On the Double Descent of Random Features Models Trained with SGD

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Abstract

We study generalization properties of random features (RF) regression in high dimensions optimized by stochastic gradient descent (SGD). In this regime, we derive precise non-asymptotics error bounds of RF regression under both constant and polynomial-decay step-size SGD setting, and observe the double descent phenomenon both theoretically and empirically. Our analysis shows how to cope with multiple randomness sources of initialization, label noise, and data sampling (as well as stochastic gradients) with no closed-form solution, and also goes beyond the commonly-used Gaussian/spherical data assumption. Our theoretical results demonstrate that, with SGD training, RF regression still generalizes well for interpolation learning, and is able to characterize the double descent behavior by the unimodality of variance and monotonic decrease of bias. Besides, we also prove that the constant step-size SGD setting incurs no loss in convergence rate when compared to the exact minimal-norm interpolator, as a theoretical justification of using SGD in practice.

1 Introduction

Harmless interpolation or benign overfitting of over-parameterized neural network models has received significant attention in the literature [1, 2, 3]. This important phenomenon is also inherently tied to the discovery of *double descent* [4] in deep learning. Indeed, many key machine learning models, including but not limited to kernel methods [5, 6, 7], and neural networks [8, 9, 10] first decrease the test error with increasing number of model parameters in the under-parameterized regime. They then yield large error when they can first interpolate the data, which is called the interpolation threshold. Finally, the test error decreases again in the over-parameterized regime in stark contrast to conventional learning theory results [2, 3, 4].

Our work partakes in this research vein and studies the random features (RF) model [11] in the context of double descent phenomenon. Briefly, RF model samples random features $\{\boldsymbol{\omega}_i\}_{i=1}^m$ from a specific distribution, corresponding to a kernel function. We then construct an explicit map: $\boldsymbol{x} \in \mathbb{R}^d \mapsto \sigma(\boldsymbol{W}\boldsymbol{x}) \in \mathbb{R}^m$, where $\boldsymbol{W} = [\boldsymbol{\omega}_1, \cdots, \boldsymbol{\omega}_m]^\top \in \mathbb{R}^{m\times d}$ is the random features matrix and $\sigma(\cdot)$ is the nonlinear (activation) function determined by the kernel. As a result, the RF model can be viewed as training a two-layer neural network where the weights in the first layer are chosen randomly and then fixed (a.k.a. the random features) and only the output layer is optimized, striking a trade-off between practical performance and accessibility to analysis. An RF model becomes an over-parameterized model if we take the number of random features m larger than that of training data n. The literature on RF under the over-parameterized regime can be split into various camps according to different assumptions on the formulation of target function, data distribution, and

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activation functions [6, 12, 13, 14, 15, 16] (see comparisons in Table 1 in Appendix A). The existing theoretical results demonstrate that the excess risk curve exhibits double descent.

Nevertheless, the analysis framework of previous work on RF regression mainly relies on the least-squares closed-form solution, including *minimal-norm* interpolator and ridge regressor. Besides, they often assume the data with specific distribution, e.g., to be Gaussian or uniformly spread on a sphere. Such dependency on the analytic solution and specific data distribution in fact mismatch practical neural networks optimized by stochastic gradient descent (SGD) based algorithms on general data distribution. Our work precisely bridges this gap: We provide a new analysis framework for the generalization properties of RF models trained with SGD, also accommodating adaptive (i.e., polynomial decay) step-size selection, and provide non-asymptotic results in under-/over-parameterized regimes on (relatively) general data distribution and activation functions. We make the following contributions:

- We characterize statistical properties of several covariance operators/matrices in RF, including $\Sigma_m := \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}[\sigma(\boldsymbol{W}\boldsymbol{x}/\sqrt{d})\sigma(\boldsymbol{W}\boldsymbol{x}/\sqrt{d})^\top]$ and its expectation version $\widetilde{\Sigma}_m := \mathbb{E}_{\boldsymbol{W}}[\Sigma_m]$. We demonstrate that, under Gaussian initialization, if the activation function $\sigma(\cdot) : \mathbb{R} \mapsto \mathbb{R}$ is Lipschitz continuous, $\mathrm{Tr}(\Sigma_m)$ is a sub-exponential random variable with $\mathcal{O}(1)$ sub-exponential norm; $\widetilde{\Sigma}_m$ has only two distinct eigenvalues at $\mathcal{O}(1)$ and $\mathcal{O}(1/m)$ order, respectively. Such analysis on the spectra of Σ_m and $\widetilde{\Sigma}_m$ (without spectral decay assumption) is helpful to obtain sharp error bounds for excess risk.
- Based on the bias-variance decomposition in stochastic approximation, we take into account multiple randomness sources of initialization, label noise, and data sampling as well as stochastic gradients. We derive non-asymptotic error bounds under the optimization effect: the error bounds for bias and variance as a function of the radio m/n are monotonic decreasing and unimodal, respectively. Importantly, our analysis holds for both constant and polynomial-decay step-size SGD setting, and is valid under (relatively) general assumptions on data distribution and activation functions.
- Our non-asymptotic results show that, RF regression trained with SGD still generalizes well for interpolation learning, and is able to capture the double descent behavior. In addition, we demonstrate that the constant step-size SGD setting incurs no loss on the convergence rate of excess risk when compared to the exact least-squares closed form solution. Our empirical evaluations support our theoretical results and findings.

Our analysis (technical contributions are discussed in Section 4) sheds light on the effect of SGD on high dimensional RF models in under-/over-parameterized regimes, and bridges the gap between the minimal-norm solution and numerical iteration solution in terms of optimization and generalization on double descent. It would be helpful for understanding large dimensional machine learning and neural network models more generally.

2 Related Work and Problem Setting

This section reviews relevant works and introduces our problem setting of RF regression with SGD.

Notation: For two operators/matrices, $A \preccurlyeq B$ means $B - A$ is positive semi-definite (PSD). For any two positive sequences $\{a_t\}_{t=1}^s$ and $\{b_t\}_{t=1}^s$, the notation $a_t \lesssim b_t$ means that there exists a positive constant C independent of s such that $a_t \leq C b_t$, and analogously for $\sim$, $\gtrsim$, and $\eqsim$. For any $a, b \in \mathbb{R}$, $a \wedge b$ denotes the minimum of a and b.

