Relaxing the Feature Covariance Assumption: Time-Variant Bounds for Benign Overfitting in Linear Regression

Jing Xu*†
xujing21@mails.tsinghua.edu.cn

Jiaye Teng*†
tjy20@mails.tsinghua.edu.cn

Andrew Chi-Chih Yao†
andrewcyao@tsinghua.edu.cn

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Abstract

Benign overfitting demonstrates that overparameterized models can perform well on test data while fitting noisy training data. However, it only considers the final min-norm solution in linear regression, which ignores the algorithm information and the corresponding training procedure. In this paper, we generalize the idea of benign overfitting to the whole training trajectory instead of the min-norm solution and derive a time-variant bound based on the trajectory analysis. Starting from the time-variant bound, we further derive a time interval that suffices to guarantee a consistent generalization error for a given feature covariance. Unlike existing approaches, the newly proposed generalization bound is characterized by a time-variant effective dimension of feature covariance. By introducing the time factor, we relax the strict assumption on the feature covariance matrix required in previous benign overfitting under the regimes of overparameterized linear regression with gradient descent. This paper extends the scope of benign overfitting, and experiment results indicate that the proposed bound accords better with empirical evidence.

1 Introduction

Deep neural networks achieve great success in practice (Silver et al., 2017; Devlin et al., 2019; Brown et al., 2020). However, their remarkable generalization ability is still one...
Figure 1: An illustration of the excess risk and training loss of overparametrized linear regression with gradient descent. We find that early stopping solution achieves low excess risk, despite the high excess risk of min-norm solution. Meanwhile, the training loss decays rapidly, which indicates that both the early stopping solution and the min-norm solution lie in the overfitting regime.

of the essential mysteries in the deep learning community, where deep neural networks achieve small test error despite fitting noisy training data, namely, *benign overfitting*.

The phenomenon of benign overfitting contradicts the traditional wisdom of learning theory (Zhang et al., 2021), as the bias-variance tradeoff implies that overfitting hurts generalization. The failure of traditional techniques is primarily because their bounds characterize the generalization behavior using various complexity measures while ignoring either the data role or algorithm role. For example, data-independent uniform convergence bounds may only yield vacuous bound even in overparameterized linear regression regimes (Nagarajan and Kolter, 2019). Therefore, understanding the generalization of neural networks requires data-dependent and algorithm-dependent analysis.

However, obtaining data-dependent or algorithm-dependent bounds in neural networks is pretty complex in practice. As a surrogate, researchers use neural tangent kernels (NTK) to approximate neural networks and study overparameterized linear models to gain intuitions for deep learning regimes, since neural networks converge to overparameterized linear models under some regularity conditions (Jacot et al., 2018; Arora et al., 2019). The seminal work pioneered by Bartlett et al. (2020) is among the most popular ones, which studies the generalization behavior of overparameterized linear models from a data-dependent perspective. Bartlett et al. (2020) demonstrates that overparameterized linear
regression can achieve small test error while fitting the noisy training data, characterized by the feature covariance matrix. Consequently, benign overfitting phenomenon indeed happens in overparameterized linear regression regimes. However, there are mainly two limitations in Bartlett et al. (2020).

**Limitation One: Algorithm-Independent Issues.** Bartlett et al. (2020) only consider the min-norm solution and ignores algorithm details. However, as discussed above, the generalization behavior highly depends on the algorithm information. Although the min-norm solution is closely related to the gradient descent (GD) algorithm since GD with a sufficiently small learning rate converges to the min-norm solution, analysis based on the whole trajectory captures more algorithmic details. Figure 1 illustrates the excess risk curve sketch for a linear regression instance, where the minimum excess risk along the trajectory can be significantly smaller than the excess risk of the final min-norm solution. Therefore, the generalization property of the entire training trajectory is pretty different from that of the min-norm solution, and a time-variant generalization bound provides a deeper understanding of benign overfitting in terms of the algorithmic information.

**Limitation Two: Strict Assumption on Feature Covariance.** To derive the benign overfitting phenomenon, Bartlett et al. (2020) requires a strict assumption on the feature covariance matrix. Bartlett et al. (2020) prove that it is essential for benign overfitting that the feature covariance has heavy tail eigenvalues. However, people have observed that benign overfitting generally happens in practice under neural network regimes. The strict data assumption in benign overfitting rules out many widely-used data distributions and hinders the applicability of the framework. Therefore, it is meaningful to derive benign overfitting with weaker assumptions on the feature covariance.

The aforementioned two limitations are naturally relevant via a time-variant generalization analysis. A time-variant bound reflects the algorithm information since it considers the whole training trajectory, and relaxes the data distribution assumption for benign overfitting since such analysis can be much more flexible. Figure 1 illustrates that the model in the middle of the trajectory (early stopping solution) enjoys better generalization than the final min-norm solution in a proper time interval.

In this paper, we propose a time-variant generalization analysis for benign overfitting in overparameterized linear regression with gradient descent. Specifically, we use a fine-grained analysis of gradient descent dynamics and prove an excess risk upper bound along the training trajectory. Based on the time-variant bound, we further derive a time interval for a wide class of feature distributions, in which the generalization error of gradient descent iterates is guaranteed to be consistent. In this way, we relax the otherwise strict assumptions on the feature covariance and demonstrate that benign overfitting holds for a broader class of input distributions. Besides, the proposed risk bound of the early stopping solution can be significantly better than the excess risk of the min-norm solution. We provide the informal version of the main theorem below.

**Theorem 1.1** (Theorem 4.1 informal). Consider an overparameterized linear regression problem with gradient descent. Let \( n \) denote the sample size, and \( k_1, k_2 \) denote the effective
dimensions of feature covariance. Then under certain regularity conditions, the excess risk at time $t$ can be bounded with high probability\footnote{In the following of the paper, we use $y \lesssim x$ and $y = O(x)$ to represent $y \leq cx$, use $y = \Theta(x)$ to represent $y = cx$, use $y = o(x)$ to represent $y < cx$, and use $y = \Omega(x)$ to represent $y \geq cx$, where $c$ is a constant.}

$$\text{excess risk} \lesssim \text{bias + variance},$$

where

$$\text{bias} = O\left(\frac{1}{t} + \frac{1}{\sqrt{n}}\right),$$

$$\text{variance} = O\left(\frac{k_1}{n} + \frac{k_2}{c(t, n)n} + \frac{c(t, n)}{n^2 t^2}\right),$$

and $c(t, n)$ is a term dependent on time $t$ and sample size $n$.

We summarize our contributions as follows:

- We derive a time-variant excess risk bound for overparameterized linear regression with gradient descent and provide a time interval in which the excess risk is consistent. Our theory extends the scope of benign overfitting from the min-norm solution analysis to a general trajectory analysis.

- The time-variant bound relaxes the strict feature covariance assumption required in previous benign overfitting by considering the time factor. We demonstrate that benign overfitting occurs for a wide range of data distributions if we consider the training algorithm and its corresponding trajectory.

- We provide various empirical evidence to verify the motivation and correctness of the time-variant benign overfitting.

## 2 Related Works

**Benign Overfitting** focuses on deriving non-asymptotic generalization guarantees for overparameterized linear models (Bartlett et al., 2020), which relies on a strict assumption of the feature covariance matrix. Some recent papers focus on deriving benign overfitting under different regimes, e.g., constant-stepsize SGD (Zou et al., 2021), ridge regression (Tsigler and Bartlett, 2020), Random Features (Li et al., 2020b), Gaussian Mixture models (Wang and Thrampoulidis, 2021). This paper relaxes the requirement on the feature covariance matrix by introducing time-variant bounds.

**Generalization** measures how models perform on unseen data. The commonly-used techniques to get the generalization bounds include uniform convergence (Koltchinskii and
Early Stopping is shown to be efficient under noisy label regimes (Li et al., 2020a; Bai et al., 2021). Another line of research focuses on the signal for early stopping (Prechelt, 2012; Forouzesh and Thiran, 2021). Unlike the existing approaches, this paper takes advantage of early stopping to relax the covariance requirements in benign overfitting regimes.

3 Preliminary

In this section, we introduce the necessary definitions, assumptions, and formally define effective dimensions of feature covariance.

3.1 Notations and Assumptions

Let \((x, y) \sim D \in \mathbb{R}^p \times \mathbb{R}\) denote the feature vector and the response, respectively\(^2\). Let \(\Sigma \triangleq \mathbb{E}[xx^\top]\) denote the feature covariance matrix, whose eigenvalue decomposition is \(\Sigma = V \Lambda V^\top = \sum_{i>0} \lambda_i v_i v_i^\top\) with decreasing eigenvalues \(\lambda_1 \geq \lambda_2 \geq \cdots\). We make the following assumptions on the distribution of the feature vector.

**Assumption 1** (Assumptions on feature distribution). We assume that

1. \(\mathbb{E}[x] = 0\).
2. \(\sum_{i>0} \lambda_i < \infty\).
3. Let \(z = \Lambda^{-\frac{1}{2}} V^\top x\). The random vector \(z\) has independent \(\sigma_x\)-subgaussian entries\(^3\).

We define the optimal parameter \(\theta^* \in \mathbb{R}^p\) which satisfies \(\mathbb{E}(y - x^\top \theta^*)^2 = \min_{\theta} \mathbb{E}(y - x^\top \theta)^2\). Let \(\varepsilon = y - x^\top \theta^*\) denote the residual. The following assumptions focus on the conditional distribution of the noise.

**Assumption 2** (Assumptions on noise distribution). We assume that

1. The conditional noise \(\varepsilon | x\) has zero mean.
2. The conditional noise \(\varepsilon | x\) is \(\sigma_y\)-subgaussian.

\(^2\)We allow \(p\) to be \(\infty\), and in this case with slightly abuse of notation, we use \(\mathbb{R}^p\) to denote a countably infinite dimensional Hilbert space.

