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 under-/over-parameterized regime. In this work, we derive precise non-asymptotic 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 minimum-norm interpolator, as a theoretical justification of using SGD in practice.

1 Introduction

Over-parameterized models, e.g., linear/kernel regression [1, 2, 3, 4] and neural networks [5, 6, 7], still generalize well even if the labels are pure noise [8]. Such high-capacity models have received significant attention recently as they go against with classical generalization theory. A paradigm for understanding this important phenomenon is *double descent* [9], in which the test error first decreases with increasing number of model parameters in the under-parameterized regime. They large error is yielded until interpolating the data, which is called the interpolation threshold. Finally, the test error decreases again in the over-parameterized regime.

Our work partakes in this research vein and studies the random features (RF) model [10], as a simplified version of neural networks, 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

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[4, 11]. 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 activation functions [4, 12, 11, 13, 14, 15] (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 *minimum-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 relatively strong data assumption in fact mismatches practical neural networks optimized by stochastic gradient descent (SGD) based algorithms. Our work precisely bridges this gap: We provide a new analysis framework for the generalization properties of RF models trained with SGD and general activation functions, also accommodating adaptive (i.e., polynomial decay) step-size selection, and provide non-asymptotic results in under-/over-parameterized regimes. We make the following contributions and findings:

First, we characterize statistical properties of 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. This is different from the least squares setting based on effective dimension [2, 16].

Second, 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 (partly) disentangle these randomness sources and 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 sub-Gaussian data and general activation functions.

Third, 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 challenges 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 minimum-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: The notation $\boldsymbol{a} \otimes \boldsymbol{a}$ denotes the tensor product of a vector $\boldsymbol{a}$. 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 $\precsim$. For any $a, b \in \mathbb{R}$, $a \wedge b$ denotes the minimum of a and b.

2.1 Related work

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 [4, 12, 13, 11].

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 [1, 4, 12, 13, 25] and from the replica method [11, 26, 14]. 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 [11, 27, 15]. 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] via 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 the convergence rate is built in [16]. This convergence rate is also demonstrated under the minimal-iterate [36] or last-iterate [37] setting in step-size SGD for noiseless least squares. We also notice a concurrent work [38] on last-iterate SGD with decaying step-size on least squares. Besides, the existence of multiple descent [39, 40] beyond double descent and SGD as implicit regularizer [41, 42] can be traced to the above two lines of work. Our work shares some similar technical tools with [31] and [16] but differs from them in several aspects. We detail the differences in Section 4.

2.2 Problem setting

We study the standard problem setting for RF least-squares regression and adopt the relevant terminologies from learning theory: *cf.*, [43, 31, 33, 25] for details. Let $X \subseteq \mathbb{R}^d$ be a metric space and $Y \subseteq \mathbb{R}$. The training data $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ are 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 $\Sigma_m : \mathbb{R}^m \to \mathbb{R}^m$

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

actually defined in $\mathcal{H}$ that is isomorphic to $\mathbb{R}^m$. This is the usually (uncentered) covariance matrix in finite dimensions,[2] 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 $\Sigma_m = J_m^* J_m$, where J_m^* denotes the adjoint operator of J_m.

[2] 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., $\widetilde{\Sigma}_m$.

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 one pass SGD with iterate averaging and adaptive step-size 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 $\boldsymbol{\theta}_0$)

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

where we use the polynomial decay step size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0, 1)$, following [31]. This setting also holds for the constant step-size case by taking $\zeta = 0$. Besides, we employ the bath size $= 1$ in an online setting style, which is commonly used in theory [31, 16, 44] for ease of analysis, which captures the key idea of SGD by combining stochastic gradients and data sampling.

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, 45, 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. *[46, 1, 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 [47, 40, 48] even though n and d tend to infinity. It holds true for linear functions with $\|f\|_{\mathcal{H}} \leqslant 4\pi$ [49], see Appendix B for details.

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

Remark: This assumption is quite general to cover commonly-used activation functions used in random features and neural networks, e.g., ReLU, Sigmoid, Logistic, and sine/cosine functions.

Recall $\Sigma_m := \mathbb{E}_{\boldsymbol{x}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]$ in Eq. (3) and its expectation $\widetilde{\Sigma}_m := \mathbb{E}_{\boldsymbol{W}}[\Sigma_m]$, we make the following fourth moment assumption that follows [29, 16, 37] to analyse SGD for least squares.

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*

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

Remark: This assumption requires the data are drawn from some not-too-heavy-tailed distribution, e.g., $\Sigma_m^{-\frac{1}{2}}\boldsymbol{x}$ has sub-Gaussian tail, common in high dimensional statistics. This condition is weaker than most previous work on double descent that requires the data to be Gaussian [1, 11, 27, 12], or uniformly spread on a sphere [4, 50], see comparisons in Table 1 in Appendix A. Note that the

assumption for any PSD operator is just for ease of description. In fact some certain PSD operators satisfying this assumption are enough for our proof. 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, 16] and holds for the standard noise model $y = f^*(\boldsymbol{x}) + \varepsilon$ with $\mathbb{E}[\varepsilon] = 0$ and $\mathbb{V}[\varepsilon] < \infty$ [1].

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. This is different from the least squares setting [2, 16] that introduces the effective dimension to separate the entire space into a "head" subspace where the error decays more quickly than the complement "tail" subspace. Instead, the following lemma shows that $\widetilde{\Sigma}_m$ has only two distinct eigenvalues at $\mathcal{O}(1)$ and $\mathcal{O}(1/m)$ order, respectively. Such fast eigenvalue decay can avoid extra data spectrum assumption for tight bound. For description simplicity, we consider the single-output activation function: $\sigma(\cdot) : \mathbb{R} \to \mathbb{R}$. Our results can be extended to multiple-output activation functions, see Appendix C.1.2 for details.

Lemma 1. *Under Assumption 1 and 3, 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.

Here we take the ReLU activation $\sigma(x) = \max\{x, 0\}$ as one example, RF actually approximates the first-order arc-cosine kernel [51] 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 $\mathrm{Tr}(\Sigma_d)/d \sim \mathcal{O}(1)$. More examples can be found in Appendix C.1.2.

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.*

Remark: This lemma characterizes the sub-exponential property of covariance operator Σ_m, which is a fundamental result for our proof since the bias and variance involve them.

The following lemma demonstrates that the behavior of the fourth moment can be bounded.

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, 16], 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 1, 2, 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*

$$\texttt{Bias} \lesssim \gamma_0 r' n^{\zeta-1}\|f^*\|^2 \sim \mathcal{O}\left(n^{\zeta-1}\right)\,.$$

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. Besides, our result on bias matches the exact formulation in [11] under the closed-form solution, i.e., monotonically decreasing bias. One slight difference is, their result on bias tends to a constant under the over-parameterized regime while our bias result can converge to zero.

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*

$$\texttt{Variance} \lesssim \gamma_0 r'\tau^2 \begin{cases} mn^{\zeta-1}, \text{ if } m \leqslant n \\ 1 + n^{\zeta-1} + \dfrac{n}{m}, \text{ if } m > n \end{cases}$$

Remark: We make the following remarks:
i) 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., [11, 27, 15].
ii) When compared to least squares, our result can degenerate to this setting by choosing $m := d$. Our upper bound is able to match the lower bound in [1, Corollary 1] with the same order, which demonstrates the tightness of our upper bound. Besides, our results can recover the result of [16] by taking the effective dimension $k^* = \min\{n, d\}$ (no data spectrum assumption is required here). 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.

