} I_{m \times d})$, by Lemma D.10, we have with probability at least $1 - \delta/6$ over the random initialization,

$$
\left\| W_1^{(0)} \right\|_F^2 \leq 1 + 2 \sqrt{\frac{\log(6/\delta)}{md}} + \frac{2 \log(6/\delta)}{md}.
\quad (33)
$$

Taking the union bound of equations (21), (22), (32) and (33), if $m \geq \text{poly} \left(n, \lambda_{\text{min}}^{-1}(\hat{\Theta}), \delta^{-1}\right)$, with probability at least $1 - \tau^{d-n+1} - \tau^d - 5\delta/6$ over the samples and random initialization $I$,

$$
\sup_{w^{(0)} \in I, (x,y) \in D} r_n(w^{(0)}) \leq \sup_{w^{(0)} \in I, (x,y) \in D} \frac{\sqrt{n \mathcal{L}_n(w^{(0)})}}{\lambda_{\text{min}}(X X^\top)}
\leq O \left( \sqrt{\left( 1 + \sqrt{\frac{\log(1/\delta)}{md}} + \frac{\log(1/\delta)}{md} \right) \frac{\log(n/\delta)}{\sqrt{n} + \sqrt{d} + \sqrt{\log(1/\delta)}} \frac{\sqrt{n} + \sqrt{d} + \sqrt{\log(1/\delta)}}{\sqrt{d} - \sqrt{n} - 1} } \right)
\leq O \left( \frac{\sqrt{\log(n/\delta)}}{\sqrt{1 + \sqrt{\log(1/\delta)/n}}} \right)
\leq O \left( \sqrt{\log(n/\delta)} \right).
\quad (34)
$$

Therefore, with probability at least $1 - \tau^{d-n+1} - \tau^d - 5\delta/6$ over the samples and random initialization,

$$
\frac{r_n(w^{(0)})}{\sqrt{n}} \leq O \left( \sqrt{\frac{\log(n/\delta)}{n}} \right).
\quad (34)
$$
For the $r$-th row of $W_1^{(t)}$, we begin to bound the distance $\|W_1^{(t)} - W_1^{(0)}\|$ for each $r \in [m]$. Notice that
\[
\left\| \frac{dW_1^{(t)}}{dt} \right\| = \left\| \nabla_{W_1^{(t)}} L_n(w^{(t)}) \right\|
\leq \frac{1}{n \sqrt{m}} \sum_{i=1}^{n} \left| f(w^{(t)}, x_i) - y_i \right|
\leq \frac{1}{\sqrt{nm}} \left\| f(w^{(t)}, X) - Y \right\|
\leq \sqrt{\frac{2L_n(w^{(0)})}{m}} \exp \left(-\lambda_{\text{min}}(\hat{\Theta}) \frac{t}{2n}\right).
\]
Hence,
\[
\left\| W_1^{(t)} - W_1^{(0)} \right\| \leq \int_{0}^{t} \left\| \frac{dW_1^{(s)}}{ds} \right\| ds \leq \frac{2n}{\lambda_{\text{min}}(\hat{\Theta})} \sqrt{\frac{2L_n(w^{(0)})}{m}} = \sqrt{\frac{2n}{m\lambda_{\text{min}}(\hat{\Theta})}} r_n(w^{(0)}).
\]
Now we apply Lemma D.11 with $B = r_n(w^{(0)})$, $R = \sup_{w^{(0)} \in \mathcal{I}, (x,y) \in \mathcal{D}} \sqrt{\frac{2n}{m\lambda_{\text{min}}(\hat{\Theta})}} r_n(w^{(0)})$, we get with probability at least $1 - \delta/12$ over the random initializaiton,
\[
\mathcal{R}_S(\mathcal{F}) \leq \frac{B}{\sqrt{2n}} \left( 1 + \left( \frac{2\log(24/\delta)}{m} \right)^{1/4} \right) + 2R^2 \sqrt{md} + R \sqrt{2 \log(24/\delta)}.
\]
Then by equation (34), if $m \geq \text{poly} \left(n, \lambda_{\text{min}}^{-1}(\hat{\Theta}), \delta^{-1}\right)$, then with probability at least $1 - \tau^{d-n+1} - \tau^d - 11\delta/12$ over the samples and random initialization,
\[
\mathcal{R}_S(\mathcal{F}) \leq \mathcal{O} \left( \sqrt{\frac{\log(n/\delta)}{n}} \right).
\]
Finally, by Lemma B.1 we have with probability at least $1 - \tau^{d-n+1} - \tau^d - \delta$ over the samples and random initialization,
\[
\mathbb{E}_{(x,y) \sim \mathcal{D}} \left[ \hat{\ell} \left(f(w^{(\infty)}, x), y \right) \right] \leq \mathcal{O} \left( \sqrt{\frac{\log(n/\delta)}{n}} \right),
\]
for some constant $\tau \in (0, 1)$ that depend only on the subgaussian moment of the entries.
This completes the proof. 
\[\square\]