2.1 Related works

A flurry of research papers are devoted to analysis of over-parameterized models on optimization [17, 18, 19], generalization (or their combination) under neural tangent kernel [20, 21, 22] and mean-field analysis regime [23, 24]. We take a unified perspective on optimization and generalization but work in the high-dimensional setting to fully capture the double descent behavior. By high-dimensional setting, we mean that m, n, and d increase proportionally, large and comparable [6, 12, 14, 13].

Double descent in random features model: Characterizing the double descent of the RF model often derives from random matrix theory (RMT) in high dimensional statistics [2, 6, 12, 14, 25] and from the replica method [13, 26, 15]. Under specific assumptions on data distribution, activation functions, target function, and initialization, these results show that the generalization error/excess risk increase when $m/n < 1$, diverge when $m/n \to 1$, and then decrease when $m/n > 1$. Further, refined results are developed on the *analysis of variance* due to multiple randomness sources [13, 27, 16]. We refer to comparisons in Table 1 in Appendix A for further details. Technically speaking, since RF (least-squares) regression involves with inverse random matrices, these two classes of methods attempt to achieve a similar target: how to disentangle the nonlinear activation function by the Gaussian equivalence conjecture. RMT utilizes calculus of deterministic equivalents (or resolvents) for random matrices and replica methods focus on some specific scalar parameters that allows for circumventing the expectation computation. In fact, most of the above methods can be asymptotically equivalent to the Gaussian covariate model [28].

Non-asymptotic stochastic approximation: Many papers on linear least-squares regression [29, 30], kernel regression [31, 32], random features [33] with SGD often work in the under-parameterized regime, where d is finite and much smaller than n. In the over-parameterized regime, under GD setting, the excess risk of least squares is controlled by the smallest positive eigenvalue in [34] by virtue of random matrix theory. Under the averaged constant step-size SGD setting, the excess risk in [35] on least squares in high dimensions can be independent of d, and is further improved to converge with n in [36]. This convergence rate is also demonstrated under the $\min$ [37] or last-iterate [38] setting in step-size SGD for noiseless least squares. We also notice a concurrent work [39] on last-iterate SGD with decaying step-size on least squares. Besides, the existence of multiple descent [40, 41] beyond double descent and SGD as implicit regularizer [42, 43] can be traced to the above two lines of work. Our work shares some similar technical tools with [31] and [36] but differs from them in several aspects. We detail the differences in Section 4.

2.2 The problem setting

We study the standard problem setting for RF least-squares regression and adopt the relevant terminologies from learning theory: *cf.*, [44, 31, 33, 25] for details. Let $X \subseteq \mathbb{R}^d$ be a metric space and $Y \subseteq \mathbb{R}$. The training data $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ is assumed to be independently drawn from a non-degenerate unknown Borel probability measure ρ on $X \times Y$. The *target function* of ρ is defined by $f_\rho(\boldsymbol{x}) = \int_Y y \,\mathrm{d}\rho(y \mid \boldsymbol{x})$, where $\rho(\cdot \mid \boldsymbol{x})$ is the conditional distribution of ρ at $\boldsymbol{x} \in X$.

RF least squares regression: We study the RF regression problem with the squared loss as follows:

$$\min_{f \in \mathcal{H}} \mathcal{E}(f), \quad \mathcal{E}(f) := \int (f(\boldsymbol{x}) - y)^2 \mathrm{d}\rho(\boldsymbol{x}, y) = \|f - f_\rho\|^2_{L^2_{\rho_X}}, \text{ with } f(\boldsymbol{x}) = \langle \boldsymbol{\theta}, \varphi(\boldsymbol{x}) \rangle \,,$$

where the optimization vector $\boldsymbol{\theta} \in \mathbb{R}^m$ and the feature mapping $\varphi(\boldsymbol{x})$ is defined as

$$\varphi(\boldsymbol{x}) := \frac{1}{\sqrt{m}} \left[\sigma(\boldsymbol{\omega}_1^\top \boldsymbol{x}/\sqrt{d}), \cdots, \sigma(\boldsymbol{\omega}_m^\top \boldsymbol{x}/\sqrt{d}) \right]^\top = \frac{1}{\sqrt{m}} \sigma(\boldsymbol{W}\boldsymbol{x}/\sqrt{d}) \in \mathbb{R}^m \,, \tag{1}$$

where $\boldsymbol{W} = [\boldsymbol{\omega}_1, \cdots, \boldsymbol{\omega}_m]^\top \in \mathbb{R}^{m \times d}$ with $W_{ij} \sim \mathcal{N}(0, 1)$ corresponds to such two-layer neural network initialized with random Gaussian weights. Then, the corresponding hypothesis space $\mathcal{H}$ is a reproducing kernel Hilbert space

$$\mathcal{H} := \left\{ f \in L^2_{\rho_X} \,\middle|\, f(\boldsymbol{x}) = \frac{1}{\sqrt{m}} \langle \boldsymbol{\theta}, \sigma(\boldsymbol{W}\boldsymbol{x}/\sqrt{d}) \rangle \right\} \,, \tag{2}$$

with $\|f\|^2_{L^2_{\rho_X}} = \int_X |f(\boldsymbol{x})|^2 \mathrm{d}\rho_X(\boldsymbol{x}) = \langle f, \Sigma_m f \rangle_{\mathcal{H}}$ with the *covariance* operator $\Sigma_m : \mathbb{R}^m \to \mathbb{R}^m$

$$\Sigma_m = \int_X \varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x}) \mathrm{d}\rho_X(\boldsymbol{x}) \,, \tag{3}$$

which is the usually (uncentered) covariance matrix in finite dimensions,[1] i.e., $\boldsymbol{\Sigma}_m = \mathbb{E}_{\boldsymbol{x}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]$. Define $J_m : \mathbb{R}^m \to L^2_{\rho_X}$ such that$(J_m \boldsymbol{v})(\cdot) = \langle \boldsymbol{v}, \varphi(\cdot) \rangle, \quad \forall \boldsymbol{v} \in \mathbb{R}^m$, we have $\Sigma_m = J_m^* J_m$,

[1] In this paper, we do not distinguish the notations Σ_m and $\boldsymbol{\Sigma}_m$. This is also suitable to other operators/matrices, e.g., $\widetilde{\Sigma}_m$.

where J_m^* denotes the adjoint operator of J_m. Clearly, Σ_m is random with respect to $\boldsymbol{W}$, and thus its deterministic version is defined as $\widetilde{\Sigma}_m = \mathbb{E}_{\boldsymbol{x},\boldsymbol{W}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]$.