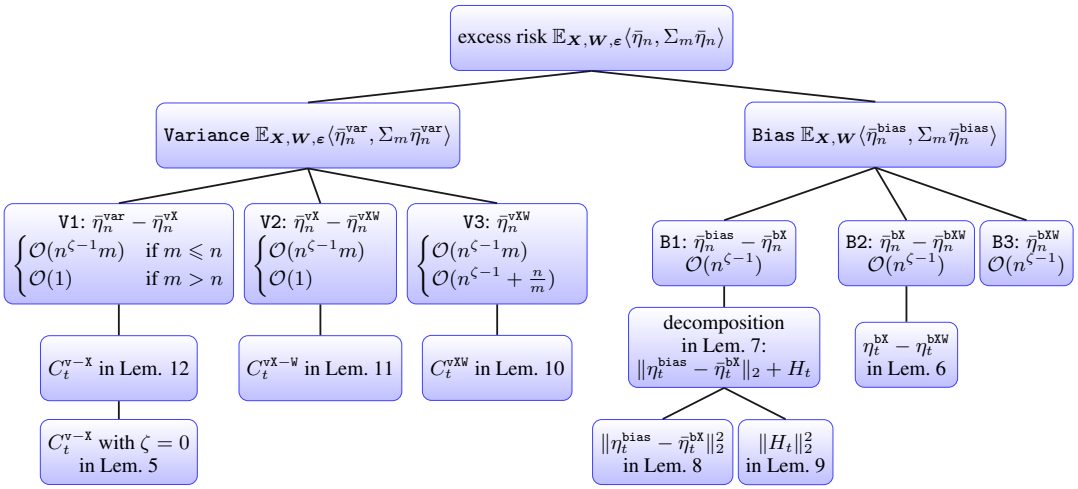


Figure 1: The roadmap of proofs.

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.

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 $\mathtt{B1} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\big[\langle \bar{\eta}_n^{\mathtt{bias}} - \bar{\eta}_n^{\mathtt{bX}}, \Sigma_m(\bar{\eta}_n^{\mathtt{bias}} - \bar{\eta}_n^{\mathtt{bX}})\rangle\big]$ and $\mathtt{B2} := \mathbb{E}_{\boldsymbol{W}}\big[\langle \bar{\eta}_n^{\mathtt{bX}} - \bar{\eta}_n^{\mathtt{bXW}}, \Sigma_m(\bar{\eta}_n^{\mathtt{bX}} - \bar{\eta}_n^{\mathtt{bXW}})\rangle\big]$ 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.

$$\eta_t^{\mathtt{vX}} := (I - \gamma_t \Sigma_m)\eta_{t-1}^{\mathtt{vX}} + \gamma_t \varepsilon_t \varphi(\boldsymbol{x}_t), \quad \eta_0^{\mathtt{vX}} = 0, \tag{8}$$

$$\eta_t^{\mathtt{vXW}} := (I - \gamma_t \widetilde{\Sigma}_m)\eta_{t-1}^{\mathtt{vXW}} + \gamma_t \varepsilon_t \varphi(\boldsymbol{x}_t), \quad \eta_0^{\mathtt{vXW}} = 0, \tag{9}$$

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).

By virtue of Minkowski inequality, the `Variance` can be decomposed as $\mathtt{Variance} \lesssim \mathtt{V1}+\mathtt{V2}+\mathtt{V3}$, where $\mathtt{V1} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\big[\langle \bar{\eta}_n^{\mathtt{var}} - \bar{\eta}_n^{\mathtt{vX}}, \Sigma_m(\bar{\eta}_n^{\mathtt{var}} - \bar{\eta}_n^{\mathtt{vX}})\rangle\big]$, $\mathtt{V2} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\big[\langle \bar{\eta}_n^{\mathtt{vX}} - \bar{\eta}_n^{\mathtt{vXW}}, \Sigma_m(\bar{\eta}_n^{\mathtt{vX}} - \bar{\eta}_n^{\mathtt{vXW}})\rangle\big]$, and $\mathtt{V3} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle \bar{\eta}_n^{\mathtt{vXW}}, \Sigma_m \bar{\eta}_n^{\mathtt{vXW}}\rangle$. Though `V1`, `V2`, `V3` still interact the multiple randomness, `V1` disentangles some randomness on data sampling, `V2` discards some randomness on initialization, and `V3` focuses on the "minimal" interaction between data sampling, label noise, and initialization. The error bounds for them can be found in Figure 1.

To bound `V3`, we focus on the formulation of the covariance operator $C_t^{\mathtt{vXW}} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\eta_t^{\mathtt{vXW}} \otimes \eta_t^{\mathtt{vXW}}]$ in Lemma 10 and the statistical properties of $\widetilde{\Sigma}_m$ and Σ_m. To bound `V2`, we need study the covariance operator $C_t^{\mathtt{vX-W}} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[(\eta_t^{\mathtt{vX}} - \eta_t^{\mathtt{vXW}}) \otimes (\eta_t^{\mathtt{vX}} - \eta_t^{\mathtt{vXW}})]$ admitting $\|C_t^{\mathtt{vX-W}}\| \lesssim \|\Sigma_m^2\|_2 \|\widetilde{\Sigma}_m\|_2$ in Lemma 11. To bound `V1`, we need study the covariance operator $C_t^{\mathtt{v-X}} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[(\eta_t^{\mathtt{var}} - \eta_t^{\mathtt{vX}}) \otimes (\eta_t^{\mathtt{var}} - \eta_t^{\mathtt{vX}})]$, as a function of $\zeta \in [0,1)$, admitting $\mathrm{Tr}[C_t^{\mathtt{v-X}}(\zeta)] \lesssim \mathrm{Tr}[C_t^{\mathtt{v-X}}(0)]$ in Lemma 5, and further $C_t^{\mathtt{v-X}} \precsim \mathrm{Tr}(\Sigma_m) I$ in Lemma 12.

4.2 Discussion on 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 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 $\boldsymbol{W}$. For instance, 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 [16] that focuses on linear regression with constant step-size SGD for benign overfitting. However, our results differ from it in 1) tackling multiple randomness, e.g., stochastic gradients, random features (Gaussian initialization), by introducing another type of error decomposition and several deterministic/randomness covariance operators. We prove nice statistical properties of them for proof, which gets rid of data spectrum assumption in [16]. 2) tackling non-constant step-size SGD setting by introducing new integral estimation techniques. Original techniques on constant step-size in [16] are invalid due to non-homogeneous update rules. The above two points make our proof relatively more intractable and largely different. Besides, their results demonstrate that linear regression with SGD generalizes well (converges with n) but has few findings on double descent. Instead, our result depends on n and m (where d is implicitly included in m), and is able to explain double descent.

Here we take the estimation for the variance in [16] under the least squares setting as an example to illustrate this.

$$\text{Variance} \lesssim \sum_{t=0}^{n-1} \Big\langle I - (I-\gamma\Sigma_d)^{n-t}, I - (I-\gamma\Sigma_d)^{t} \Big\rangle \qquad \text{[Eq. (4.10) in [16]]}$$

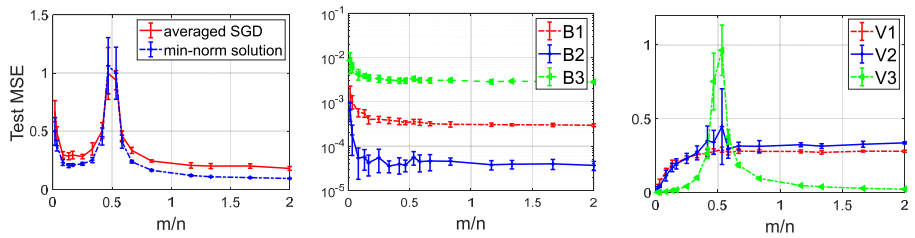
In this setting, the effective dimension to tackle $I - (I-\gamma\Sigma_d)^{n-t}$; while our result is based on fast eigenvalue decay of $\widetilde{\Sigma}_m$ in Lemma 1 can direct to bound this. Besides, the homogeneous markov chain under the constant step-size setting is employed [16] for $(I-\gamma\Sigma_d)^{n-t}$, which is naturally invalid under our decaying step-size setting. Instead, we introduce integral estimation techniques to tackle adaptive step-size, see Appendix E for details.