\(^3\)We say a random variable \(X\) is \(\sigma\)-subgaussian if \(\mathbb{E}[e^{\lambda X}] \leq e^{\frac{\lambda^2 \sigma^2}{2}}\) for any \(\lambda\).
Note that both Assumption 1 and Assumption 2 are mild and commonly considered in related literature (Bartlett et al., 2020; Tsigler and Bartlett, 2020; Zou et al., 2021).

Given a training set \( \{(x_i, y_i)\}_{1 \leq i \leq n} \) with \( n \) pairs independently sampled from the population distribution \( D \), we define \( X \triangleq (x_1, \ldots, x_n)^\top \in \mathbb{R}^{n \times p} \) as the design matrix, \( Y \triangleq (y_1, \ldots, y_n)^\top \in \mathbb{R}^n \) as the corresponding response vector, and \( \varepsilon \triangleq Y - X\theta^* \) as the residual vector. Let the singular value decomposition (SVD) of \( X \) be \( X = U\tilde{\Lambda}\tilde{W}^\top \), with \( \tilde{\Lambda} = \text{diag}\{\mu_1, \ldots, \mu_n\} \in \mathbb{R}^{n \times p}, \mu_1 \geq \cdots \geq \mu_n \).

We consider the overparametrized regime where the feature dimension is much larger than the sample size, namely, \( p \gg n \). Under the overparameterized regimes, Assumption 3 guarantees that \( \text{rank}(X) = n \) almost surely.

**Assumption 3 (Linear Independent Training Set).** For any \( n < p \), we assume that a independently sampled training set \( \{x_1, x_2, \cdots, x_n\} \) is linearly independent almost surely.

### 3.2 Gradient Descent on Linear Regression

We formulate the population loss of linear regression as

\[
\min_{\theta} L(\theta) \triangleq \frac{1}{2} \mathbb{E}_{(x,y) \sim D} (x^\top \theta - y)^2,
\]

where \( \theta \in \mathbb{R}^p \) is the weight vector to be optimized. As defined above, the minimizer of the population loss is \( \theta^* \).

Given the dataset \((X, Y)\), we define the empirical loss function as

\[
\hat{L}(\theta) \triangleq \frac{1}{2n} \|X\theta - Y\|^2.
\]

We apply full-batch gradient descent (GD) with a constant learning rate \( \lambda \) to solve the empirical risk minimization problem. In this case, the update rule for the optimization trajectory \( \{\theta_t\}_{t \geq 0} \) is formulated as

\[
\theta_{t+1} = \theta_t - \frac{\lambda}{n} X\tilde{W}^\top (X\theta_t - Y).
\]

The following Lemma 3.1 provides the explicit form of the optimization trajectory \( \{\theta_t\}_{t \geq 0} \) at step \( t \).

**Lemma 3.1.** The trajectory of \( \{\theta_t\}_{t \geq 0} \) satisfies

\[
\theta_t = \left( I - \frac{\lambda}{n} X\tilde{W}^\top X \right)^t (\theta_0 - X\dagger Y) + X\dagger Y,
\]

where \( X\dagger \) denotes the pseudo-inverse of matrix \( X \).
Without loss of generality, we consider zero initialization \( \theta_0 = 0 \) in this paper. In this case, for a sufficiently small learning rate \( \lambda \), \( \theta_t \) converges to the min-norm solution \( \tilde{\theta} = X^\top (XX^\top)^{-1}Y \) as \( t \) goes to infinity. Previous researches [Bartlett et al., 2020] mainly consider the min-norm solution, and we discuss the training trajectory in this paper.

In this paper, we mainly focus on the excess risk of estimator \( \theta \) due to label noise, defined as
\[
R(\theta) \triangleq \mathbb{E}_{(x,y) \sim D} \left[ (x^\top \theta - y)^2 - (x^\top \theta^* - y)^2 \right].
\]
Specifically, we consider the excess risk along the entire training trajectory \( \{R(\theta_t)\}_{t \geq 0} \).

### 3.3 Effective Dimensions

We define the effective rank of \( \Sigma \) as
\[
r(\Sigma) \triangleq \frac{\sum_{i>0} \lambda_i}{\lambda_1}.
\]

In this paper, we use three types of effective dimension. We will use these quantities to characterize the excess risk of gradient descent iterates in Section 4.

**Definition 3.1 (Effective Dimension).** Given a feature covariance matrix \( \Sigma \), we define three types of effective dimension as
\[
\begin{align*}
k_0 & \triangleq \min \left\{ l \geq 0 : \lambda_{l+1} \leq \frac{c_0 \sum_{i>0} \lambda_i}{n} \right\}, \\
k_1 & \triangleq \min \left\{ l \geq 0 : \lambda_{l+1} \leq \frac{c_1 \sum_{i>0} \lambda_i}{n} \right\}, \\
k_2 & \triangleq \min \left\{ l \geq 0 : \sum_{i>l} \lambda_i + n \lambda_{l+1} \leq c_2 c(t,n) \sum_{i>0} \lambda_i \right\},
\end{align*}
\]

where \( c_0, c_1, c_2 \) are constants independent of the dimension \( d \), sample size \( n \), and time \( t \). The term \( c(t,n) \) is a function to be discussed later. Although the effective dimension \( k_0, k_1, k_2 \) is dependent on \( c_0, c_1, c_2, c(t,n) \), when the context is clear, we omit these dependencies and only denote them by \( k_0, k_1, k_2 \).

**Discussion for** \( k_0 \) **and** \( k_1 \). The quantity \( k_0 \) is previously proposed in [Bartlett et al., 2020] as the effective dimension of the feature covariance matrix \( \Sigma \). In this work, we introduce a new quantity \( k_1 \) to characterize the effective dimension of \( \Sigma \) instead of \( k_0 \), which divides the eigenvalues of \( \Sigma \) based on a threshold of \( \Theta (1/n) \). Note that \( k_1 < k_0 \) and in some cases it holds that \( k_1 \ll k_0 \) (See section 4.2 for more discussion).

**Discussion for** \( k_2 \). The quantity \( k_2 \) represents the effective dimension of matrix \( XX^\top \), which is a crucial ingredient in analyzing the gradient descent trajectory. The term \( k_2 \) bounds the number of eigenvalues \( \mu_j \) of matrix \( XX^\top \) that are larger than a time-dependent and sample-dependent threshold function \( c(t,n) \).

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4Constants may depend on \( \sigma_x \), and we omit this dependency thereafter for clarity.
4 Time-Variant Bound

In this section, we present our main theorem in Theorem 4.1, which derives an upper bound of excess risk $R(\theta_t)$ for any given time $t > 0$. Compared to the existing bound (Bartlett et al., 2020), Theorem 4.1 focuses on investigating the role of training epoch $t$ in the excess risk.

Theorem 4.1 (Time Variant Bound). Suppose Assumption 1, 2 and 3 hold. For any fixed training epoch $t$ and function $c(t, n)$, we define $k_0, k_1, k_2$ as in Definition 7. Given $\delta \in (0, 1)$, assume that $k_0 \leq \frac{n}{c}$, $\log \frac{1}{\delta} \leq \frac{n}{c}$, $0 \leq \lambda \leq \frac{1}{c\sum_{i > 0} \lambda_i}$ for a large enough constant $c$. Then with probability at least $1 - \delta$,

$$R(\theta_t) \lesssim B(\theta_t) + V(\theta_t),$$

where

$$B(\theta_t) = \|\theta^*\|^2 \left( \frac{1}{\lambda t} + \|\Sigma\| \max \left\{ \sqrt{\frac{r(\Sigma)}{n}}, \frac{r(\Sigma)}{n}, \frac{\log(\frac{1}{\delta})}{n} \right\} \right),$$

$$V(\theta_t) = \sigma^2 \log \left( \frac{1}{\delta} \right) \left( \frac{k_1}{n} + \frac{k_2}{c(t, n)n} + c(t, n) \left( \frac{\lambda t}{n} \sum_{i > 0} \lambda_i \right)^2 \right).$$

Theorem 4.1 first decomposes $R(\theta_t)$ into the bias term and the variance term, and bounds them with $B(\theta_t)$ and $V(\theta_t)$, respectively. We note that there is a tradeoff between $B(\theta_t)$ and $V(\theta_t)$, where $B(\theta_t)$ decreases with time $t$ while $V(\theta_t)$ increases with time $t$.

**Bias Term.** The bias upper bound consists of two parts. The first part decays with rate $O(1/t)$, which comes from the optimization error. The second part is time-independent with order $\Theta(1/\sqrt{n})$, which comes from the approximation error where we use $\frac{1}{n}XX^\top$ to approximate $\Sigma$. Therefore, $t = \Omega(\sqrt{n})$ is sufficient to guarantee that $B(\theta_t)$ is of order $\Theta(1/\sqrt{n})$.

**Variance Term.** The variance upper bound is characterized by three quantities $k_1, k_2$ and $c(t, n)$. Firstly, the term $k_1$ represents the number of large eigenvalues in the covariance matrix $\Sigma$, which divides the eigenvalues $\lambda_i$ into small parts and large parts based on a threshold $\Theta(1/n)$. Secondly, the term $k_2$ implicitly represents the number of large eigenvalues in the matrix $XX^\top$. Different from $k_1$, the term $k_2$ divides the eigenvalues $\mu_j$ based on a threshold function $c(t, n)$, which is time-dependent and sample-dependent.

Unlike the bias term, which tends to zero when the sample size $n$ tends to infinity, the variance term is vacuous unless $k_1, k_2$ is small compared with $n$ for a suitably chosen $c(t, n)$. We finally remark that due to the implicit dependency between $k_2$ and $c(t, n)$, one cannot directly calculate the best $c(t, n)$ based on basic inequality by simply setting

$$\frac{k_2}{c(t, n)n} = c(t, n) \left( \frac{\lambda t}{n} \sum_{i > 0} \lambda_i \right)^2.$$
a proper $c(t, n)$. Basically, a general criterion is to find minimal $c(t, n)$ such that $k_2 = o(n)$. However, we may simplify the criterion in practice. In the subsequent sections, we show how to derive non-vacuous risk bounds for different time $t$, based on different choices of $c(t, n)$.