SGD with averaging: Regarding the stochastic approximation, we consider the polynomial-decay step-size SGD with iterate averaging at each iteration t, after a training sample $(\boldsymbol{x}_t, y_t) \sim \rho$ is observed, we update the decision variable as below (initialized at $\boldsymbol{\theta}_0$)

$$\boldsymbol{\theta}_t = \boldsymbol{\theta}_{t-1} + \gamma_t[y_t - \langle \boldsymbol{\theta}_{t-1}, \varphi(\boldsymbol{x}_t)\rangle]\varphi(\boldsymbol{x}_t), \qquad t = 1, 2, \ldots \tag{4}$$

This averaged SGD with bath size $= 1$ is commonly used in theory [31, 36, 45] for ease of analysis, which captures the key idea of SGD by combining stochastic gradients and data sampling. Here the step-size is given by $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0, 1)$, following [31], which naturally holds for the constant step-size case by taking $\zeta = 0$. The final output is defined as the average of the iterates: $\bar{\boldsymbol{\theta}}_n := \frac{1}{n}\sum_{t=0}^{n-1} \boldsymbol{\theta}_t$. Here we sum up $\{\theta_t\}_{t=0}^{n-1}$ with n terms for notational simplicity. The optimality condition for Eq. (4) implies $\mathbb{E}_{(\boldsymbol{x},y)\sim\rho}[(y - \langle \boldsymbol{\theta}^*, \varphi(\boldsymbol{x})\rangle)\varphi(\boldsymbol{x})] = \mathbf{0}$, which corresponds to $f^* = J_m\boldsymbol{\theta}^*$ if we assume that $f^* = \operatorname{argmin}_{f\in\mathcal{H}} \mathcal{E}(f)$ exists (see Assumption 2 in the next section). Likewise, we have $f_t = J_m\boldsymbol{\theta}_t$ and $\bar{f}_n = J_m\bar{\boldsymbol{\theta}}_n$.

In this paper, we study the averaged excess risk $\mathbb{E}\|\bar{f}_n - f^*\|^2_{L^2_{\rho_X}}$ instead of $\mathbb{E}\|\bar{f}_n - f_\rho\|^2_{L^2_{\rho_X}}$, that follows [31, 46, 33, 25], as f^* is the best possible solution in $\mathcal{H}$ and the mis-specification error $\|f^* - f_\rho\|^2_{L^2_{\rho_X}}$ pales into insignificance. Note that the expectation used here is considered with respect to the random features matrix $\boldsymbol{W}$, and the distribution of the training data $\{(\boldsymbol{x}_t, y_t)\}_{t=1}^n$ (note that $\|\bar{f}_n - f^*\|^2_{L^2_{\rho_X}}$ is itself a different expectation over ρ_X).

3 Main results

In this section, we present our main theoretical results on the generalization properties employing error bounds for bias and variance of RF regression in high dimensions optimized by averaged SGD.

3.1 Assumptions

Before we present our result, we list the assumptions used in this paper, refer to Appendix B for more discussions.

Assumption 1. *[47, 2, high dimensional setting] We work in the large d, n, m regime with $c \leqslant \{d/n, m/n\} \leqslant C$ for some constants $c, C > 0$ such that m, n, d are large and comparable. The data point $\boldsymbol{x} \in \mathbb{R}^d$ is assumed to satisfy $\|\boldsymbol{x}\|_2^2 \sim \mathcal{O}(d)$ and the sample covariance operator $\Sigma_d := \mathbb{E}_{\boldsymbol{x}}[\boldsymbol{x} \otimes \boldsymbol{x}]$ with bounded spectral norm $\|\Sigma_d\|_2$ (finite and independent of d).*

Assumption 2. *There exists $f^* \in \mathcal{H}$ such that $f^* = \operatorname{argmin}_{f\in\mathcal{H}} \mathcal{E}(f)$ with bounded Hilbert norm.*

Remark: This bounded Hilbert norm assumption is commonly used in [48, 41, 49] even though n and d tend to infinity. Bach [50] provides an example satisfying this assumption, *cf.*, Appendix B.

This is a standard assumption in learning theory, e.g., [46, 33]. Assuming the existence of $f^* \in \mathcal{H}$ implies that $\|f\|_{\mathcal{H}}$ is bounded in Eq. (2), which is in fact indispensable and standard.

Assumption 3. *The activation function $\sigma(\cdot)$ is assumed to be Lipschitz continuous.*

Assumption 4 (Fourth moment condition)**.** *Assume there exists some positive constants $r', r \geqslant 1$, such that for any PSD operator A, it holds that*

$$\mathbb{E}_{\boldsymbol{W}}[\Sigma_m A \Sigma_m] \preccurlyeq \mathbb{E}_{\boldsymbol{W}}\left(\mathbb{E}_{\boldsymbol{x}}\left([\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]A[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]\right)\right) \preccurlyeq r'\mathbb{E}_{\boldsymbol{W}}[\operatorname{Tr}(\Sigma_m A)\Sigma_m] \preccurlyeq r\operatorname{Tr}(\widetilde{\Sigma}_m A)\widetilde{\Sigma}_m.$$

Remark: This assumption follows [36] that requires the data are drawn from some not-too-heavy-tailed distribution, e.g., $\Sigma_m^{-\frac{1}{2}}\boldsymbol{x}$ has sub-Gaussian, or sub-exponential tails, common in high dimensional statistics. This condition is weaker than most previous work on double descent that requires the data to be Gaussian [2, 13, 27, 12], or uniformly spread on a sphere [6, 51], see comparisons in Table 1 in Appendix A. Besides, a special case of this assumption with $A := I$ is proved by Lemma 3, and thus this assumption can be regarded as a natural extension, with more discussions in Appendix B.