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 [52], following the experimental setting of [13, 53], to study the generalization performance of minimum-norm solution, see Figure 2(a). More results on regression dataset refer to Appendix H.



(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).

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[3] corrupted with zero-mean, unit-variance Gaussian noise. The experiments are repeated 10 times and the test MSE (mean±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 2(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 validated 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 2(b) and 2(c), respectively. 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 $\eta_t^{\texttt{bias}}$ in Eq. (5), $\eta_t^{\texttt{bX}}$, and $\eta_t^{\texttt{bXW}}$ in Eq. (7), respectively, which is further used to approximately compute $\texttt{B1} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\left[\langle \bar{\eta}_n^{\texttt{bias}} - \bar{\eta}_n^{\texttt{bX}}, \Sigma_m(\bar{\eta}_n^{\texttt{bias}} - \bar{\eta}_n^{\texttt{bX}})\rangle\right]$ (red line) and $\texttt{B2} := \mathbb{E}_{\boldsymbol{W}}\left[\langle \bar{\eta}_n^{\texttt{bX}} - \bar{\eta}_n^{\texttt{bXW}}, \Sigma_m(\bar{\eta}_n^{\texttt{bX}} - \bar{\eta}_n^{\texttt{bXW}})\rangle\right]$ (blue line) and $\texttt{B3} := \langle \bar{\eta}_n^{\texttt{bXW}}, \widetilde{\Sigma}_m \bar{\eta}_n^{\texttt{bXW}}\rangle$ (green line). The (approximate) computation for `Variance` can be similar achieved by this process.

Error bounds for bias: Figure 2(b) shows the trends of (scaled) `B1`, `B2`, and `B3`. Recall our error bound: `B1`, `B2`, `B3` $\sim \mathcal{O}(n^{\zeta-1})$, we find that, all of them monotonically decreases at a certain convergence rate when m increases from the under-parameterized regime to the over-parameterized regime. These experimental results coincide with our error bound on them.

[3] 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.

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 increase 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 [11, 27, 15]: 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 double descent 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 converges to $\mathcal{O}(1)$ order, that depends on noise parameter(s).

Our work centers around the RF model, which is still a bit far away from practical neural networks. Theoretical understanding the generalization properties of over-parameterized neural networks is a fundamental but difficult problem. We believe that a comprehensive and thorough understanding of shallow neural networks, e.g., the RF model, is a necessary first step. Besides, we consider the single-pass SGD in our work for simplicity rather than multiple-pass SGD used in practice. This is also an interesting direction for understanding the optimization effect of SGD in the double descent.

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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 Conclusion.
   (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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   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
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   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

The outline of the appendix is stated as follows.

- Appendix A summarizes representative results on random features regarding to double descent under various settings and discusses the tightness of our derived upper bounds.
- Appendix B presents more discussion on the used assumptions, especially Assumptions 2 and 4, demonstrating the rationale behind these assumptions.
- Appendix C provides the proofs of lemmas in Section 3.2 on statistical properties of Σ_m and $\widetilde{\Sigma}_m$.
- Appendix D introduces preliminaries on PSD operators in stochastic approximation.
- Appendix E provides estimation for several typical integrals that are needed for our proof.
- Appendix F gives error bounds for `Bias`.
- Appendix G provides the error bounds for `Variance`.
- Appendix H provides more experiments including different initialization, step-size on various datasets to support our theory.

A Comparisons with previous work

A.1 Problem settings

Here we summarize various representative approaches in Table 1 according to the used data assumption, the type of solution, and the derived results.

Table 1: Comparison of problem settings on analysis of high dimensional random features on double descent.

	data assumption	solution	result
[1]	Gaussian	closed-form	variance $\nearrow\searrow$
[12]	Gaussian	GD	variance $\nearrow\searrow$
[4]	i.i.d on sphere	closed-form	variance, bias $\nearrow\searrow$
[11]	Gaussian	closed-form	refined [2]
[14]	Gaussian	closed-form	$\nearrow\searrow$
[27]	Gaussian	closed-form	refined
[54]	Gaussian	closed-form	$\nearrow\searrow$
[28]	Gaussian	closed-form	$\nearrow\searrow$
[13]	general	closed-form	$\nearrow\searrow$
[15]	isotropic features with finite moments	closed form	refined
[25]	correlated features with polynomial decay on Σ_d	closed form	interpolation learning
Ours	sub-Gaussian data	SGD	variance $\nearrow\searrow$, bias $\searrow$

[1] A refined decomposition on variance is conducted by sources of randomness on data sampling, initialization, label noise to possess each term [11] or their full decomposition in [27, 15].

Here we discuss the used assumption on data distribution and the discussion on other assumptions is deferred to Appendix B. It can be found that, most papers assume the data to be Gaussian or uniformly distributed on the sphere. The following papers admit weaker assumption on data. Given a correlated features model that is commonly used in high dimensional statistics [1]

$$\boldsymbol{x} = \Sigma_d^{\frac{1}{2}} \boldsymbol{t}\,, \quad \mathbb{E}[t_i] = 0, \mathbb{V}[t_i] = 1, \quad \text{with } \Sigma_d := \mathbb{E}_{\boldsymbol{x}}[\boldsymbol{x}\boldsymbol{x}^\top]\,, \tag{10}$$

where $\boldsymbol{t} \in \mathbb{R}^d$ has i.i.d entries t_i ($i = 1, 2, \ldots, d$) with zero mean and unit variance. In [25], they further require that each entry is i.i.d sub-Gaussian and Σ_d admits polynomial decay on eigenvalues. In [15], the authors consider isotropic features with finite moment, i.e., taking $\Sigma_d := I$ in Eq. (10) and $\mathbb{E}[t_i^{8+\eta}] < \infty$ for any arbitrary positive constant $\eta > 0$. Our model holds for sub-Gaussian, and thus the used data assumption 4 is weaker than them. We also remark that, no assumption on data

distribution is employed [13] but they require that test data "behave" statistically like the training data by concentrated random vectors. Indeed, their data assumption is weaker than ours, but their analysis framework builds on the exact closed-form solution from random matrix theory. Instead, we focus on the SGD setting and thus take a unified perspective on optimization and generalization.

Here we briefly discuss our result 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 [13]. 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 [11, 27, 15], e.g., the interaction effect can dominate the variance (between samples and initialization); the unimodality of variance is a prevalent phenomenon.

A.2 Discussion on the tightness of our results

We present the upper bounds of excess risk in this work, and it is natural to ask whether the lower bound can be derived by our proof framework. Unfortunately, the first step in our proof is based on Minkowski inequality such that $\texttt{Bias} \leqslant 3(\texttt{B1} + \texttt{B2} + \texttt{B3})$ and $\texttt{Variance} \leqslant 3(\texttt{V1} + \texttt{V2} + \texttt{V3})$. This could be a limitation of this work, but our derived results are still tight when compared to previous work in both under- and over-parameterized regimes.