4.1 Varying $t$, Constant $c(t, n)$

Theorem 4.1 provides an excess risk upper bound for any fixed time $t$. As discussed above, the remaining question is how to decide the term $c(t, n)$. This section shows how to derive the generalization bound by setting $c(t, n)$ a constant.

Corollary 4.1 (Constant $c(t, n)$). Under the settings in Theorem 4.1, we fix a constant $c(t, n)$. Given $\delta \in (0, 1)$, assume that $k_0 \leq \frac{n}{c}, \log \frac{1}{\delta} \leq \frac{n}{c}, \lambda = \frac{a}{\sum_{i=0}^{n} \lambda_i}$ for some appropriate constants $a, c$, then with probability at least $1 - \delta$, for any $t \in [\Theta(\sqrt{n}), \Theta(\sqrt{\max\{k_1, 1\} n})$ we have

\[
R(\theta_t) \leq \|\theta^*\|^2 \left( \frac{1}{\lambda \sqrt{n}} + \|\Sigma\| \max \left\{ \sqrt{\frac{r(\Sigma)}{n}}, \frac{r(\Sigma)}{n}, \sqrt{\frac{\log(\frac{1}{\delta})}{n}} \right\} \right) + \sigma_y^2 \log \left( \frac{1}{\delta} \right) \frac{\max\{k_1, 1\}}{n}.
\]

If we additionally assume $k_1 = o(n)$, the excess risk is consistent, namely,

\[
\lim_{n \to \infty} R(\theta_t) \to 0,
\]

where we omit the dependency between $R(\theta_t)$ and $n$.

Corollary 4.1 indicates that for a time interval $t \in [\Theta(\sqrt{n}), \Theta(\sqrt{\max\{k_1, 1\} n})$, the excess risk is always consistent. We remark that the interval is dependent on the form of the feature covariance matrix via the term $k_1$. Therefore, the bound proposed in Corollary 4.1 is data-dependent. In the next section, we will provide several concrete examples to show how to apply Corollary 4.1 in practice under different data distributions.

4.2 Examples

We now apply our bound in Corollary 4.1 to several examples. In each example, we show the data distribution, the time interval, and the corresponding generalization bound. These distributions are widely discussed in (Bartlett et al., 2020; Zou et al., 2021)

Example 4.1. Under the same conditions as Theorem 4.1 let $\Sigma$ denote the feature covariance matrix. We show the following examples:

1. (Inverse Polynominal). If the spectrum of $\Sigma$ satisfies

\[
\lambda_k = \frac{1}{k^\alpha},
\]

If we additionally assume $k_1 = o(n)$, the excess risk is consistent, namely,

\[
\lim_{n \to \infty} R(\theta_t) \to 0,
\]

where we omit the dependency between $R(\theta_t)$ and $n$.
Table 1: Comparison of excess risk bound with Bartlett et al. (2020) and Zou et al. (2021). We provide four types of feature covariance with eigenvalues $\lambda_k$, including Inverse Polynomial ($\lambda_k = \frac{1}{k^\alpha}$, $\alpha > 1$), Inverse Log Polynomial ($\lambda_k = \frac{1}{k \log^\beta(k+1)}$, $\beta > 1$), Constant ($\lambda_k = \frac{1}{n^{1+\varepsilon}}$, $1 \leq k \leq n^{1+\varepsilon}$, $\varepsilon > 0$), and Piecewise Constant ($\lambda_k = \frac{1}{s}$ if $1 \leq k \leq s$ and $\lambda_k = \frac{1}{d-s}$ if $s+1 \leq k \leq d$, where $s = n^r$, $d = n^q$, $0 < r < 1$, $q \geq 1$). We refer to Section 4.2 for more distribution details. In light of these bounds, Ours outperforms Bartlett et al. (2020) in all the cases, and outperforms Zou et al. (2021) in Constant / Piecewise Constant cases if $\varepsilon < \frac{1}{2}$ and $q < \min\{2 - r, \frac{3}{2}\}$.

| DISTRIBUTIONS | OURS | BARTLETT ET AL. (2020) | ZOU ET AL. (2021) |
|---------------|------|------------------------|-------------------|
| INVERSE POLYNOMIAL | $O \left( n^{-\min\{\frac{\alpha-1}{\alpha}, \frac{1}{2} \}} \right)$ | $O(1)$ | $O \left( n^{-\frac{\alpha-1}{\alpha}} \right)$ |
| INVERSE LOG POLYNOMIAL | $O \left( \frac{1}{\log^\beta n} \right)$ | $o(1)$ | $O \left( \frac{1}{\log^\beta n} \right)$ |
| CONSTANT | $O \left( n^{-\frac{1}{2}} \right)$ | $O \left( n^{-\min\{\frac{\varepsilon}{2}, \frac{1}{2} \}} \right)$ | $O \left( n^{-\min\{\varepsilon, 1 \}} \right)$ |
| PIECEWISE CONSTANT | $O \left( n^{-\min\{1-r, \frac{1}{2} \}} \right)$ | $O \left( n^{-\min\{1-r, q-1, \frac{1}{2} \}} \right)$ | $O \left( n^{-\min\{1-r, q-1 \}} \right)$ |

for some $\alpha > 1$, we derive that $k_0 = \Theta(n)$, $k_1 = \Theta \left( n^{\frac{1}{2}} \right)$. Therefore, $V(\theta_t) = O \left( n^{\frac{1-\alpha}{\alpha}} \right)$ and

$$R(\theta_t) = O \left( n^{-\min\{\frac{\alpha-1}{\alpha}, \frac{1}{2} \}} \right),$$

for $t \in \left[ \Theta \left( \frac{n^{1}}{2} \right), \Theta \left( n^{\frac{\alpha+1}{2}} \right) \right]$.

2. (Inverse Log-Polynomial). If the spectrum of $\Sigma$ satisfies

$$\lambda_k = \frac{1}{k \log^\beta(k+1)},$$

for some $\beta > 1$, we derive that $k_0 = \Theta \left( \frac{n}{\log n} \right)$, $k_1 = \Theta \left( \frac{n}{\log^\beta n} \right)$. Therefore, $V(\theta_t) = O \left( \frac{1}{\log^\beta n} \right)$ and

$$R(\theta_t) = O \left( \frac{1}{\log^\beta n} \right),$$

for $t \in \left[ \Theta \left( \frac{n^{1}}{2} \right), \Theta \left( \frac{n}{\log^\beta n} \right) \right]$.

3. (Constant). If the spectrum of $\Sigma$ satisfies

$$\lambda_k = \frac{1}{n^{1+\varepsilon}}, 1 \leq k \leq n^{1+\varepsilon},$$
for some $\varepsilon > 0$, we derive that $k_0 = 0$, $k_1 = 0$. Therefore, $V(\theta_t) = O\left(\frac{1}{n}\right)$ and

$$R(\theta_t) = O\left(\frac{1}{\sqrt{n}}\right),$$

for $t = \Theta(\sqrt{n})$.

4. (Piecewise Constant). If the spectrum of $\Sigma$ satisfies

$$\lambda = \begin{cases} \frac{1}{s} & 1 \leq k \leq s, \\ \frac{1}{d-s} & s+1 \leq k \leq d, \end{cases}$$

where $s = n^r, d = n^q, 0 < r \leq 1, q \geq 1$. We derive that $k_0 = n^r$, $k_1 = n^r$. Therefore, $V(\theta_t) = O(n^{r-1})$ and

$$R(\theta_t) = O\left(n^{-\min\{1-r, \frac{1}{2}\}}\right),$$

for $t \in \left[\Theta\left(n^\frac{r}{2}\right), \Theta\left(n^{\frac{r+1}{2}}\right)\right]$.

4.3 Comparisons with Previous Results

We summarize the results in Bartlett et al. (2020); Zou et al. (2021) and our results in Table 1 and provide a detailed comparison below.

Comparison to Bartlett et al. (2020). In this seminal work, the authors study the excess risk of the min-norm solution. As discussed above, the min-norm solution is the convergence point of gradient descent in the overparameterized linear regression regime. One of the main results in Bartlett et al. (2020) is providing a tight bound for the variance part

$$V(\hat{\theta}) = O\left(\frac{k_0}{n} + \frac{n}{R_k(\Sigma)}\right),$$

where $\hat{\theta} = X^T(XX^T)^{-1}Y$ denotes the min-norm solution, and $R_k(\Sigma) = (\sum_{i<k} \lambda_i^2) / (\sum_{i>k} \lambda_i^2)$ denote another type of effective rank.

By introducing the time factor, Theorem 4.1 improves over Equation (2) in at least two aspects. Firstly, Theorem 4.1 guarantees the consistency of the gradient descent dynamics for a broad range of step number $t$, while Bartlett et al. (2020) only study the limiting behavior of the dynamics of $t \to \infty$. Secondly, Theorem 4.1 implies that the excess risk of early stopping gradient descent solution can be much better than the min-norm solution. For example, as derived in Corollary 4.1, the excess risk satisfies

$$R(\theta_t) = O\left(\frac{1}{n}\right)$$

for $t = \Theta(\sqrt{n})$. Compared to the bound in Equation (2), the bound in Corollary 4.1(a.) replaces $k_0$ with a much smaller quantity $k_1$; and (b.) drops the second

\footnote{We do not compare the bias component in the excess risk bound here since our bound for the bias component follows Bartlett et al. (2020).}
term involving $R_{k_0}(\Sigma)$. Therefore, we can derive a consistent bound for overparameterized linear regression for an early-stopping solution, even though the excess risk of limiting point (min-norm solution) can be $\Omega(1)$ (See the first example in [4.1]). We can further derive a data-dependent time interval in which the bound is consistent, which cannot be directly obtained in Bartlett et al. (2020).