Assumption 5 (Noise condition)**.** *There exists $\tau > 0$ such that $\Xi := \mathbb{E}_{\boldsymbol{x}}[\varepsilon^2 \varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})] \preccurlyeq \tau^2 \Sigma_m$, where the noise $\varepsilon := y - f^*(\boldsymbol{x})$.*

Remark: This noise assumption is standard in [31, 36] and holds for the standard noise model $y = f^*(\boldsymbol{x}) + \varepsilon$ with $\mathbb{E}[\varepsilon] = 0$ and $\mathbb{V}[\varepsilon] < \infty$ [2].

3.2 Properties of covariance operators

Before we present the main results, we study statistical properties of Σ_m and $\widetilde{\Sigma}_m$ by the following lemmas (with proof deferred to Appendix C), that will be needed for our main result.

Lemma 1. *Under Assumption 1 and 3, if we further require $\sigma(\cdot)$ is single-output, then the expected covariance operator $\widetilde{\Sigma}_m := \mathbb{E}_{\boldsymbol{x},\boldsymbol{W}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})] \in \mathbb{R}^{m\times m}$ has the same diagonal elements and the same non-diagonal element*

$$(\widetilde{\Sigma}_m)_{ii} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]^2 \sim \mathcal{O}(1/m)\,, \quad (\widetilde{\Sigma}_m)_{ij} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\Big(\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]\Big)^2 \sim \mathcal{O}(1/m)\,.$$

Accordingly, $\widetilde{\Sigma}_m$ has only two distinct eigenvalues

$$\widetilde{\lambda}_1 = (\widetilde{\Sigma}_m)_{ii} + (m-1)(\widetilde{\Sigma}_m)_{ij} \sim \mathcal{O}(1)\,, \quad \widetilde{\lambda}_2 = (\widetilde{\Sigma}_m)_{ii} - (\widetilde{\Sigma}_m)_{ij} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\mathbb{V}[\sigma(z)] \sim \mathcal{O}(1/m).$$

Remark: Lemma 1 implies $\mathrm{tr}(\widetilde{\Sigma}_m) < \infty$. In fact, $\mathbb{E}_{\boldsymbol{x}}\mathbb{V}[\sigma(z)] > 0$ holds almost surely as $\sigma(\cdot)$ is not a constant, and thus $\widetilde{\Sigma}_m$ is positive definite. For description simplicity, we mainly focus on the single-output activation function in this paper, but it can be easily extended to a multiple-output version, as discussed in below.

Here we take two examples with different activation functions $\sigma(\cdot)$ for demonstration. The calculation details can be found in Appendix C.1.2.

1) If we choose the ReLU activation $\sigma(x) = \max\{x, 0\}$, RF actually approximates the first-order arc-cosine kernel [52] with $\varphi(\boldsymbol{x}) \in \mathbb{R}^m$. We have $(\widetilde{\Sigma}_m)_{ii} = \frac{1}{2md}\mathrm{Tr}(\Sigma_d)$ and $(\widetilde{\Sigma}_m)_{ij} = \frac{1}{2md\pi}\mathrm{Tr}(\Sigma_d)$ by recalling $\Sigma_d := \mathbb{E}_{\boldsymbol{x}}[\boldsymbol{x}\boldsymbol{x}^\top]$ and $\mathrm{Tr}(\Sigma_d)/d \sim \mathcal{O}(1)$.

2) If we choose $\sigma(x) = [\cos(x), \sin(x)]^\top$, a multiple-output version, RF actually approximates the Gaussian kernel with $\varphi(\boldsymbol{x}) \in \mathbb{R}^{2m}$ in Eq. (1), resulting in $\widetilde{\Sigma}_m \in \mathbb{R}^{2m\times 2m}$. In this case, $\widetilde{\Sigma}_m = S_1 \oplus S_2$ is a block diagonal matrix, where $\oplus$ is the direct sum. By denoting $\vartheta := \|\boldsymbol{x}\|_2^2/d$, the matrix $S_1 \in \mathbb{R}^{m\times m}$ has the same diagonal elements $[S_1]_{ii} = \frac{1}{2m}\mathbb{E}_{\boldsymbol{x}}\left[1 + \exp\left(-2\vartheta\right)\right]$, and the same non-diagonal elements $\frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\left[\exp\left(-\vartheta\right)\right]$. The matrix S_2 is diagonal with $[S_2]_{ii} = \frac{1}{2m}\mathbb{E}_{\boldsymbol{x}}\left[1 - \exp\left(-2\vartheta\right)\right]$. In this case, $\widetilde{\Sigma}_m$ admits three distinct eigenvalues: the largest eigenvalue at $\mathcal{O}(1)$ order, and the remaining two eigenvalues at $\mathcal{O}(1/m)$ order.

Lemma 2. *Under Assumptions 1 and 3, random variables $\|\Sigma_m\|_2$, $\|\Sigma_m - \widetilde{\Sigma}_m\|_2$, and $\mathrm{Tr}(\Sigma_m)$ are sub-exponential, and have sub-exponential norm at $\mathcal{O}(1)$ order.*

Lemma 3. *Under Assumptions 1,and 3, there exists a constant $r > 0$ such that $\mathbb{E}_{\boldsymbol{W}}\left(\Sigma_m^2\right) \preccurlyeq \mathbb{E}_{\boldsymbol{x},\boldsymbol{W}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})] \preccurlyeq r\mathrm{Tr}(\widetilde{\Sigma}_m)\widetilde{\Sigma}_m$.*

Lemma 4. *Under Assumptions 1 and 3, we have $\mathrm{Tr}[\widetilde{\Sigma}_m^{-1}\mathbb{E}_{\boldsymbol{W}}(\Sigma_m^2)] \sim \mathcal{O}(1)$.*

We remark here that Lemma 3 is a special case of Assumption 4 if we take $A := I$ and $r := 1 + \mathcal{O}\left(\frac{1}{m}\right)$; and Lemma 4 is a direct corollary of Lemma 3.