First, we compare our result with classical random features regression with SGD in the under-parameterized regime [33]. Under the same standard assumptions, e.g., $f^* \in H$ and label noise with bounded variance, without refined assumptions, e.g., source condition describing the smoothness of f^* and capacity condition describing the "size" of the corresponding $\mathcal{H}$ [45], by taking one-pass over the data (the same setting with our result) and the random features $m = \mathcal{O}(\sqrt{n})$, the excess risk [33] achieves at a certain $\mathcal{O}(1/\sqrt{n})$ rate. Under the same setting with the constant-step size, i.e., $\gamma = 0$, we have

$$\mathbb{E}\|\bar{f}_n - f^*\|^2_{L^2_{\rho_X}} = \underbrace{\texttt{Bias}}_{\mathcal{O}(\frac{1}{n})} + \underbrace{\texttt{Variance}}_{\mathcal{O}(\frac{1}{\sqrt{n}})} \lesssim \frac{1}{\sqrt{n}} \,,$$

which achieves the same learning rate with [33], and has been proved to be optimal in a minimax sense [55] under the standard assumptions. That means, the constant step-size SGD setting incurs no loss in convergence rate when compared to the exact kernel ridge regression.

Second, in the over-parameterized regime, previous work using random matrix theory and replica method provide an exact formulation of the excess risk. Nevertheless, it appears difficult to compare the specific convergence rate due to their complex formulations, and thus we in turn study the tendency. Here we take [11] as an example for comparison. They use conditional expectations to split the variance into label noise, initialization, and data sampling, and the first two terms dominates the variance.
(i) Our result on bias matches their exact formulation, i.e., monotonically decreasing bias. One slight difference is, their result on bias tends to a constant under the over-parameterized regime while our bias result can converge to zero.
(ii) Our result on variance admits the same tendency with their result, leading to unimodal variance, where some part(s) are with phase transition and some part(s) firstly monotonically increase during the under-parameterized regime and then remain unchanged during the over-parameterized regime. More importantly, both of the above two results demonstrate that, the variance will finally converge to a constant order, that depends on the variance of label noise τ^2. That means, our (upper bound) result is tight to describe phase transition and the final convergence state (depending on the noise level) when compared to the exact formulation results.

Third, though convergence rates of random features for double descent is non-easy to compare, results on least squares [2, 16] under the over-parameterized regime or interpolation are possible for comparison. Here we take our result by choosing $m := d$ and the constant step-size for least squares setting, and compare their lower bound results to demonstrate the tightness of our result. By virtue of

Lemma 1, we can reformulate our result as

$$\mathbb{E}\|\bar{f}_n - f^*\|^2_{L^2_{\rho_X}} \lesssim \gamma_0 \tau^2 \begin{cases} \frac{1}{n} + \frac{d}{n}, \text{ if } d \leqslant n \\ 1 + \frac{1}{n} + \frac{n}{d}, \text{ if } d > n \end{cases}$$

which matches the same order with [1, Corollary 1].

Besides, when compared to [16], if taking the effective dimension $k^* = \min\{n, d\}$ (no data spectrum assumption is required here), we can recover their result. In fact, our result is able to match their lower bound [2, 16]: `excess risk` $\gtrsim \tau^2(\frac{1}{n} + \frac{n}{d})$ with only one difference on an extra constant when $d > n$.

Based on the above discussion, our upper bound matches previous work with exact formulation or lower bound under various settings, which demonstrates the tightness of our upper bound, and accordingly, our result is able to recover the double descent phenomenon.

B Discussion on the used assumptions

Here we give more discussion on the used assumptions, especially Assumptions 2 and 4, which are fair and attainable.

Discussion on Assumption 2: $i)$ *bounded Hilbert norm:* In high-dimensional asymptotics, this bounded Hilbert norm assumption is commonly used in kernel regression [47, 40, 56], and RF model [48] even though n and d tend to infinity. Here we give an example satisfying this assumption, which is provided by [49, Proposition 4], i.e., linear functions on the sphere can have bounded Hilbert norm for all d.

To be specific, assume $f : \mathbb{S}^d \to \mathbb{R}$ such that $f(\boldsymbol{x}) = \boldsymbol{v}^\top \boldsymbol{x}$ for a certain $\boldsymbol{v} \in \mathbb{S}^d$, if we consider the following reproducing kernel

$$k(\boldsymbol{x}, \boldsymbol{x}') = \int_{\mathbb{S}^d} 1_{\{\boldsymbol{\omega}^\top \boldsymbol{x} \geq 0\}} 1_{\{\boldsymbol{\omega}^\top \boldsymbol{x}' \geq 0\}} \mathrm{d}\mu(\boldsymbol{\omega}) \,,$$

where μ is the probability measure of $\boldsymbol{\omega}$, leading to a zero-order arc-cosine kernel [51] by taking Gaussian measure. Then we have

$$\|f\|_{\mathcal{H}} = \frac{2d\pi}{d-1} \leqslant 4\pi \,,$$

which verifies that our assumption on bounded Hilbert norm is attainable.

We also need to remark that, unbounded Hilbert norm of functions can be achieved [49, 57] when $d \to \infty$ in some cases. For example, if we consider the above problem setting but employ the first-order arc-cosine kernel, we have $\|f\|_{\mathcal{H}} \asymp C\sqrt{d}$ for some constant C independent of d.

Accordingly, apart from directly regarding it as an assumption, we also give an example such that a function can have bounded Hilbert norm. In fact, in practice d is fixed (larger or smaller than n), and accordingly it is reasonable for a fixed ground truth with bounded Hilbert norm.

$ii)$ *optimal solution:* We assume that $\mathcal{E}(f)$ admits a unique global optimum. If multiple solutions exist, we choose the minimum norm solution of $\mathbb{E}(f)$, i.e.,

$$f^* = \operatorname*{argmin}_{f \in \mathcal{H}} \|f\|_{\mathcal{H}} \quad \text{s.t. } f \in \operatorname*{argmin}_{f \in \mathcal{H}} \mathcal{E}(f) \,,$$

which follows the setting [16, 38].

Discussion on Assumption 4: This assumption follows the spirit of [16, Assumption 2.2]. According to [58, Theorem 5.2.15], assume $\boldsymbol{x}$ is a sub-Gaussian random vector with density of the form $p(\boldsymbol{x}) = \exp(-U(\boldsymbol{x}))$ for the strongly convex function $U : \mathbb{R}^d \to \mathbb{R}$. Accordingly, $\Sigma_m^{-\frac{1}{2}} \boldsymbol{x}$ is sub-Gaussian, and then for any fixed $\boldsymbol{W}$ and PSD operator A, we have

$$\mathbb{E}_{\boldsymbol{x}}[\varphi^\top(\boldsymbol{x}) A \varphi(\boldsymbol{x}) \Sigma_m] \lesssim \mathrm{Tr}(A\Sigma_m)\Sigma_m \,.$$

The proof is similar to [16, Lemma A.1], and thus we omit the proof for simplicity. The sub-Gaussian assumption is common in high dimensional statistics [2], which is weaker than most previous work

on double descent that requires the data to be Gaussian [1, 11, 27, 12], or uniformly spread on a sphere [4, 50], as discussed in Appendix A.

In fact, our proof only requires Assumption 4 valid to some specific PSD operators, e.g., $S^{\mathtt{W}}$, $\mathbb{E}_{\boldsymbol{X}}[\Sigma_m - \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]^2$ defined in Appendix D. For description simplicity, we present the requirement on all PSD operators in Assumption 4. Besides, one special case of Assumption 4 by taking $A := I$ is proved by Lemma 3, and accordingly this assumption can be regarded as a natural extension.