Comparison to Zou et al. (2021). Zou et al. (2021) study a very different regime from this paper, which focuses on the online stochastic gradient descent solution of linear regression. The authors prove a bound for the excess risk as

$$R(\bar{\theta}_t) = O\left(\frac{k_1}{n} + \frac{n \sum_{i > k_1} \lambda_i^2}{(\sum_{i > 0} \lambda_i)^2}\right), \quad (3)$$

where $\bar{\theta}_t$ denotes the parameter obtained using stochastic gradient descent (SGD) with constant step size at epoch $t$. Similar to our bound, Equation (3) also uses the effective dimension $k_1$ to characterize the variance term. However, we emphasize that Zou et al. (2021) derive the bound in a pretty different scenario from ours, which is one-path SGD scenario. During the one-path SGD training, we use a fresh data point to perform stochastic gradient descent in each epoch, and therefore they set $t = \Theta(n)$ by default. As a comparison, we apply the standard full-batch gradient descent, and thus the time can be more flexible. Besides, our results in Corollary 4.1 improve the bound in Equation (3) by dropping the second term. We refer to the third and fourth example in Example 4.1 for more details, where our bound outperforms Zou et al. (2021) when $\varepsilon < 1/2$ or $q < \min\{2 - r, 3/2\}$.

4.4 Varying $t$, Varying $c(t, n)$

In previous sections, we set $c(t, n)$ as a constant by default and demonstrate that Theorem 4.1 yields a non-vacuous bound of $O(k_1/n)$ for $t \in [\Theta(\sqrt{n}), \Theta(\sqrt{k_1 n})]$. In practice, the choice of $c(t, n)$ can be much more flexible. In this section, we provide a concrete example and demonstrate that by setting $c(t, n)$ a non-constant, Theorem 4.1 can indeed guarantee the consistency of the excess risk for a much larger range of $t$.

**Example 4.2 (The first example in Example 4.1 revisited).** Under the same conditions as Theorem 4.1 let $\Sigma$ denote the feature covariance matrix. If the spectrum of $\Sigma$ satisfies $\lambda_k = \frac{1}{k^\alpha}$ for some $\alpha > 1$, we set $c(t, n) = \Theta\left(\frac{n^{\alpha+1-2\alpha \tau}}{2\alpha+1}\right)$ for a given $\frac{\alpha+1}{2\alpha} \leq \tau \leq \frac{3\alpha+1}{2\alpha+2}$.

Then for $t = \Theta(n^\tau)$, we derive that $V(\theta_t) = O\left(\frac{n^{2\alpha \tau - 3\alpha + 2\tau - 1}}{2\alpha+1}\right)$.

Example 4.2 shows that by choosing $c(t, n)$ as a non-constant, we broader the scope of Theorem 4.1. Note that when setting $c(t, n)$ as a constant, the support of time $t$ is $[\Theta(n^{1/2}), \Theta(n^{(\alpha+1)/2\alpha})]$ (See Example 4.2). By relaxing $c(t, n)$ as a non-constant, we...
can provide the bound for \( t \in \left[ \Theta(n^{(\alpha+1)/2\alpha}), \Theta(n^{(3\alpha+1)/(2\alpha+2)}) \right] \). Note that when \( t = \Theta(n^{(\alpha+1)/2\alpha}) \), we derive that \( V(\theta_t) = O(n^{(1-\alpha)/\alpha}) \) in Example 4.2, which coincides with the bound of setting \( c(t, n) \) as a constant in Example 4.2. Therefore, by setting \( c(t, n) \) as a non-constant, we broaden the support of time \( t \) and extends the result of constant \( c(t, n) \).

Example 4.2 implies that we can derive types of bounds from Theorem 4.1 benefiting from the flexibility of \( c(t, n) \). Although setting \( c(t, n) \) to a constant is intuitive and straightforward, we may improve the bounds by setting different types of \( c(t, n) \).

5 Experiments

In this section, we provide numerical studies of overparameterized linear regression problems. The empirical results demonstrate that (a.) **benign overfitting occurs in early-stopping gradient descent** for a wide range of input distributions, where optimal early-stopping solution indeed lies in the overfitting time region; (b.) **the optimal excess risk of early stopping solution is significantly lower than that of min-norm solution**, which

Figure 2: Excess risk curve and training loss curve for different distributions. We plot the lowest point (red point) on the excess risk curve (blue line). Besides, we plot the smallest time (brown point) where the training error curve (orange line) reaches \( \sigma_y^2/2 \) (green dotted line), indicating that overfitting has already happened. The figures illustrate that (a.) the models have already become overfitting when they achieve minimal excess risk since the red points always lie on the right of the brown points; and (b.) the faster \( \lambda_i \) decays, the better early stopping solution generalizes, which corroborates with our theory (See Table 2 for more details).
Table 2: The effective dimension $k_1$, the optimal early stopping excess risk and the min-norm excess risk for different feature distributions. The table shows that early stopping solution generalizes significantly better than min-norm solution, and reveals a positive correlation between the effective dimension $k_1$ and generalization performance of early stopping solution. We calculate the 95% confidence interval for the excess risk.

| DISTRIBUTIONS | $k_1$ | OPTIMAL EXCESS RISK | MIN-NORM EXCESS RISK |
|---------------|-------|---------------------|----------------------|
| $\lambda_i = \frac{1}{i}$ | $\Theta(n)$ | 4.799 ± 0.0123 | 48.142 ± 0.4895 |
| $\lambda_i = \frac{1}{i^2}$ | $\Theta(n^{\frac{1}{2}})$ | 0.428 ± 0.0101 | 86.945 ± 1.2927 |
| $\lambda_i = \frac{1}{i^3}$ | $\Theta(n^{\frac{3}{2}})$ | 0.154 ± 0.0010 | 20.801 ± 0.5946 |
| $\lambda_i = \frac{1}{i \log(i+1)}$ | $\Theta(\frac{n}{\log n})$ | 1.395 ± 0.0106 | 179.844 ± 1.9182 |
| $\lambda_i = \frac{1}{i \log^2(i+1)}$ | $\Theta(\frac{n}{\log^2 n})$ | 0.596 ± 0.0107 | 164.825 ± 1.8540 |
| $\lambda_i = \frac{1}{i \log^3(i+1)}$ | $\Theta(\frac{n}{\log^3 n})$ | 0.373 ± 0.0093 | 76.289 ± 1.1723 |

justifies our motivation of considering the entire training trajectory; (c.) the optimal excess risk is lower when the eigenvalues of feature covariance decay faster, which accords with Theorem 4.1.

Setup. We consider six overparametrized linear regression instances with input dimension $p = 1000$ and sample size $n = 100$. We provide additional experiments for sample size $n = 50$ and $n = 200$ in appendix B. The feature vectors are independently sampled from zero-mean Gaussian distributions, whose covariances are diagonal with entries $\lambda_i = \frac{1}{i}, \frac{1}{i^2}, \frac{1}{i^3}, \frac{1}{i \log(i+1)}, \frac{1}{i \log^2(i+1)}, \frac{1}{i \log^3(i+1)}$, respectively. Note that we only consider finite dimensional case here, so the assumption of $\sum_{i>0} \lambda_i < \infty$ is naturally satisfied. For each instance, the ground truth $\theta^*$ is sampled from a $d$-dimensional standard Gaussian distribution. For each feature $x$, we construct the response as $y = x^T \theta^* + \epsilon$, where the residual $\epsilon$ is sampled from a standard Gaussian distribution. We conduct gradient descent with learning rate $\lambda = 0.001$ on the above instances. Figure 2 shows the excess risk curves and the training loss curves.

Observation One: Optimal early stopping solution already overfits. We select $\sigma_y^2/2$ (green dotted line) as a threshold for overfitting in our experiment, as the model fits at least half of the data noise if the training loss has dropped below $\sigma_y^2/2$. As indicated by figure 2, the training error quickly drops below the overfitting threshold in just a few epochs (marked by the brown dot). As a comparison, the model achieves minimum excess risk after a decent number of training epochs (marked by the red dot). Therefore, even though early-stopping may mitigate the influence of overfitting, the optimal model in the gradient descent trajectory already overfits the data. Note that corollary 4.1 naturally implies that $\min_t R(\theta_t) = O(\max(\frac{k_1 \sqrt{n}}{n}, \frac{\sqrt{n}}{n}))$. Hence, our theory provides non-vacuous generalization results in the overfitting regime.

Observation Two: Optimal early stopping solution generalizes significantly better
than the min-norm solution. We calculate the excess risk of optimal early stopping solutions and min-norm solutions from 1000 independent trials, and list the results in Table 2. To avoid numerical instability, we apply weight decay on parameter $\theta$ with parameter $1 \times 10^{-4}$ when computing min-norm excess risk. The results demonstrate that the early stopping solution enjoys much better generalization property, and therefore highlights the benefits of time-variant generalization analysis.

**Observation Three: The faster covariance spectrum decays, the lower optimal excess risk is.** Figure 2 shows a positive correlation between the decaying rate of $\lambda_i$ and the generalization performance of the early-stopping solution. In each of the experiments, we calculate the minimum excess risk from 1000 independent trials and show results in Table 2. The experiment results accord with Theorem 4.1 showing that the excess risk is better for a smaller effective dimension $k_1$, where small $k_1$ indicates a faster-decaying eigenvalue $\lambda_i$. We additionally note that such phenomenon also illustrates the difference between minimum-norm and early-stopping solutions in linear regression, since Bartlett et al. (2020) demonstrate that the min-norm solution is not consistent when the eigenvalues decay too fast. By comparison, early-stopping solutions do not suffer from this restriction.

6 Conclusion

In this paper, we follow the idea of benign overfitting and derive time-variant bounds in the regime of overparametrized linear regression with gradient descent. Compared to the previous results, the newly-proposed bounds consider the whole training trajectory instead of the min-norm solution, and therefore require a milder assumption on the feature covariance matrix. We conduct several experiments on linear models to validate the utility of the theorem. Our theorem does not aim at providing the tightest bound. Instead, this paper provides the possibility for broader application of benefit overfitting: reducing the assumptions for benefit overfitting by considering the influence of other factors, for example, time.

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Appendix

We give the whole proof in Appendix A and provide the experimental details in Appendix B.