3.3 Results for error bounds

Recall the definition of the noise $\boldsymbol{\varepsilon} = [\varepsilon_1, \cdots, \varepsilon_n]^\top$ with $\varepsilon_t = y_t - f^*(\boldsymbol{x}_t)$, $t = 1, 2, \ldots, n$, the averaged excess risk can be expressed as

$$\mathbb{E}\|\bar{f}_n - f^*\|_{L^2_{\rho_X}}^2 := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\|\bar{f}_n - f^*\|_{L^2_{\rho_X}}^2 = \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle \bar{f}_n - f^*, \Sigma_m(\bar{f}_n - f^*)\rangle = \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle \bar{\eta}_n, \Sigma_m\bar{\eta}_n\rangle,$$

where $\bar{\eta}_n := \frac{1}{n}\sum_{t=0}^{n-1}\eta_t$ with the centered SGD iterate $\eta_t := f_t - f^*$. Following the standard bias-variance decomposition in stochastic approximation [31, 30, 36], it admits

$$\eta_t = [I - \gamma_t \varphi(\boldsymbol{x}_t)\otimes\varphi(\boldsymbol{x}_t)](f_{t-1} - f^*) + \gamma_t\varepsilon_t\varphi(\boldsymbol{x}_t)\,,$$

where the first term corresponds to the bias

$$\eta_t^{\texttt{bias}} = [I - \gamma_t \varphi(\boldsymbol{x}_t)\otimes\varphi(\boldsymbol{x}_t)]\eta_{t-1}^{\texttt{bias}}, \quad \eta_0^{\texttt{bias}} = f^*\,, \tag{5}$$

and the second term corresponds to the variance

$$\eta_t^{\texttt{var}} = [I - \gamma_t \varphi(\boldsymbol{x}_t)\otimes\varphi(\boldsymbol{x}_t)]\eta_{t-1}^{\texttt{var}} + \gamma_t\varepsilon_t\varphi(\boldsymbol{x}_t), \quad \eta_0^{\texttt{var}} = 0\,. \tag{6}$$

Accordingly, we have $f_t = \eta_t^{\texttt{bias}} + \eta_t^{\texttt{var}} + f^*$ due to $\mathbb{E}_{\boldsymbol{\varepsilon}}\bar{f}_n = \bar{\eta}_n^{\texttt{bias}} + f^*$ and $\|f\|^2_{L^2_{\rho_X}} = \langle f, \Sigma_m f\rangle$.

Proposition 1. *Based on the above setting, the averaged excess risk admits the following bias-variance decomposition*

$$\mathbb{E}\|\bar{f}_n - f^*\|^2_{L^2_{\rho_X}} = \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\|\bar{f}_n - \mathbb{E}_{\boldsymbol{\varepsilon}}\bar{f}_n + \mathbb{E}_{\boldsymbol{\varepsilon}}\bar{f}_n - f^*\|^2_{L^2_{\rho_X}} = \underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\langle\bar{\eta}_n^{\texttt{bias}}, \Sigma_m\bar{\eta}_n^{\texttt{bias}}\rangle}_{:=\texttt{Bias}} + \underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle\bar{\eta}_n^{\texttt{var}}, \Sigma_m\bar{\eta}_n^{\texttt{var}}\rangle}_{:=\texttt{Variance}}\,.$$

By (partly) decoupling the multiple randomness sources of initialization, label noise, and data sampling (as well as stochastic gradients), we give precise non-asymptotic error bounds for bias and variance as below.

Theorem 1. *(Error bound for bias) Under Assumptions 2, 1, 3, 4 with $r' \geqslant 1$, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0,1)$ satisfies $\gamma_0 \lesssim \frac{1}{r'\mathrm{Tr}(\widetilde{\Sigma}_m)} \sim \mathcal{O}(1)$, the* `Bias` *in Proposition 1 holds by*

$$\texttt{Bias} \lesssim \frac{\gamma_0 r' n^{\zeta-1}}{\sqrt{\mathbb{E}[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]^4}}\|f^*\|^2 \sim \mathcal{O}\left(n^{\zeta-1}\right)\,.$$

Remark: The error bound for `Bias` is monotonically decreasing at $\mathcal{O}(n^{\zeta-1})$ rate. For the constant step-size setting, it converges at $\mathcal{O}(1/n)$ rate, which is better than $\mathcal{O}(\sqrt{\log n/n})$ in [25] relying on closed-form solution under correlated features with polynomial decay on Σ_d.

Theorem 2. *(Error bound for variance) Under Assumptions 1, 3, 4 with $r' \geqslant 1$, and Assumption 5 with $\tau > 0$, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0,1)$ satisfies $\gamma_0 \lesssim \frac{1}{r'\mathrm{Tr}(\widetilde{\Sigma}_m)} \sim \mathcal{O}(1)$, the* `Variance` *defined in Proposition 1 holds*

$$\texttt{Variance} \lesssim \frac{\gamma_0 r'\tau^2}{\sqrt{\mathbb{E}[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]^2}}\begin{cases} mn^{\zeta-1}, \text{ if } m \leqslant n \\ 1 + n^{\zeta-1} + \dfrac{n}{m}, \text{ if } m > n \end{cases}$$

Remark: The error bound for `Variance` is demonstrated to be unimodal: increasing with m in the under-parameterized regime and decreasing with m in the over-parameterized regime, and finally converge to a constant order (that depends on noise parameter τ^2), which matches recent results relying on closed-form solution for (refined) variance, e.g., [13, 27, 16]. More discussion on our derived results refers to Appendix A.

4 Proof Outline and Discussion

In this section, we first introduce the structure of the proofs with high level ideas, and then discuss our work with previous literature in terms of the used techniques and the obtained results.

4.1 Proof outline

We (partly) disentangle the multiple randomness sources on the data $\boldsymbol{X}$, the random features matrix $\boldsymbol{W}$, the noise $\boldsymbol{\varepsilon}$, make full use of statistical properties of covariance operators Σ_m and $\widetilde{\Sigma}_m$ in Section 3.2, and provide the respective (bias and variance) upper bounds in terms of multiple randomness sources, as shown in Figure 1.