This assumption is also similar to the bounded fourth moment in stochastic approximation, see [29, 31, 30, 36, 37] for details.

C Results on covariance operators

In this section, we present the proofs of Lemmas 1, 2, 3, 4 on statistical properties of Σ_m and $\widetilde{\Sigma}_m$.

C.1 Proof of Lemma 1 and examples

Here we present the proof of Lemma 1 and then give two examples by taking different activation functions.

C.1.1 Proof of Lemma 1

Proof. Recall the definition of $\widetilde{\Sigma}_m$, we have

$$\widetilde{\Sigma}_m := \mathbb{E}_{\boldsymbol{x},\boldsymbol{W}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})] = \frac{1}{m}\mathbb{E}_{\boldsymbol{x},W_{ij}\sim\mathcal{N}(0,1)}\left[\sigma\left(\frac{\boldsymbol{W}\boldsymbol{x}}{\sqrt{d}}\right)\sigma\Big(\frac{\boldsymbol{W}\boldsymbol{x}}{\sqrt{d}}\Big)^\top\right] \in \mathbb{R}^{m\times m}\,.$$

We consider the diagonal and non-diagonal elements of $\widetilde{\Sigma}_m$ separately.

Diagonal element: The diagonal entry $(\widetilde{\Sigma}_m)_{ii} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x},\boldsymbol{\omega}_i}[\sigma(\frac{\boldsymbol{\omega}_i^\top\boldsymbol{x}}{\sqrt{d}})\sigma(\frac{\boldsymbol{\omega}_i^\top\boldsymbol{x}}{\sqrt{d}})] = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\mathbb{E}_{\boldsymbol{\omega}}[\sigma(\frac{\boldsymbol{\omega}^\top\boldsymbol{x}}{\sqrt{d}})]^2$ is the same. In fact, $\mathbb{E}_{\boldsymbol{\omega}}\left[\sigma\left(\frac{\boldsymbol{\omega}^\top\boldsymbol{x}}{\sqrt{d}}\right)\right]^2$ is actually a one-dimensional integration by considering the basis $(e_1, e_2, \cdots, e_d)$ with $\boldsymbol{e}_1 = \boldsymbol{x}/\|\boldsymbol{x}\|_2$, and $\boldsymbol{e}_2, \cdots, \boldsymbol{e}_d$ any completion of the basis. This technique is commonly used in [59, 60]. The random feature $\boldsymbol{\omega}$ admits the coordinate representation $\boldsymbol{\omega} = \bar{\omega}_1\boldsymbol{e}_1 + \bar{\omega}_2\boldsymbol{e}_2 + \cdots + \bar{\omega}_d\boldsymbol{e}_d$, and thus

$$\boldsymbol{\omega}^\top\boldsymbol{x} = (\bar{\omega}_1\boldsymbol{e}_1 + \bar{\omega}_2\boldsymbol{e}_2 + \cdots + \bar{\omega}_d\boldsymbol{e}_d)^\top(\|\boldsymbol{x}\|\boldsymbol{e}_1) = \|\boldsymbol{x}\|\bar{\omega}_1\,,$$

which implies

$$\begin{aligned}
\mathbb{E}_{\boldsymbol{\omega}}\left[\sigma\left(\frac{\boldsymbol{\omega}^\top\boldsymbol{x}}{\sqrt{d}}\right)\right]^2 &= (2\pi)^{-\frac{d}{2}}\int_{\mathbb{R}^d}\left[\sigma\left(\frac{\boldsymbol{\omega}^\top\boldsymbol{x}}{\sqrt{d}}\right)\right]^2\exp\left(-\frac{1}{2}\|\boldsymbol{\omega}\|_2^2\right)\mathrm{d}\boldsymbol{\omega} \\
&= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\left[\sigma\left(\frac{\bar{\omega}_1\|\boldsymbol{x}\|_2}{\sqrt{d}}\right)\right]^2\exp\left(-\frac{\bar{\omega}_1^2}{2}\right)\mathrm{d}\bar{\omega}_1 \\
&= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}[\sigma(z)]^2\exp\left(-\frac{z^2}{2\|\boldsymbol{x}\|^2/d}\right)\frac{\sqrt{d}}{\|\boldsymbol{x}\|_2}\mathrm{d}z \\
&= \mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]^2\,,
\end{aligned}$$

where we change the integral variable $z := \frac{\bar{\omega}_1\|\boldsymbol{x}\|_2}{\sqrt{d}}$. Hence we have $(\widetilde{\Sigma}_m)_{ii} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]^2$.

Non-diagonal element: The non-diagonal entry $(\widetilde{\Sigma}_m)_{ij} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x},\boldsymbol{\omega}_i,\boldsymbol{\omega}_j}[\sigma(\frac{\boldsymbol{\omega}_i^\top\boldsymbol{x}}{\sqrt{d}})\sigma(\frac{\boldsymbol{\omega}_j^\top\boldsymbol{x}}{\sqrt{d}})^\top] = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}[\mathbb{E}_{\boldsymbol{\omega}}\sigma(\frac{\boldsymbol{\omega}^\top\boldsymbol{x}}{\sqrt{d}})]^2$ is the same due to the independence between $\boldsymbol{\omega}_i$ and $\boldsymbol{\omega}_j$. Likewise, it can be represented as a one-dimensional integration

$$(\widetilde{\Sigma}_m)_{ij} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\left[\mathbb{E}_{\boldsymbol{\omega}}\sigma\left(\frac{\boldsymbol{\omega}^\top\boldsymbol{x}}{\sqrt{d}}\right)\right]^2 = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\left[\mathbb{E}_{z\sim\mathcal{N}(0,1)}\sigma\left(\frac{z\|\boldsymbol{x}\|}{\sqrt{d}}\right)\right]^2 = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\left(\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]\right)^2\,.$$

Accordingly, by denoting $a := (\widetilde{\Sigma}_m)_{ii}$ and $b := (\widetilde{\Sigma}_m)_{ij}$, the covariance operator $\widetilde{\Sigma}_m$ can be represented as

$$\widetilde{\Sigma}_m = (a-b)I_m + b\mathbf{1}\mathbf{1}^\top \in \mathbb{R}^{m\times m}\,, \tag{11}$$

with its determinant $\det(\widetilde{\Sigma}_m) = (1+\frac{mb}{a-b})(a-b)^m$. Hence, the eigenvalues of $\widetilde{\Sigma}_m$ can be naturally obtained by the matrix determinant lemma: $\widetilde{\lambda}_1(\widetilde{\Sigma}_m) = a-b+bm$ and the remaining eigenvalues are $a-b$.