A Proofs for the Main Results

A.1 Proof Sketch

We start with a standard bias-variance decomposition following [Bartlett et al. (2020)], which derives that the time-variant excess risk $R(\theta_t)$ can be bounded by a bias term and a variance term. We refer to Appendix A.3 for more details.

For the bias part, we first decompose it into an optimization error and an approximation error. For the optimization error, we use the spectrum analysis to bound it with $O(1/t)$ where $t$ denotes the time. For the approximation error, we bound it with $O(1/\sqrt{n})$ where $n$ denotes the sample size, inspired by Bartlett et al. (2020). We refer to Appendix A.4 for more details.

For the variance part, a key step is to bound the term $(I - \frac{\lambda}{n}XX^\top)^t$, where $X$ is the design matrix. The difficulty arises from the different scales of the eigenvalues of $XX^\top$, where the largest eigenvalue has order $\Theta(n)$ while the smallest eigenvalue has order $O(1)$, according to Lemma 10 in Bartlett et al. (2020). To overcome this issue, we divide the matrix $XX^\top$ based on whether its eigenvalues is larger than $c(t, n)$, which is a flexible term dependent on time $t$ and sample size $n$. Therefore, we split the variance term based on eigenvalues of covariance matrix $\Sigma$ (leading to the $k_1$-related term) and based on the eigenvalues of $XX^\top$ (leading to the $k_2$-related term). We refer to Appendix A.5 for more details.

A.2 Preliminaries

First, we cite a result from Bartlett et al. (2020), which bounds the eigenvalues of $XX^\top$.

Lemma A.1. (Lemma 10 in Bartlett et al. (2020)) For any $\sigma_x$, there exists a constant $c$, such that for any $k \geq 0$, with probability at least $1 - e^{-\frac{n}{c}}$, $\mu_{k+1} \leq c \left( \sum_{i > k} \lambda_i + \lambda_{k+1} n \right)$.

This implies that as long as the step size $\lambda$ is small than a threshold independent of sample size $n$, gradient descent is stable.

Corollary A.1. There exists a constant $c$, such that with probability at least $1 - e^{-\frac{n}{c}}$, for any $0 \leq \lambda \leq \frac{1}{c \sum_{i > 0} \lambda_i}$ we have

$$O \leq I - \frac{\lambda}{n}XX^\top \leq I.$$
Proof. The right hand side of the inequality is obvious since $\lambda > 0$. For the left hand side, we have to show that the eigenvalues of $I - \frac{\lambda}{n} X^\top X$ is non-negative. Since $X^\top X$ and $XX^\top$ have the same non-zero eigenvalues, we know that with probability at least $1 - e^{-\frac{c}{n}}$, the smallest eigenvalue of $I - \frac{\lambda}{n} X^\top X$ can be lower bounded by

$$
\mu_p \left( I - \frac{\lambda}{n} X^\top X \right) = 1 - \frac{\lambda}{n} \mu_1
\geq 1 - c\lambda \left( \frac{\sum_{i>0} \lambda_i}{n} + \lambda_{k+1} \right)
\geq 1 - 2c\lambda \sum_{i>0} \lambda_i
\geq 0.
$$

where the second inequality uses lemma A.1 and the last inequality holds if $\lambda \leq \frac{1}{2c \sum_{i>0} \lambda_i}$.

A.3 Proof for the Bias-Variance Decomposition

The following lemma gives a closed form expression for $\theta_t$.

Lemma A.2. (Lemma 3.1 restated) The dynamics of $\{\theta_t\}_{t \geq 0}$ satisfies

$$
\theta_t = \left( I - \frac{\lambda}{n} X^\top X \right)^t (\theta_0 - X^\top Y) + X^\top Y.
$$

Proof. We prove the lemma using induction. The equality holds at $t = 0$ as both sides are $\theta_0$. Recall that $\theta_t$ is updated as

$$
\theta_{t+1} = \theta_t + \frac{\lambda}{n} X^\top (Y - X \theta_t).
$$

Suppose that the dynamic holds up to the $t$-th step. Plug the expression for $\theta_t$ into the above recursion and note that $X^\top XX^\top = X^\top$, we get

$$
\theta_{t+1} = \left( I - \frac{\lambda}{n} X^\top X \right) \theta_t + \frac{\lambda}{n} X^\top Y
= \left( I - \frac{\lambda}{n} X^\top X \right)^{t+1} (\theta_0 - X^\top Y) + \left( I - \frac{\lambda}{n} X^\top X \right) X^\top Y + \frac{\lambda}{n} X^\top Y
= \left( I - \frac{\lambda}{n} X^\top X \right)^{t+1} (\theta_0 - X^\top Y) + X^\top Y.
$$

which finishes the proof.

Next we prove two identities which will be used in further proof.
Lemma A.3. The following two identities hold for any matrix $X$ and non-negative integer $t$:

\[
I - X^\dagger X + \left(I - \frac{\lambda}{n} X^\top X\right)^t X^\dagger X = \left(I - \frac{\lambda}{n} X^\top X\right)^t ,
\]

\[
\left[I - \left(I - \frac{\lambda}{n} X^\top X\right)^t \right] X^\dagger XX^\top = X^\top \left[I - \left(I - \frac{\lambda}{n} XX^\top\right)^t \right] .
\]

Proof. Note that $X^\top XX^\dagger = X^\top$, we can expand the left hand side of the first identity above using binomial theorem and eliminate the pseudo-inverse $X^\dagger$:

\[
I - X^\dagger X + \left(I - \frac{\lambda}{n} X^\top X\right)^t X^\dagger X
\]

\[
= I - X^\dagger X + \sum_{k=0}^{t} \binom{t}{k} \left(-\frac{\lambda}{n} X^\top X\right)^k X^\dagger X
\]

\[
= I - X^\dagger X + X^\dagger X + \sum_{k=1}^{t} \binom{t}{k} \left(-\frac{\lambda}{n}\right)^k (X^\top X)^{k-1} X^\top XX^\dagger X
\]

\[
= I + \sum_{k=1}^{t} \binom{t}{k} \left(-\frac{\lambda}{n}\right)^k (X^\top X)^k
\]

\[
= \left(I - \frac{\lambda}{n} X^\top X\right)^t .
\]

The second identity can be proved in a similar way:

\[
\left[I - \left(I - \frac{\lambda}{n} X^\top X\right)^t \right] X^\dagger XX^\top
\]

\[
= - \sum_{k=1}^{t} \binom{t}{k} \left(-\frac{\lambda}{n} X^\top X\right)^k X^\dagger XX^\top
\]

\[
= - \sum_{k=1}^{t} \binom{t}{k} \left(-\frac{\lambda}{n}\right)^k (X^\top X)^{k-1} X^\top XX^\dagger X
\]

\[
= - \sum_{k=1}^{t} \binom{t}{k} \left(-\frac{\lambda}{n}\right)^k (X^\top X)^{k-1} XX^\top
\]

\[
= - \sum_{k=1}^{t} \binom{t}{k} \left(-\frac{\lambda}{n}\right)^k X^\top (XX^\top)^k
\]

\[
= X^\top \left[I - \left(I - \frac{\lambda}{n} XX^\top\right)^t \right] .
\]
We are now ready to prove the main result of this section.

**Lemma A.4.** The excess risk at the $t$-th epoch can be upper bounded as

$$R(\theta_t) \leq 2\theta^*^\top B\theta^* + 2\varepsilon^\top C\varepsilon,$$

where

$$B = \left(I - \frac{\lambda}{n} X^\top X\right)^t \Sigma \left(I - \frac{\lambda}{n} X^\top X\right)^t,$$

$$C = (XX^\top)^{-1} \left[I - \left(I - \frac{\lambda}{n} XX^\top\right)^t\right] XX^\top \left[I - \left(I - \frac{\lambda}{n} XX^\top\right)^t\right] \left(I - \frac{\lambda}{n} XX^\top\right)^{-1},$$

which characterizes bias term and variance term in the excess risk. Furthermore, there exists constant $c$ such that with probability at least $1 - \delta$ over the randomness of $\varepsilon$, we have

$$\varepsilon^\top C\varepsilon \leq c\sigma_y^2 \log \frac{1}{\delta} \text{Tr}[C].$$

**Proof.** First we express the excess risk as follows

$$R(\theta_t) = \mathbb{E}[(y - x^\top \theta_t)^2 - (y - x^\top \theta^*)^2]$$

$$= \mathbb{E}[(y - x^\top \theta^* + x^\top \theta^* - x^\top \theta_t)^2 - (y - x^\top \theta^*)^2]$$

$$= \mathbb{E}[(x^\top (\theta_t - \theta^*))^2 + 2(y - x^\top \theta^*)(x^\top \theta^* - x^\top \theta_t)]$$

$$= \mathbb{E}[x^\top (\theta_t - \theta^*)]^2.$$

Recall that $\theta_0 = 0$ and $Y = X\theta^* + \varepsilon$ and we can further simplify the formula for $\theta_t$ in lemma 3.1

$$\theta_t = \left(I - \frac{\lambda}{n} X^\top X\right)^t (\theta_0 - X^\top Y) + X^\top Y$$

$$= \left[I - \left(I - \frac{\lambda}{n} XX^\top\right)^t\right] X^\top (X\theta^* + \varepsilon).$$

Plug it into the above expression for $R(\theta_t)$, we have

$$R(\theta_t) = \mathbb{E} \left[ x^\top \left[I - \left(I - \frac{\lambda}{n} XX^\top\right)^t\right] X^\top (X\theta^* + \varepsilon) - x^\top \theta^* \right]^2$$

$$= \mathbb{E} \left[ x^\top \left(X^\top X - \left(I - \frac{\lambda}{n} XX^\top\right)^t X^\top X - I\right) \theta^* + x^\top \left[I - \left(I - \frac{\lambda}{n} XX^\top\right)^t\right] X^\top \varepsilon \right]^2.$$
Applying lemma A.3, we obtain
\[
R(\theta_t) = \mathbb{E}\left[ -x^\top \left( I - \frac{\lambda}{n} X^\top X \right)^t \theta^* + x^\top X^\top \left( I - \left( I - \frac{\lambda}{n} X X^\top \right)^t \right) (XX^\top)^{-1} \varepsilon \right]^2 \\
\leq 2 \mathbb{E}\left[ x^\top \left( I - \frac{\lambda}{n} X^\top X \right)^t \theta^* \right]^2 \\
+ 2 \mathbb{E}\left[ x^\top X^\top \left( I - \left( I - \frac{\lambda}{n} X X^\top \right)^t \right) (XX^\top)^{-1} \varepsilon \right]^2 \\
:= 2 \theta^*\top B \theta^* + 2 \varepsilon\top C \varepsilon.
\]
which proves the first claim in the theorem. The second part of the theorem directly follows from lemma 18 in Bartlett et al. (2020).