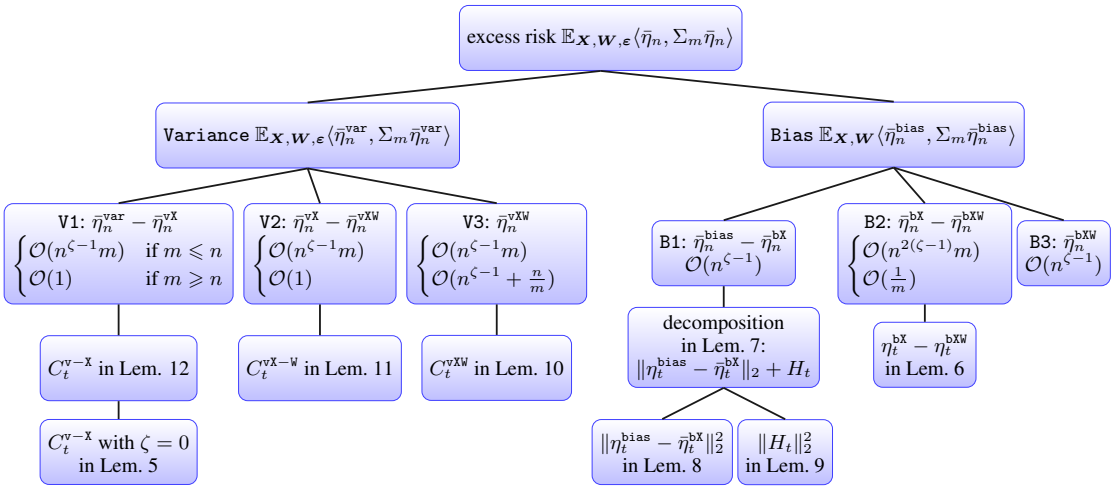


Figure 1: The roadmap of proofs.

Bias: To bound $\mathtt{Bias}$, we need some auxiliary notations. Recall $\Sigma_m = \mathbb{E}_{\boldsymbol{x}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]$ and $\widetilde{\Sigma}_m = \mathbb{E}_{\boldsymbol{x},\boldsymbol{W}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]$, define

$$\eta_t^{\mathtt{bX}} = (I - \gamma_t\Sigma_m)\eta_{t-1}^{\mathtt{bX}}, \quad \eta_0^{\mathtt{bX}} = f^*, \qquad \eta_t^{\mathtt{bXW}} = (I - \gamma_t\widetilde{\Sigma}_m)\eta_{t-1}^{\mathtt{bXW}}, \quad \eta_0^{\mathtt{bXW}} = f^*, \tag{7}$$

with the average $\bar{\eta}_n^{\mathtt{bX}} := \frac{1}{n}\sum_{t=0}^{n-1}\bar{\eta}_t^{\mathtt{bX}}$ and $\bar{\eta}_n^{\mathtt{bXW}} := \frac{1}{n}\sum_{t=0}^{n-1}\bar{\eta}_t^{\mathtt{bXW}}$. Accordingly, $\eta_t^{\mathtt{bX}}$ can be regarded as a "deterministic" version of $\eta_t^{\mathtt{bias}}$: we omit the randomness on $\boldsymbol{X}$ (data sampling, stochastic gradients) by replacing $[\varphi(\boldsymbol{x})\varphi(\boldsymbol{x})^\top]$ with its expectation Σ_m. Likewise, $\eta_t^{\mathtt{bXW}}$ is a deterministic version of $\eta_t^{\mathtt{vX}}$ by replacing Σ_m with its expectation $\widetilde{\Sigma}_m$ (randomness on initialization).

By Minkowski inequality, the $\mathtt{Bias}$ can be decomposed as $\mathtt{Bias} \lesssim \mathtt{B1} + \mathtt{B2} + \mathtt{B3}$, where $\mathtt{B1} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\left[\langle\bar{\eta}_n^{\mathtt{bias}} - \bar{\eta}_n^{\mathtt{bX}}, \Sigma_m(\bar{\eta}_n^{\mathtt{bias}} - \bar{\eta}_n^{\mathtt{bX}})\rangle\right]$ and $\mathtt{B2} := \mathbb{E}_{\boldsymbol{W}}\left[\langle\bar{\eta}_n^{\mathtt{bX}} - \bar{\eta}_n^{\mathtt{bXW}}, \Sigma_m(\bar{\eta}_n^{\mathtt{bX}} - \bar{\eta}_n^{\mathtt{bXW}})\rangle\right]$ and $\mathtt{B3} := \langle\bar{\eta}_n^{\mathtt{bXW}}, \widetilde{\Sigma}_m\bar{\eta}_n^{\mathtt{bXW}}\rangle$. Here $\mathtt{B3}$ is a deterministic quantity that is closely connected to model (intrinsic) bias without any randomness; while $\mathtt{B1}$ and $\mathtt{B2}$ evaluate the effect of randomness from $\boldsymbol{X}$ and $\boldsymbol{W}$ on the bias, respectively. The error bounds for them can be directly found in Figure 1.

To bound $\mathtt{B3}$, we directly focus on its formulation by virtue of spectrum decomposition and integral estimation. To bound $\mathtt{B2}$, we have $\mathtt{B2} = \frac{1}{n^2}\mathbb{E}_{\boldsymbol{W}}\left\|\Sigma_m^{\frac{1}{2}}\sum_{t=0}^{n-1}(\eta_t^{\mathtt{bX}} - \eta_t^{\mathtt{bXW}})\right\|^2$, where the key part $\eta_t^{\mathtt{bX}} - \eta_t^{\mathtt{bXW}}$ can be estimated by Lemma 6. To bound $\mathtt{B1}$, it can be further decomposed as (here we use inaccurate expression for description simplicity) $\mathtt{B1} \lesssim \sum_t \|\eta_t^{\mathtt{bX}} - \eta_t^{\mathtt{bXW}}\|_2^2 + \sum_t \mathbb{E}_{\boldsymbol{X}}\|H_t\|^2$ in Lemma 7, where $H_{t-1} := [\Sigma_m - \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\eta_{t-1}^{\mathtt{bX}}$. The first term can be upper bounded by $\sum_t \|\eta_t^{\mathtt{bX}} - \eta_t^{\mathtt{bXW}}\|_2^2 \lesssim \mathrm{Tr}(\Sigma_m)n^\zeta\|f^*\|^2$ in Lemma 8, and the second term admits $\sum_t \mathbb{E}_{\boldsymbol{X}}\|H_t\|^2 \lesssim \mathrm{Tr}(\Sigma_m)\|f^*\|^2$ in Lemma 9.