According to [61, Theorem 2.26], by virtue of the Lipschitz function $\sigma(\cdot)$ of Gaussian variables, we have

$$\mathbb{P}\left[\left|\sigma\left(\frac{\boldsymbol{\omega}^\top\boldsymbol{x}}{\sqrt{d}}\right) - \mathbb{E}_{\boldsymbol{\omega}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I}_d)}\sigma\left(\frac{\boldsymbol{\omega}^\top\boldsymbol{x}}{\sqrt{d}}\right)\right| \geqslant t\right] \leqslant c\exp(-t^2),\ \ \forall t\geqslant 0\,,$$

which implies that $\sigma\big(\frac{\boldsymbol{\omega}^\top\boldsymbol{x}}{\sqrt{d}}\big)$ is a sub-Gaussian random variable due to its expectation in the $\mathcal{O}(1)$ order. Accordingly, for $z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)$, we have $\mathbb{E}_{\boldsymbol{x}}\mathbb{V}[\sigma(z)]\sim\mathcal{O}(1)$ as $\sigma(z)$ is sub-Gaussian with $\mathcal{O}(1)$ norm and its finite second moment, i.e., $\mathbb{V}[\sigma(z)]\sim\mathcal{O}(1)$, which implies $\widetilde{\lambda}_2 = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\mathbb{V}[\sigma(z)]\sim\mathcal{O}(1/m)$. Finally, we conclude the proof. □

C.1.2 Examples

In our analysis, we assume $\sigma(\cdot):\mathbb{R}\to\mathbb{R}$ with single-output for description simplicity. In fact, our results can be easily extended to multiple-output cases, e.g., the Gaussian kernel corresponding to $\sigma(x) = [\cos(x),\sin(x)]^\top$. Here we give two examples, including single- and multiple-output: arc-cosine kernel that corresponds to the ReLU function $\sigma(x)=\max\{0,x\}$; and the Gaussian kernel.

Arc-cosine kernel: We begin with calculation of arc-cosine kernels due to its related single-output activation function. Denote $\widetilde{z} := \max\{0,z\}$ with $z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)$, it is subject to the Rectified Gaussian distribution admitting (refer to [25])

$$\mathbb{E}[\widetilde{z}] = \frac{\|\boldsymbol{x}\|_2}{\sqrt{2d\pi}}\,,\quad \mathbb{E}[\widetilde{z}]^2 = \frac{\|\boldsymbol{x}\|_2^2}{2d}\,,\quad \mathbb{V}[\widetilde{z}] = \frac{\|\boldsymbol{x}\|_2^2}{2d}\left(1-\frac{1}{\pi}\right).$$

Accordingly, recall the sample covariance operator $\Sigma_d := \mathbb{E}_{\boldsymbol{x}}[\boldsymbol{x}\boldsymbol{x}^\top]$, the diagonal elements are the same

$$(\widetilde{\Sigma}_m)_{ii} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]^2 = \frac{1}{2md}\mathbb{E}_{\boldsymbol{x}}\|\boldsymbol{x}\|_2^2 = \frac{1}{2md}\mathrm{Tr}(\Sigma_d)\,,\quad i=1,2,\ldots,m\,,$$

and the non-diagonal elements are the same

$$(\widetilde{\Sigma}_m)_{ij} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\left(\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]\right)^2 = \frac{1}{2md\pi}\mathrm{Tr}(\Sigma_d)\,,\quad i,j=1,2,\ldots,m \text{ with } i\neq j\,.$$

Gaussian kernels: Briefly, 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.

According to Bochner's theorem [62], we have $\mathbb{E}[\cos(\boldsymbol{\omega}^\top\boldsymbol{z})] = \exp(-z^2/2)$ and $\mathbb{E}[\cos^2(\boldsymbol{\omega}^\top\boldsymbol{z})] = \frac{1+\exp(-2z^2)}{2}$ for $\boldsymbol{\omega}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I}_d)$ and $z := \|\boldsymbol{z}\|_2$. In fact, this can be computed by two steps: first transforming the d-dimensional integration to a one-dimensional integral as discussed before; and then computing the integral by virtue of the Euler's formula $\exp(-\mathrm{i}x) = \cos x + \mathrm{i}\sin x$. For instance,

$$\begin{aligned}
\mathbb{E}[\cos(\boldsymbol{\omega}^\top\boldsymbol{z})] = \mathbb{E}_{x\sim\mathcal{N}(0,\|\boldsymbol{z}\|_2^2)}\cos x &= \frac{1}{\sqrt{2\pi}\|\boldsymbol{z}\|_2}\mathrm{Re}\left[\int_{\mathbb{R}}\exp(-\frac{x^2}{2\|\boldsymbol{z}\|_2^2})\exp(\mathrm{i}x)\mathrm{d}x\right]\\
&= \exp\left(-\frac{\|\boldsymbol{z}\|_2^2}{2}\right)\mathrm{Re}\left[\frac{1}{\sqrt{2\pi}\|\boldsymbol{z}\|_2}\int_{\mathbb{R}}\exp\left(-\frac{(x-\mathrm{i}\|\boldsymbol{z}\|_2^2)}{2\|\boldsymbol{z}\|_2^2}\right)\mathrm{d}x\right]\\
&= \exp\left(-\frac{\|\boldsymbol{z}\|_2^2}{2}\right)\,.
\end{aligned}$$

Similarly, we have $\mathbb{E}[\sin(\boldsymbol{\omega}^\top \boldsymbol{z})] = 0$ and $\mathbb{E}[\sin^2(\boldsymbol{\omega}^\top \boldsymbol{z})] = \frac{1-\exp(-2z^2)}{2}$ for $\boldsymbol{\omega} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I}_d)$ and $z := \|\boldsymbol{z}\|_2$.

Based on the above results, for the Gaussian kernel, the expected covariance operator $\widetilde{\Sigma}_m$ is a block diagonal matrix

$$\widetilde{\Sigma}_m = \left[\begin{array}{c|c} \boldsymbol{S}_1 & \boldsymbol{0} \\ \hline \boldsymbol{0} & \boldsymbol{S}_2 \end{array}\right] \in \mathbb{R}^{2m \times 2m},$$

where $\boldsymbol{S}_1 \in \mathbb{R}^{m \times m}$ has the same diagonal elements and the same non-diagonal elements:

$$[\boldsymbol{S}_1]_{ii} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x},\boldsymbol{\omega}}\left[\cos\left(\frac{\boldsymbol{\omega}^\top \boldsymbol{x}}{\sqrt{d}}\right)\right]^2 = \frac{1}{2m}\mathbb{E}_{\boldsymbol{x}}\left[1 + \exp\left(-2\frac{\|\boldsymbol{x}\|_2^2}{d}\right)\right], \quad i = 1, 2, \ldots, m,$$

$$[\boldsymbol{S}_1]_{ij} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\left[\mathbb{E}_{\boldsymbol{\omega}}\cos\left(\frac{\boldsymbol{\omega}^\top \boldsymbol{x}}{\sqrt{d}}\right)\right]^2 = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\left[\exp\left(-\frac{\|\boldsymbol{x}\|_2^2}{d}\right)\right], \quad i, j = 1, 2, \ldots, m \text{ with } i \neq j.$$

The matrix $\boldsymbol{S}_2 \in \mathbb{R}^{m \times m}$ is diagonal with

$$[\boldsymbol{S}_2]_{ii} = \frac{1}{m}\mathbb{E}_{\boldsymbol{x},\boldsymbol{\omega}}\left[\sin\left(\frac{\boldsymbol{\omega}^\top \boldsymbol{x}}{\sqrt{d}}\right)\right]^2 = \frac{1}{2m}\mathbb{E}_{\boldsymbol{x}}\left[1 - \exp\left(-2\frac{\|\boldsymbol{x}\|_2^2}{d}\right)\right], \quad i = 1, 2, \ldots, m.$$

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

$$\begin{aligned}
\widetilde{\lambda}_1 &= \mathbb{E}_{\boldsymbol{x}}\left[\exp\left(-\frac{\|\boldsymbol{x}\|_2^2}{d}\right)\right] + \frac{1}{2m}\mathbb{E}_{\boldsymbol{x}}\left[1 - \exp\left(-\frac{\|\boldsymbol{x}\|_2^2}{d}\right)\right]^2 \sim \mathcal{O}(1), \\
\widetilde{\lambda}_2 &= \frac{1}{2m}\mathbb{E}_{\boldsymbol{x}}\left[1 - \exp\left(-2\frac{\|\boldsymbol{x}\|_2^2}{d}\right)\right] \sim \mathcal{O}\left(\frac{1}{m}\right), \\
\widetilde{\lambda}_3 &= \frac{1}{2m}\mathbb{E}_{\boldsymbol{x}}\left[1 - \exp\left(-\frac{\|\boldsymbol{x}\|_2^2}{d}\right)\right]^2 \sim \mathcal{O}\left(\frac{1}{m}\right).
\end{aligned}$$

In this case, we can also get the similar claim on spectra of $\widetilde{\Sigma}_m$ with the single-output version: $\widetilde{\Sigma}_m$ admits the largest eigenvalue at $\mathcal{O}(1)$ order, and the remaining eigenvalues are at $\mathcal{O}(1/m)$ order.