A.4 Proof for the Bias Upper Bound

The next lemma guarantees that the sample covariance matrix $\frac{1}{n} X^\top X$ concentrates well around $\Sigma$.

**Lemma A.5.** (Lemma 35 in Bartlett et al. (2020)) There exists constant $c$ such that for any $0 < \delta < 1$ with probability as least $1 - \delta$,

\[
\left\| \Sigma - \frac{1}{n} X^\top X \right\| \leq c \left\| \Sigma \right\| \max \left\{ \sqrt{\frac{r(\Sigma)}{n}}, \frac{r(\Sigma)}{n}, \sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{n}}, \frac{\log\left(\frac{1}{\delta}\right)}{n} \right\}.
\]

The following inequality will be useful in our proof to characterize the decaying rate of the bias term with $t$.

**Lemma A.6.** For any positive semidefinite matrix $P$ which satisfies $\|P\| \leq 1$, we have

\[
\|P(1 - P)^t\| \leq \frac{1}{t}.
\]

**Proof.** Assume without loss of generality that $P$ is diagonal. Then it suffices to consider separately each eigenvalue $\sigma$ of $P$, and show that $\sigma(1 - \sigma)^t \leq \frac{1}{t}$.

In fact, by AM-GM inequality we have

\[
\sigma(1 - \sigma)^t \leq \frac{1}{t} \left[ t\sigma + (1 - \sigma)t \right]^{t+1} \leq \frac{1}{t},
\]
which completes the proof.

Next we prove the main result of this section.
Lemma A.7. There exists constant $c$ such that if $0 \leq \lambda \leq \frac{1}{\sum_{i>0} \lambda_i}$, then for any $0 < \delta < 1$, with probability at least $1 - \delta$ the following bound on the bias term holds for any $t$

$$\theta^\top B \theta^* \leq c \|\theta^*\|^2 \left( \frac{1}{\lambda t} + \|\Sigma\| \max \left\{ \sqrt{\frac{r(\Sigma)}{n}}, \frac{r(\Sigma)}{n}, \sqrt{\frac{\log(\frac{1}{\delta})}{n}}, \frac{\log(\frac{1}{\delta})}{n} \right\} \right).$$

Proof. The bias can be decomposed into the following two terms

$$\theta^\top B \theta^* = \theta^\top \left( I - \frac{\lambda}{n} X^\top X \right)^t \left( \Sigma - \frac{1}{n} X^\top X \right) \left( I - \frac{\lambda}{n} X^\top X \right)^t \theta^*$$

$$+ \theta^\top \left( \frac{1}{n} X^\top X \right) \left( I - \frac{\lambda}{n} X^\top X \right)^{2t} \theta^*.$$

For sufficiently small learning rate $\lambda$ as given by corollary A.1, we know that with high probability

$$\left\| I - \frac{\lambda}{n} X^\top X \right\| \leq 1,$$

which together with lemma A.5 gives a high probability bound on the first term:

$$\theta^\top \left( I - \frac{\lambda}{n} X^\top X \right)^t \left( \Sigma - \frac{1}{n} X^\top X \right) \left( I - \frac{\lambda}{n} X^\top X \right)^t \theta^*$$

$$\leq c \|\Sigma\| \|\theta^*\|^2 \max \left\{ \sqrt{\frac{r(\Sigma)}{n}}, \frac{r(\Sigma)}{n}, \sqrt{\frac{\log(\frac{1}{\delta})}{n}}, \frac{\log(\frac{1}{\delta})}{n} \right\} \theta^*.$$

For the second term, invoke lemma A.6 with $P = \frac{\lambda}{n} X^\top X$ and we get

$$\theta^\top \left( \frac{1}{n} X^\top X \right) \left( I - \frac{\lambda}{n} X^\top X \right)^{2t} \theta^* \leq \frac{1}{\lambda} \|\theta^*\|^2 \left\| \left( \frac{\lambda}{n} X^\top X \right) \left( I - \frac{\lambda}{n} X^\top X \right)^{2t} \right\|$$

$$\leq \frac{1}{2\lambda t} \|\theta^*\|^2.$$

Putting these two bounds together gives the proof for the main theorem.

\[\square\]

### A.5 Proof for the Variance Upper Bound

Recall that $X = U \tilde{\Lambda}^{\frac{1}{2}} W^\top$ is the singular value decomposition of data matrix $X$, where $U = (u_1, \cdots, u_n)$, $W = (w_1, \cdots, w_n)$, $\tilde{\Lambda} = \text{diag}\{\mu_1, \cdots, \mu_n\}$ with $\mu_1 \geq \mu_2 \geq \cdots \mu_n$. 

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Recall that
\[
k_0 = \min\{l \geq 0 : \lambda_{l+1} \leq \frac{c_0 \sum_{i > l} \lambda_i}{n}\},
\]
\[
k_1 = \min\{l \geq 0 : \lambda_{l+1} \leq \frac{c_1 \sum_{i > 0} \lambda_i}{n}\},
\]
\[
k_2 = \min\{l \geq 0 : \sum_{i > l} \lambda_i + n\lambda_{l+1} \leq c_2 c(t, n) \sum_{i > 0} \lambda_i\},
\]
for some constant \(c_0, c_1, c_2\) and function \(c(t, n)\).

We further define
\[
k_3 = \min\{l \geq 0 : \mu_{l+1} \leq c_3 c(t, n) \sum_{i > 0} \lambda_i\},
\]
for some constant \(c_3\).

The next lemma shows that we can appropriately choose constants to ensure that \(k_3 \leq k_2\) holds with high probability, and in some specific cases we have \(k_2 \leq k_1\).

**Lemma A.8.** For any function \(c(t, n)\) and constant \(c_2\), there exists constants \(c, c_3\), such that \(k_3 \leq k_2\) with probability at least \(1 - e^{-\frac{n}{c}}\). Furthermore, if \(c(t, n)\) is a positive constant function, for any \(c_1\), there exists \(c_2\) such that \(k_2 \leq k_1\).

**Proof.** According to lemma A.1 there exists a constant \(c\), with probability at least \(1 - e^{-\frac{n}{c}}\) we have
\[
\mu_{k_2+1} \leq c \left( \sum_{i > k_2} \lambda_i + n\lambda_{k_2+1} \right) \leq cc_2 c(t, n) \sum_{i > 0} \lambda_i.
\]
Therefore, we know that \(k_3 \leq k_2\) for \(c_3 = cc_2\).

By the definition of \(k_1\), we have
\[
\sum_{i > k_1} \lambda_i + n\lambda_{k_1+1} \leq (c_1 + 1) \sum_{i > 0} \lambda_i,
\]
which implies that \(k_2 \leq k_1\) for \(c_2 = \frac{c_1 + 1}{c(t, n)}\), if \(c(t, n)\) is a positive constant. \(\square\)

Next we bound \(\text{Tr}[C]\), which implies an upper bound on the variance term.

**Theorem A.1.** There exist constants \(c, c_0, c_1, c_2\) such that if \(k_0 \leq \frac{n}{c}\), then with probability at least \(1 - e^{-\frac{n}{c}}\), the trace of the variance matrix \(C\) has the following upper bound
\[
\text{Tr}[C] \leq c \left( \frac{k_1}{n} + \frac{k_2}{c(t, n)n} + c(t, n) \left( \frac{\lambda_1}{n} \sum_{i > 0} \lambda_i \right)^2 \right).
\]
Proof. We divide the eigenvalues of $XX^\top$ into two groups based on whether they are greater than $c_3 c(t, n) \sum_{i>0} \lambda_i$. The first group consists of $\mu_1 \cdots \mu_{k_3}$, and the second group consists of $\mu_{k_3+1} \cdots \mu_n$. For $1 \leq j \leq k_3$, we have

$$1 - \left(1 - \frac{\lambda}{n} \mu_j\right)^t \leq 1.$$ 

Therefore we have the following upper bound on $\left[ I - \left(I - \frac{\lambda}{n} XX^\top\right)^t \right]^2$:

$$\left[ I - \left(I - \frac{\lambda}{n} XX^\top\right)^t \right]^2 = U \text{diag} \left\{ \left[ 1 - \left(1 - \frac{\lambda}{n} \mu_1 \right)^t \right]^2, \ldots, \left[ 1 - \left(1 - \frac{\lambda}{n} \mu_n \right)^t \right]^2 \right\} U^\top$$

$$\leq U \text{diag} \left\{ \underbrace{\left[ 1 - \left(1 - \frac{\lambda}{n} \mu_1 \right)^t \right]^2, \ldots, \left[ 1 - \left(1 - \frac{\lambda}{n} \mu_n \right)^t \right]^2}_{k_3 \text{ times}}, \underbrace{0, \ldots, 0}_{n-k_3 \text{ times}} \right\} U^\top$$

$$= U \text{diag} \left\{ \underbrace{0, \ldots, 0}_{k_3 \text{ times}}, \underbrace{\left[ 1 - \left(1 - \frac{\lambda}{n} \mu_1 \right)^t \right]^2, \ldots, \left[ 1 - \left(1 - \frac{\lambda}{n} \mu_n \right)^t \right]^2}_{n-k_3 \text{ times}} \right\} U^\top.$$ 