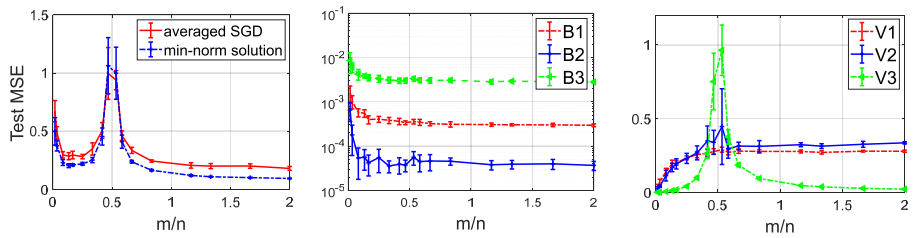
Variance: To bound $\mathtt{Variance}$, we need some auxiliary notations.

$$\eta_t^{\mathtt{vX}} := (I-\gamma_t\Sigma_m)\eta_{t-1}^{\mathtt{vX}}+\gamma_t\varepsilon_t\varphi(\boldsymbol{x}_t), \quad \eta_0^{\mathtt{vX}} = 0, \quad \eta_t^{\mathtt{vXW}} := (I-\gamma_t\widetilde{\Sigma}_m)\eta_{t-1}^{\mathtt{vXW}}+\gamma_t\varepsilon_t\varphi(\boldsymbol{x}_t), \quad \eta_0^{\mathtt{vXW}} = 0.$$

with the averaged quantities $\bar{\eta}_n^{\mathtt{vX}} := \frac{1}{n}\sum_{t=0}^{n-1}\bar{\eta}_t^{\mathtt{vX}}$, $\bar{\eta}_n^{\mathtt{vXW}} := \frac{1}{n}\sum_{t=0}^{n-1}\bar{\eta}_t^{\mathtt{vXW}}$. Accordingly, $\eta_t^{\mathtt{vX}}$ can be regarded as a "semi-stochastic" version of $\eta_t^{\mathtt{var}}$: we keep the randomness due to the noise ε_t but omit the randomness on $\boldsymbol{X}$ (data sampling) by replacing $[\varphi(\boldsymbol{x})\varphi(\boldsymbol{x})^\top]$ with its expectation Σ_m. Likewise, $\eta_t^{\mathtt{vXW}}$ can be regarded as a "semi-stochastic" version of $\eta_t^{\mathtt{vX}}$ by replacing Σ_m with its expectation $\widetilde{\Sigma}_m$ (randomness on initialization). The proof outline of **Variance** is similar to **Bias** as above mentioned, and thus is deferred to Appendix G due to page limit.

4.2 Discussion with previous work

Difference in techniques: Our proof framework follows [31] that focuses on kernel regression with stochastic approximation in the under-parameterized regimes (d is regarded as finite and much



(a) SGD vs. min-norm solution (b) `Bias` (c) `Variance`

Figure 2: Test MSE (mean±std.) of RF regression as a function of the ratio m/n on MNIST data set (digit 3 vs. 7) across the Gaussian kernel, for $d = 784$ and $n = 600$ in (a). The interpolation threshold occurs at $m/n = 0.5$ as the Gaussian kernel outputs the $2m$-feature mapping (instead of m), i.e., $\sigma(\boldsymbol{W}\boldsymbol{x}) \in \mathbb{R}^{2m}$. Under this setting, the trends of `Bias` and `Variance` are empirically given in (b) and (c).

smaller than n). Nevertheless, even in the under-parameterized regime, their results can not be directly extended to random features model due to the extra randomness on $\boldsymbol{W}$, coupling with other randomness sources on noise and data sampling, which makes their proof framework invalid: their results depend on [29, Lemma 1] by taking conditional expectation to bridge the connection between $\mathbb{E}[\|\alpha_t\|_2]$ and $\mathbb{E}\langle \alpha_t, \Sigma_m \alpha_t \rangle$. This is valid for `B1` but expires on other quantities.

Some technical tools used in this paper follow [36] that focuses on linear regression with constant step-size SGD in over-parameterized regime. However, our results differ from it in 1) tackling (extra) multiple randomness, e.g., stochastic gradients, random features, by introducing deterministic/randomness covariance operators. We prove nice statistical properties of them operator approximation theory in Hilbert spaces to help our proof. 2) tackling non-constant step-size SGD setting by introducing integral estimation techniques. Original techniques on constant step-size in [36] are invalid due to non-homogeneous update rules.

Comparison with previous work: Compared to [12] on RF optimized by gradient descent under the Gaussian data in an asymptotic view, our non-asymptotic result holds for more general data distribution under the SGD setting. In fact, our data assumption is weaker than most previous work assuming the data to be Gaussian, uniformly spread on a sphere, or isotropic/correlated features (with spectral decay assumption), except [14]. Nevertheless, we extend their asymptotic results relying on the least-squares closed-form solution to non-asymptotic results under the SGD setting, which takes the effect of optimization into consideration. Besides, our result coincides several findings with refined variance decomposition in [13, 27, 16], e.g., the interaction effect can dominate the variance (between samples and initialization); the unimodality of variance is a prevalent phenomenon.

5 Numerical Validation

In this section, we provide some numerical experiments in Figure 2 to support our theoretical results and findings. Note that our results go beyond Gaussian data assumption and can be empirically validated on real-world datasets. More experiments can be found in Appendix H.

5.1 Behavior of RF for interpolation learning

Here we evaluate the test mean square error (MSE) of RFF regression on the MNIST data set [53], following the experimental setting of [14, 54], to study the generalization performance of minimum-norm solution, see Figure 3(a). More results on regression dataset refer to Appendix H.