C.2 Proof of Lemma 2

Proof. As discussed before, $\sigma\left(\frac{\boldsymbol{\omega}^\top \boldsymbol{x}}{\sqrt{d}}\right)$ is a sub-Gaussian random variable with the $\mathcal{O}(1)$ sub-Gaussian norm order. Hence, $\|\Sigma_m - \widetilde{\Sigma}_m\|_2$ is a sub-exponential random variable with

$$\begin{aligned}
\|\Sigma_m - \widetilde{\Sigma}_m\|_2 \leqslant \|\Sigma_m\|_2 + \|\widetilde{\Sigma}_m\|_2 &= \frac{1}{m}\left\|\mathbb{E}_{\boldsymbol{x}}\left[\sigma\left(\frac{\boldsymbol{W}\boldsymbol{x}}{\sqrt{d}}\right)\sigma\left(\frac{\boldsymbol{W}\boldsymbol{x}}{\sqrt{d}}\right)^\top\right]\right\|_2 + \mathcal{O}(1) \quad \text{[using Lemma 1]} \\
&\leqslant \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\left\|\sigma\left(\frac{\boldsymbol{W}\boldsymbol{x}}{\sqrt{d}}\right)\right\|_2^2 + \mathcal{O}(1) \quad \text{[Jensen's inequality]} \\
&\lesssim \frac{1}{m}\left(\mathbb{E}_{\boldsymbol{x}}\|\sigma(\boldsymbol{0}_m)\|_2^2 + \mathbb{E}_{\boldsymbol{x}}\left\|\frac{\boldsymbol{W}\boldsymbol{x}}{\sqrt{d}}\right\|_2^2\right) + \mathcal{O}(1) \quad [\sigma\text{: Lipschitz continuous}] \\
&\lesssim \mathcal{O}(1) + \frac{1}{md}\sum_{i=1}^m \boldsymbol{\omega}_i^\top \mathbb{E}_{\boldsymbol{x}}[\boldsymbol{x}\boldsymbol{x}^\top]\boldsymbol{\omega}_i \quad [\text{using } \|\Sigma_d\|_2 < \infty] \\
&\lesssim \frac{1}{d}\|\boldsymbol{\omega}\|_2^2 \quad [\text{here } \boldsymbol{\omega} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I}_d)],
\end{aligned}$$

where $\|\boldsymbol{\omega}\|_2^2$ is a $\chi^2(d)$ random variable, and thus $\|\Sigma_m - \widetilde{\Sigma}_m\|_2$ has sub-exponential norm at $\mathcal{O}(1)$ order. Accordingly, the high moment $\mathbb{E}\|\Sigma_m\|_2^p < \infty$ holds for finite p. Following the above derivation, we can also conclude that $\mathrm{Tr}(\Sigma_m)$ has the sub-exponential norm $\mathcal{O}(1)$, i.e.

$$\mathrm{Tr}(\Sigma_m) = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\mathrm{Tr}\left[\sigma\left(\frac{\boldsymbol{W}\boldsymbol{x}}{\sqrt{d}}\right)\sigma\left(\frac{\boldsymbol{W}\boldsymbol{x}}{\sqrt{d}}\right)^\top\right] = \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\left\|\sigma\left(\frac{\boldsymbol{W}\boldsymbol{x}}{\sqrt{d}}\right)\right\|_2^2 \lesssim \frac{1}{d}\|\boldsymbol{\omega}\|_2^2.$$

Likewise, we can derive $\mathrm{Tr}(\Sigma_m^2) < \infty$ in the similar fashion. □

C.3 Proof of Lemma 3

Proof. The first inequality naturally holds, and so we focus on the second inequality. Denote $\Phi := \mathbb{E}_{\boldsymbol{x},\boldsymbol{W}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]$, its diagonal elements are the same

$$\Phi_{ii} = \frac{m-1}{m^2}\mathbb{E}_{\boldsymbol{x}}\left(\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]^2\right)^2 + \frac{1}{m^2}\mathbb{E}_{\boldsymbol{x}}\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]^4 \sim \mathcal{O}\left(\frac{1}{m}\right).$$

Its non-diagonal elements Φ_{ij} with $i \neq j$ are the same

$$\begin{aligned}\Phi_{ij} = &\frac{m-3}{m^2}\mathbb{E}_{\boldsymbol{x}}\left[\left(\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]\right)^2 \mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]^2\right] \\ &+ \frac{2}{m^2}\mathbb{E}_{\boldsymbol{x}}\left[\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]^3\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]\right],\end{aligned}$$

where the first term is in $\mathcal{O}(\frac{1}{m})$ order and the second term is in $\mathcal{O}(\frac{1}{m^2})$ order. By denoting $a := (\widetilde{\Sigma}_m)_{ii}$, $b := (\widetilde{\Sigma}_m)_{ij}$ as given by Lemma 1, $A := \Phi_{ii}$, and $B := \Phi_{ij}$, the operator $r\mathrm{Tr}(\widetilde{\Sigma}_m)\widetilde{\Sigma}_m - \Phi$ can be represented as

$$r\mathrm{Tr}(\widetilde{\Sigma}_m)\Sigma_m - \Phi = [rm(a-b) - A + B]\, I_m + (rmab - B)\mathbf{1}\mathbf{1}^\top,$$

of which the smallest eigenvalue is $rma(a-b) - A + B$. Accordingly, to ensure the positive definiteness of $r\mathrm{Tr}(\widetilde{\Sigma}_m)\widetilde{\Sigma}_m - \Phi$, which implies $\mathbb{E}_{\boldsymbol{W}}\left(\mathbb{E}_{\boldsymbol{x}}\left([\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]A[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]\right)\right) \preccurlyeq r\mathrm{Tr}(\widetilde{\Sigma}_m)\widetilde{\Sigma}_m$, we require its smallest eigenvalue is non-negative, i.e., $rma(a-b) - A + B \geqslant 0$. That means, r should satisfies

$$r \geqslant \frac{A-B}{ma(a-b)} = \frac{A-B}{\frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\mathbb{E}_{z\sim\mathcal{N}(0,\|\boldsymbol{x}\|_2^2/d)}[\sigma(z)]^2\mathbb{E}_{\boldsymbol{x}}\mathbb{V}[\sigma(z)]}. \tag{12}$$

Since $A - B$ admits

$$A - B \leqslant \frac{1}{m}\mathbb{E}_{\boldsymbol{x}}\mathbb{E}_z[\sigma(z)]^2\mathbb{E}_{\boldsymbol{x}}\mathbb{V}[\sigma(z)] + \mathcal{O}\left(\frac{1}{m^2}\right),$$

then by taking $r := 1 + \mathcal{O}\left(\frac{1}{m}\right)$, the condition in Eq. (12) satisfies, and thus $r\mathrm{Tr}(\widetilde{\Sigma}_m)\widetilde{\Sigma}_m - \Phi$ is positive definite, which concludes the proof. □

D Preliminaries on PSD operators

In this section, we first define some stochastic/deterministic PSD operators that follow [63, 16] in stochastic approximation, and then present Lemma 5 that is based on PSD operators and is needed to estimate `B1` and `V1`. Note that, the PSD operators will make the notation in our proof simple and clarity but do not change the proof itself.