For positive semidefinite matrices $P, Q, R$ which satisfies $Q \preceq R$, it holds that
\[ \text{Tr}[PQ] \leq \text{Tr}[PR] \]. It implies the following upperbound of \( \text{Tr}[C] \):

\[
\text{Tr}[C] = \text{Tr} \left[ I - \left( I - \frac{\lambda}{n} XX^\top \right) \right]^2 \left( XX^\top \right)^{-2} XX^\top \]
\leq \text{Tr} \left[ \underbrace{U \text{diag} \left\{ 1, \cdots, 1, 0, \cdots, 0 \right\}}_{(1)} \right] \left( XX^\top \right)^{-2} XX^\top
\]

\[\begin{align*}
&+ \text{Tr} \left[ \underbrace{U \text{diag} \left\{ \underbrace{0, \cdots, 0}_{n-k_3 \text{ times}}, \left[ 1 - \left( 1 - \frac{\lambda}{n} \mu_{k_3+1} \right) \right]^{t_2}, \cdots, \left[ 1 - \left( 1 - \frac{\lambda}{n} \mu_n \right) \right]^{t_2} \right\}}_{(2)} \right] \left( XX^\top \right)^{-2} XX^\top
\end{align*}\]

(4)

**Bounding (1)**

Noticing \( X = U \tilde{\Lambda}^{\frac{1}{2}} W^\top \) and \( \Sigma = \sum_{i \geq 1} \lambda_i v_i v_i^\top \), we express the first term as sums of eigenvector products,

\[
(1) = \text{Tr} \left[ U \text{diag} \left\{ \underbrace{1, \cdots, 1}_{k_3 \text{ times}}, \underbrace{0, \cdots, 0}_{n-k_3 \text{ times}} \right\} \right] \left( XX^\top \right)^{-2} XX^\top
\]

\[\begin{align*}
&= \text{Tr} \left[ U \text{diag} \left\{ \underbrace{1, \cdots, 1}_{k_3 \text{ times}}, \underbrace{0, \cdots, 0}_{n-k_3 \text{ times}} \right\} \right] \left( XX^\top \right)^{-2} XX^\top \left( \tilde{\Lambda}^{-2} U^\top U \tilde{\Lambda}^{\frac{1}{2}} W^\top \right) \Sigma W \tilde{\Lambda}^{\frac{1}{2}} U^\top
\end{align*}\]

\[\begin{align*}
&= \text{Tr} \left[ \text{diag} \left\{ \underbrace{1, \cdots, 1}_{k_3 \text{ times}}, \underbrace{0, \cdots, 0}_{n-k_3 \text{ times}} \right\} \right] \tilde{\Lambda}^{-1} W^\top \Sigma W
\]

\[\begin{align*}
&= \sum_{i \geq 1} \lambda_i \text{Tr} \left[ \text{diag} \left\{ \underbrace{1, \cdots, 1}_{k_3 \text{ times}}, \underbrace{0, \cdots, 0}_{n-k_3 \text{ times}} \right\} \right] \tilde{\Lambda}^{-1} W^\top v_i v_i^\top W
\end{align*}\]

\[\begin{align*}
&= \sum_{i \geq 1} \sum_{1 \leq j \leq k_3} \frac{\lambda_i}{\mu_j} \left( v_i^\top w_j \right)^2.
\end{align*}\]

Next we divide the above summation into \( 1 \leq i \leq k_1 \) and \( i > k_1 \). For the first part,
notice that
\[
\sum_{1 \leq j \leq k_3} \frac{\lambda_i}{\mu_j} (v_i^\top w_j)^2 \leq \sum_{1 \leq j \leq n} \frac{\lambda_i}{\mu_j} (v_i^\top w_j)^2
\]
\[
= \lambda_i v_i^\top \left( \sum_{1 \leq j \leq n} \frac{1}{\mu_j} w_j^\top \right) v_i
\]
\[
= \lambda_i v_i^\top W \tilde{\Lambda}^{-1} W^\top v_i
\]
\[
= \lambda_i v_i^\top W \tilde{\Lambda}^{-1} U^\top U \tilde{\Lambda}^{-2} U^\top W \tilde{\Lambda}^{-1} W^\top v_i
\]
\[
= \lambda_i^2 z_i^\top (XX^\top)^{-2} z_i,
\]

where \(z_i\) is defined as \(z_i = \frac{X v_i}{\sqrt{\lambda_i}} = \frac{U \tilde{\Lambda}^{-1} W^\top v_i}{\sqrt{\lambda_i}}\).

From the proof of lemma 11 in Bartlett et al. (2020), we know that for any \(\sigma_x\), there exists a constant \(c_0\) and \(c\) such that if \(k_0 \leq \frac{n}{c}\), with probability at least \(1 - e^{-\frac{n}{c}}\) the first part can be bounded as

\[
\sum_{1 \leq i \leq k_1} \sum_{1 \leq j \leq k_3} \frac{\lambda_i}{\mu_j} (v_i^\top w_j)^2 \leq \sum_{1 \leq i \leq k_1} \lambda_i^2 z_i^\top (XX^\top)^{-2} z_i \leq c \frac{k_1}{n},
\]

which gives a bound for the first part.

For the second part we interchange the order of summation and have

\[
\sum_{i \geq k_1} \sum_{1 \leq j \leq k_3} \frac{\lambda_i}{\mu_j} (v_i^\top w_j)^2 = \sum_{1 \leq j \leq k_3} \sum_{i \geq k_1} \frac{\lambda_i}{\mu_j} (v_i^\top w_j)^2
\]
\[
\leq c_3 c(t, n) \sum_{i > 0} \lambda_i \sum_{1 \leq j \leq k_3} \sum_{i \geq k_1} (v_i^\top w_j)^2
\]
\[
= \frac{\lambda_{k_1+1}}{c_3 c(t, n) \sum_{i > 0} \lambda_i} \sum_{1 \leq j \leq k_3} \sum_{i \geq k_1} (v_i^\top w_j)^2
\]
\[
\leq \frac{\lambda_{k_1+1}}{c_3 c(t, n) \sum_{i > 0} \lambda_i} \sum_{1 \leq j \leq k_3} 1
\]
\[
= \frac{\lambda_{k_1+1} k_3}{c_3 c(t, n) \sum_{i > 0} \lambda_i}
\]
\[
\leq c \frac{k_3}{c(t, n) n}.
\]

for \(c\) large enough.

Putting 5 and 6 together, and noting that \(k_3 \leq k_2\) with high probability as given in lemma A.8, we know there exists a constant \(c\) that with probability at least \(1 - e^{-\frac{n}{c}}\),

\[
\sum_{1 \leq j \leq n} \frac{\lambda_i}{\mu_j} (v_i^\top w_j)^2 \leq c \frac{k_1}{n} + c \frac{k_2}{c(t, n) n}.
\]
Bounding (2)
Similar to the first step in bounding (1), we note that

\[
2 = \text{Tr} \left[ U \text{diag} \left\{ \underbrace{0, \cdots, 0}_{k_3 \text{ times}}, \left[ 1 - \left(1 - \frac{\lambda}{n} \mu_{k_3+1}\right)^t \right]^2, \cdots, \left[ 1 - \left(1 - \frac{\lambda}{n} \mu_n\right)^t \right]^2 \right\} \right]
\]

\[
U \tilde{\Lambda}^{-2} U^T U \tilde{\Lambda}^{\frac{1}{2}} W^T \Sigma W \tilde{\Lambda}^{\frac{1}{2}} U^T \]

\[
= \text{Tr} \left[ \text{diag} \left\{ \underbrace{0, \cdots, 0}_{k_3 \text{ times}}, \frac{1}{\mu_{k_3+1}} \left[ 1 - \left(1 - \frac{\lambda}{n} \mu_{k_3+1}\right)^t \right]^2, \cdots, \frac{1}{\mu_n} \left[ 1 - \left(1 - \frac{\lambda}{n} \mu_n\right)^t \right]^2 \right\} \right]
\]

\[
W^T \Sigma W \right].
\]

From Bernoulli's inequality and the definition of \( k_3 \), for any \( k_3 + 1 \leq j \leq n \), we have

\[
\frac{1}{\mu_k} \left[ 1 - \left(1 - \frac{\lambda}{n} \mu_k\right)^t \right]^2 \leq \frac{1}{\mu_k} \left( \frac{\lambda}{n} \mu_k t \right)^2 = \left( \frac{\lambda t}{n} \right)^2 \mu_k \leq c_3 \left( \frac{\lambda t}{n} \right)^2 c(t, n) \sum_{i>0} \lambda_i, \tag{7}
\]

Hence,

\[
2 \leq c_3 c(t, n) \left( \frac{\lambda t}{n} \right)^2 \sum_{i>0} \lambda_i \text{Tr}[W^T \Sigma W]
\]

\[
= c_3 c(t, n) \left( \frac{\lambda t}{n} \sum_{i>0} \lambda_i \right)^2.
\]

Putting things together
From the bounds for (1) and (2) given above, we know that there exists a constant \( c \) such that with probability at least \( 1 - e^{-\frac{n}{2}} \), the trace of the variance matrix \( C \) has the following upper bound

\[
\text{Tr}[C] \leq c \left( \frac{k_1}{n} + \frac{k_2}{c(t, n)n} + c(t, n) \left( \frac{\lambda t}{n} \sum_{i>0} \lambda_i \right)^2 \right).
\]

\[
\square
\]

Corollary A.2. If we take \( \lambda = \frac{a_1}{\sum_{i>0} \lambda_i} \), \( c(t, n) = a_2 \), \( t \leq a_3 \sqrt{\max\{k_1, 1\} n} \) for some appropriate constant \( a_1, a_2, a_3 \), then there exist constants \( c, c_0, c_1 \), such that if \( k_0 \leq \frac{n}{e} \) then
with probability at least $1 - e^{-\frac{n}{2}}$, the trace of the variance matrix $C$ has the following upper bound

$$\text{Tr}[C] \leq c \frac{\max \{k_1, 1\}}{n}.$$ 

**Proof.** When $c(t, n)$ is a constant, we know that $k_2 \leq k_1$ with high probability as given in lemma [A.8](#). Moreover, if $t \leq a_3 \sqrt{\max \{k_1, 1\} n}$, we have $\frac{k}{n} \sum_{i>0} \lambda_i \leq a_1 a_3 \sqrt{\max \{k_1, 1\}} n$. These two observations gives the required bound. \qed

### A.6 Omitted Calculations in Section 4.2

1. **Calculations for $\lambda_k = \frac{1}{k^\alpha}, \alpha > 1$**

   Define $r_k(\Sigma) = \sum_{i \geq k} \frac{\lambda_i}{\lambda_{k+1}}$ as in [Bartlett et al. (2020)](#). Since $\sum_{i \geq k} \frac{1}{i} = \Theta(\frac{1}{k^{\alpha-1}})$, we have $r_k(\Sigma) = \Theta\left(\frac{1}{k^{\alpha-1}}\right) = \Theta(k)$. Hence, $k_0 = \Theta(n)$, and the conditions of theorem 4.1 is satisfied.