Experimental settings: We take digit 3 vs. 7 as an example, and randomly select 300 training data in these two classes, resulting in $n = 600$ for training. Hence, our setting with $n = 600$, $d = 784$, and tuning m satisfies our realistic high dimensional assumption. The Gaussian kernel $k(\boldsymbol{x}, \boldsymbol{x}') = \exp(-\|\boldsymbol{x} - \boldsymbol{x}'\|_2^2/(2\sigma_0^2))$ is used, where the kernel width σ_0 is chosen as $\sigma_0^2 = d$ in high dimensional settings such that $\|\boldsymbol{x}\|_2^2/d \sim \mathcal{O}(1)$ in Assumption 1. In our experiment, the initial

step-size is set to $\gamma_0 = 1$ and we take the initial point $\boldsymbol{\theta}_0$ near the min-norm solution[2] corrupted with zero-mean, unit-variance Gaussian noise. The experiments are repeated 10 times and the test MSE (mean$\pm$std.) can be regarded as a function of the ratio m/n by tuning m. Results on different initialization and more epochs of SGD refer to Appendix H.

SGD vs. minimal-norm solution: Figure 3(a) shows the test MSE of RF regression with averaged SGD (we take $\zeta = 0.5$ as an example; red line) and minimal-norm solution (blue line). First, we observe the double descent phenomenon: a phase transition on the two sides of the interpolation threshold at $2m = n$ when these two algorithms are employed. Second, in terms of test error, RF with averaged SGD is slightly inferior to that with min-norm solution, but still generalizes well.

5.2 Behavior of our error bounds

We have experimentally validate the phase transition and corresponding double descent in the previous section, and here we aim to semi-quantitatively assess our derived bounds for `Bias` and `Variance`, see Figure 3(d) and 2(c). Results of these quantities on different step-size refer to Appendix H.

Experimental settings: Since the target function f^*, the covariance operators Σ_d, Σ_m, and the noise $\boldsymbol{\varepsilon}$ are unknown on the MNIST data set, our experimental evaluation need some assumptions to calculate `Bias` and `Variance`. First, we assume the label noise $\varepsilon \sim \mathcal{N}(0, 1)$, which can in turn obtain $f^*(\boldsymbol{x})$ on both training and test data due to $f^*(\boldsymbol{x}) = y - \varepsilon$. Second, the covariance matrices Σ_d and Σ_m are estimated by the related sample covariance matrices. When using the Gaussian kernel, the covariance matrix $\widetilde{\Sigma}_m$ can be directly computed, see the remark in Lemma 1, where the expectation on $\boldsymbol{x}$ is approximated by Monte Carlo sampling with n training samples. Accordingly, based on the above results, we are ready to calculate $\eta_t^{\mathtt{bias}}$ in Eq. (5), $\eta_t^{\mathtt{bX}}$, and $\eta_t^{\mathtt{bXW}}$ in Eq. (7), respectively, which is further used to approximately compute $\mathtt{B1} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\left[\langle \bar{\eta}_n^{\mathtt{bias}} - \bar{\eta}_n^{\mathtt{bX}}, \Sigma_m(\bar{\eta}_n^{\mathtt{bias}} - \bar{\eta}_n^{\mathtt{bX}})\rangle\right]$ (red line) and $\mathtt{B2} := \mathbb{E}_{\boldsymbol{W}}\left[\langle \bar{\eta}_n^{\mathtt{bX}} - \bar{\eta}_n^{\mathtt{bXW}}, \Sigma_m(\bar{\eta}_n^{\mathtt{bX}} - \bar{\eta}_n^{\mathtt{bXW}})\rangle\right]$ (blue line) and $\mathtt{B3} := \langle \bar{\eta}_n^{\mathtt{bXW}}, \widetilde{\Sigma}_m \bar{\eta}_n^{\mathtt{bXW}}\rangle$ (green line). The (approximate) computation for `Variance` can be similar achieved by this process.

Error bounds for bias: Figure 3(d) shows the trends of (scaled) `B1`, `B2`, and `B3`. Recall our error bound: $\mathtt{B1}, \mathtt{B3} \sim \mathcal{O}(n^{\zeta-1})$; $\mathtt{B2} \sim \mathcal{O}(mn^{(2\zeta-2)})$ for $m < n$ and $\mathcal{O}(1/m)$ for $m > n$. We find that, all of them monotonically decreases when m increases from the under-parameterized regime to the over-parameterized regime. When $m < n$, `B2` converges faster than `B1` and `B3`. These experimental results coincide with our error bound on them.

Error bounds for variance: Figure 2(c) shows the trends of (scaled) `V1`, `V2`, and `V3`. Recall our error bound: in the under-parameterized regime, `V1`, `V2`, and `V3` increases with m at a certain $\mathcal{O}(n^{\zeta-1}m)$ rate; and in the over-parameterized regime, `V1` and `V2` are in $\mathcal{O}(1)$ order while `V3` decreases with m. Figure 2(c) shows that, when $2m < n$, `V1` and `V2` monotonically increases with m and then remain unchanged when $2m > n$. Besides, `V3` is observed to be unimodal: firstly increasing when $2m < n$, reaching to the peak at $2m = n$, and then decreasing when $2m > n$, which admits the phase transition at $2m = n$. Accordingly, these findings accord with our theoretical results, and also matches refined results in [13, 27, 16]: the unimodality of variance is a prevalent phenomenon.

6 Conclusion

We present non-asymptotic results for RF regression under the averaged SGD setting for understanding benign overfitting under the optimization effect. Our theoretical and empirical results demonstrate that, the error bounds for variance and bias can be unimodal and monotonically decreasing, respectively, which is able to recover the double descent phenomenon. Regarding to constant/adaptive step-size setting, there is no difference between the constant step-size case and the exact minimal-norm solution on the convergence rate; while the polynomial-decay step-size case will slow down the learning rate, but does not change the error bound for variance in over-parameterized regime that remains $\mathcal{O}(1)$ order, that depends on noise parameter(s).

[2] In our numerical experiments, we only employ single-pass SGD, and thus the initialization is chosen close to minimum norm solution, with more discussion in Appendix H. We take the regularization parameter fixed with 10^{-8} to avoid non-singular.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] We clearly discuss the limitation of this work in the Conclusion section.
   (c) Did you discuss any potential negative societal impacts of your work? [No] Our work is theoretical and generally will have no negative societal impacts.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] The assumptions are clearly stated and well discussed.
   (b) Did you include complete proofs of all theoretical results? [Yes] All of the proofs can be found in the Appendix.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes]
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