   As $\sum_{i>0} \lambda_i < \infty$, By its definition we know that $k_1$ is the smallest $l$ such that $\lambda_{l+1} = O\left(\frac{1}{l}\right)$. Therefore, $k_1 = \Theta\left(n^{\frac{1}{\alpha}}\right)$.

2. **Calculations for $\lambda_k = \frac{1}{k \log^\beta(k+1)}, \beta > 1$**

   $$\sum_{i > k} \frac{1}{i \log^\beta(i+1)} = \Theta\left(\int_k^{\infty} \frac{1}{x \log^\beta x} dx\right) = \Theta\left(\frac{1}{\log^\beta(k+1)}\right),$$

   which implies $r_k(\Sigma) = k \log k$.

   Solving $k_0 \log k_0 = \Theta(n)$, we have $k_0 = \Theta\left(\frac{n}{\log n}\right)$.

   By the definition of $k_1$, we know that $k_1$ is the smallest $l$ such that $l \log^\beta(l+1) = \Theta(n)$. Therefore, $k_1 = \Theta\left(\frac{n}{\log^\beta n}\right)$.

3. **Calculations for $\lambda_i = \frac{1}{i^{1+\epsilon}}, 1 \leq i \leq n^{1+\epsilon}, \epsilon > 0$**

   Since $r(\Sigma) = n^{1+\epsilon}$, we have $k_0 = 0$. By the definition of $k_1$, we also have $k_1 = 0$.

4. **Calculations for $\lambda = \begin{cases} \frac{1}{s} & 1 \leq k \leq s \\ \frac{1}{d-s} & s+1 \leq k \leq d \end{cases}, s = n^r, d = n^q, 0 < r \leq 1, q \geq 1$**

   For $0 \leq k < s$, $r_k(\Sigma) = \Theta\left(\frac{1}{s}\right) = \Theta(n^r) = o(n)$, while $r_s(\Sigma) = \frac{1}{s^{r-1}} = \Theta(n^q) = \omega(n)$. Therefore, $k_0 = s = n^r$.

   Similarly, noting that $\lambda_k = \frac{1}{n^r} = \omega(n)$ for $0 \leq k < s$ and $\lambda_s = \Theta\left(\frac{1}{n^q}\right) = o(n)$, we know that $k_1 = s = n^r$. 

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Table 3: The effective dimension $k_1$, the optimal early stopping excess risk and min-norm excess risk for different feature distributions, with sample size $n = 50$. The table shows that early stopping solution generalizes significantly better than min-norm solution, and reveals a positive correlation between the effective dimension $k_1$ and generalization performance of early stopping solution. We calculate the 95% confidence interval for the excess risk.

| DISTRIBUTIONS | $k_1$ | OPTIMAL EXCESS RISK | MIN-NORM EXCESS RISK |
|---------------|------|---------------------|----------------------|
| $\lambda_i = \frac{1}{i}$ | $\Theta(n)$ | $5.063 \pm 0.0138$ | $25.264 \pm 0.3205$ |
| $\lambda_i = \frac{1}{i^{0.5}}$ | $\Theta(n^{0.5})$ | $0.329 \pm 0.0044$ | $100.988 \pm 1.8757$ |
| $\lambda_i = \frac{1}{i^{2}}$ | $\Theta(n^2)$ | $0.0861 \pm 0.0017$ | $26.416 \pm 0.9112$ |
| $\lambda_i = \frac{1}{i^{3}}$ | $\Theta\left(\frac{n}{\log n}\right)$ | $1.466 \pm 0.0099$ | $93.412 \pm 1.3966$ |
| $\lambda_i = \frac{1}{i^{3}(i+1)}$ | $\Theta\left(\frac{n}{\log^2 n}\right)$ | $0.566 \pm 0.0070$ | $148.846 \pm 2.2944$ |
| $\lambda_i = \frac{1}{i^{4}(i+1)}$ | $\Theta\left(\frac{n}{\log^3 n}\right)$ | $0.284 \pm 0.0038$ | $86.090 \pm 1.6695$ |

A.7 Omitted Calculations for $\lambda_k = \frac{1}{k^\alpha}$, $\alpha > 1$ in Section 4.4

Set $c(t, n) = \frac{1}{n^\beta}$, where $\beta > 0$ will be chosen later. First we calculate $k_2$ under this choice of $c(t, n)$. Note that $\sum_{i > k_2} \frac{1}{i^{\alpha}} = \Theta\left(\frac{1}{k_2^{\alpha-1}}\right)$. Therefore, $k_2$ is the smallest $k$ such that $\frac{1}{k_2^{\alpha-1}} + \frac{n}{k_2^{\alpha}} = O\left(\frac{1}{n^{\beta}}\right)$. For the bound on $V(\theta_t)$ to be non-vacuous, we need $k_2 = o(n)$. Hence, $\frac{1}{k_2^{\alpha-1}} = O\left(\frac{1}{n^{\beta-1}}\right)$, which implies $k_2 = n^{\frac{\beta+1}{\alpha}}$.

Plugging the value of $c(t, n)$ and $k_2$ into our bound, we have

$$V(\theta_t) = O\left(\frac{n^{\frac{\beta+1}{\alpha}-2\beta-1} + n^{2\beta-2}}{\alpha}\right)$$

which attains its minimum $\Theta\left(n^{\frac{2\alpha-3\alpha+2\beta-1}{2\alpha+2}}\right)$ at $\beta = \Theta\left(\frac{2\alpha-3\alpha+2\beta-1}{2\alpha+2}\right)$.

For $V(\theta) = O(1)$, we need $\tau \leq \frac{3\alpha+1}{2\alpha+2}$. For $\beta \geq 0$, we need $\tau \geq \frac{\alpha+1}{2\alpha}$. Putting them together gives the range of $t$ in which the above calculation applies.

B Additional Experiment Results

In this section, we provide the experiment results of sample size $n = 50$ and $n = 200$. The settings are the same as the experiments in the main text, except for the sample size. The optimal excess risk and min-norm excess risk are provided in Table 3 and Table 4. The excess risk curve and training loss curve are provided in Table 3 and Table 4. The tables and figures indicate that the three observations given in section 5 hold for different sample size $n$. 
Table 4: The effective dimension $k_1$, the optimal early stopping excess risk and min-norm excess risk for different feature distributions, with sample size $n = 200$. The table shows that early stopping solution generalizes significantly better than min-norm solution, and reveals a positive correlation between the effective dimension $k_1$ and generalization performance of early stopping solution. We calculate the 95% confidence interval for the excess risk.

| DISTRIBUTIONS | $k_1$ | OPTIMAL EXCESS RISK | MIN-NORM EXCESS RISK |
|---------------|-------|---------------------|----------------------|
| $\lambda_i = \frac{1}{\gamma}$ | $\Theta(n)$ | 4.492 ± 0.0126 | 104.752 ± 0.8042 |
| $\lambda_i = \frac{1}{\gamma^2}$ | $\Theta(n^{\frac{1}{2}})$ | 0.323 ± 0.0078 | 74.040 ± 0.9807 |
| $\lambda_i = \frac{1}{\gamma^3}$ | $\Theta(n^{\frac{1}{3}})$ | 0.0695 ± 0.0010 | 16.398 ± 0.4626 |
| $\lambda_i = \frac{1}{\log(n+1)}$ | $\Theta(\frac{n}{\log n})$ | 1.254 ± 0.0049 | 305.402 ± 2.2147 |
| $\lambda_i = \frac{1}{\log^2(n+1)}$ | $\Theta(\frac{n}{\log^2 n})$ | 0.425 ± 0.0048 | 167.100 ± 1.5191 |
| $\lambda_i = \frac{1}{\log^3(n+1)}$ | $\Theta(\frac{n}{\log^3 n})$ | 0.293 ± 0.0059 | 66.925 ± 0.9100 |

Figure 3: Excess risk curve and training loss curve for different distributions, with sample size $n = 50$. We plot the lowest point (red point) on the excess risk curve (blue line). Besides, we plot the smallest time (brown point) where the training error curve (orange line) reaches $\frac{\sigma^2}{2}$ (green dotted line), indicating that overfitting has already happened. The figures illustrate that (a.) the models have already become overfitting when they achieve minimal excess risk, since the red points always lie on the right of the brown points; and (b.) the faster $\lambda_i$ decays, the better early stopping solution generalizes, which corroborates with our theory.
Figure 4: Excess risk curve and training loss curve for different distributions, with sample size $n = 200$. We plot the lowest point (red point) on the excess risk curve (blue line). Besides, we plot the smallest time (brown point) where the training error curve (orange line) reaches $\frac{1}{2} i^2$ (green dotted line), indicating that overfitting has already happened. The figures illustrate that (a.) the models have already become overfitting when they achieve minimal excess risk, since the red points always lie on the right of the brown points; and (b.) the faster $\lambda_i$ decays, the better early stopping solution generalizes, which corroborates with our theory.