Following [63, 16], we define several stochastic PSD operators as below. Given the random features matrix $\boldsymbol{W}$ and any PSD operator A, define

$$\begin{aligned}&S^{\mathtt{W}} := \mathbb{E}_{\boldsymbol{x}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})], \quad \widetilde{S}^{\mathtt{W}} := \Sigma_m \otimes \Sigma_m, \\ &S^{\mathtt{W}} \circ A := \mathbb{E}_{\boldsymbol{x}}\left[\varphi(\boldsymbol{x})^\top\varphi(\boldsymbol{x})A\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})\right], \quad \widetilde{S}^{\mathtt{W}} \circ A := \Sigma_m A \Sigma_m,\end{aligned}$$

where the superscript `W` denotes the randomness dependency on the random feature matrix $\boldsymbol{W}$. Besides, for any γ_i ($i = 1, 2, \ldots, n$), define the following operators

$$\begin{aligned}&(I - \gamma_i T^{\mathtt{W}}) \circ A := \mathbb{E}_{\boldsymbol{x}}\left([I - \gamma_i\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]A[I - \gamma_i\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]\right) \\ &(I - \gamma_i\widetilde{T}^{\mathtt{W}}) \circ A := (I - \gamma_i\Sigma_m)A(I - \gamma_i\Sigma_m),\end{aligned}$$

associated with two corresponding operators (that depend on γ_i)

$$T^{\mathtt{W}} := \Sigma_m \otimes I + I \otimes \Sigma_m - \gamma_i S^{\mathtt{W}}, \quad \widetilde{T}^{\mathtt{W}} := \Sigma_m \otimes I + I \otimes \Sigma_m - \gamma_i\widetilde{S}^{\mathtt{W}}.$$

Clearly, the above operators $S^{\mathtt{W}}$, $\widetilde{S}^{\mathtt{W}}$, $(I-\gamma_i T^{\mathtt{W}})$, $(I-\gamma_i \widetilde{T}^{\mathtt{W}})$, $T^{\mathtt{W}}$, and $\widetilde{T}^{\mathtt{W}}$ are PSD, and $S^{\mathtt{W}} \succcurlyeq \widetilde{S}^{\mathtt{W}}$. The proof is similar to [16, Lemma B.1] and thus we omit it here.

Further, if $\gamma_0 < 1/\mathrm{Tr}(\Sigma_m)$, the PSD operator $I-\gamma_i\Sigma_m$ $(i=1,2,\ldots,n)$ is a contraction map, and thus for any PSD operator A and step-size γ_i, the following exists

$$\sum_{t=0}^{\infty}(I-\gamma_i\widetilde{T}^{\mathtt{W}})^t \circ A = \sum_{t=0}^{\infty}(I-\gamma_i\Sigma_m)^t A (I-\gamma_i\Sigma_m)^t \,.$$

Hence, $(\widetilde{T}^{\mathtt{W}})^{-1} := \gamma_i \sum_{t=0}^{\infty}(I-\gamma_i\widetilde{T}^{\mathtt{W}})^t$ exists and is PSD. We need to remark that, though $\mathrm{Tr}(\Sigma_m)$ is a random variable, it is with a sub-exponential $\mathcal{O}(1)$ norm. That means, this holds with exponentially high probability.

Based on the above stochastic operators, we define several deterministic PSD ones by taking the expectation over $\boldsymbol{W}$ as below. For any given γ_i $(i=1,2,\ldots,n)$, we have the following PSD operators

$$\begin{aligned}
&S := \mathbb{E}_{\boldsymbol{W}}[\Sigma_m \otimes \Sigma_m], \quad \widetilde{S} := \widetilde{\Sigma}_m \otimes \widetilde{\Sigma}_m \,,\\
&T := \widetilde{\Sigma}_m \otimes I + I \otimes \widetilde{\Sigma}_m - \gamma_i S, \quad \widetilde{T} := \widetilde{\Sigma}_m \otimes I + I \otimes \widetilde{\Sigma}_m - \gamma_i \widetilde{S} \,,\\
&S \circ A := \mathbb{E}_{\boldsymbol{W}}[\Sigma_m A \Sigma_m], \quad \widetilde{S} \circ A := \widetilde{\Sigma}_m A \widetilde{\Sigma}_m \,,\\
&(I-\gamma_i T)\circ A := \mathbb{E}_{\boldsymbol{W}}[(I-\gamma_i\Sigma_m)A(I-\gamma_i\Sigma_m)], \quad (I-\gamma_i\widetilde{T})\circ A := (I-\gamma_i\widetilde{\Sigma}_m)A(I-\gamma_i\widetilde{\Sigma}_m) \,,
\end{aligned}$$

which implies $\widetilde{T} - T = \gamma_i(S-\widetilde{S})$.

Based on the above PSD operators, we present a lemma here that is used to estimate B1 and V1.[4]

Lemma 5. *Under Assumptions 1, 2, 3, 4 with $r' \geqslant 1$, denote*

$$D_t^{\mathtt{v-x}} := \sum_{s=1}^{t}\prod_{i=s+1}^{t}(I-\gamma_i T^{\mathtt{W}}) \circ \gamma_s^2 B \Sigma_m \,, \tag{13}$$

with a scalar B independent of k, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0,1)$ satisfies

$$\gamma_0 < \min\left\{\frac{1}{r'\mathrm{Tr}(\Sigma_m)}, \frac{1}{c'\mathrm{Tr}(\Sigma_m)}\right\} \,,$$

where the constant c' is defined as

$$c' := \begin{cases} 1, \ \textit{if}\ \zeta = 0 \,, \\ \dfrac{1}{1-2^{-\zeta}}, \ \textit{if}\ \zeta \in (0,1) \,. \end{cases} \tag{14}$$

Then $D_t^{\mathtt{v-x}}$ can be upper bounded by

$$D_t^{\mathtt{v-x}} \preccurlyeq \frac{\gamma_0 B}{1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)} I \,.$$

Remark: The PSD operator $I-\gamma_i T^{\mathtt{W}}$ cannot be guaranteed as a contraction map since we cannot directly choose $\gamma_0 < \frac{1}{\mathrm{Tr}[\varphi(\boldsymbol{x})\varphi(\boldsymbol{x})^\top]}$ for general data $\boldsymbol{x}$. However, its summation in Eq. (13) can be still bounded by our lemma. In our work, we set $B := r'\mathrm{Tr}(\Sigma_m)$ for estimate B1, and $B := \tau^2 r'\gamma_0[\mathrm{Tr}(\Sigma_m) + \gamma_0 \mathrm{Tr}(\Sigma_m^2)]$ to bound V1, respectively.

Proof. Our proof can be divided into two parts: one is to prove $\mathrm{Tr}[D_t^{\mathtt{v-x}}(\zeta)] \leqslant \mathrm{Tr}[D_t^{\mathtt{v-x}}(0)]$ for any $\zeta \in [0,1)$; the other is to provide the upper bound of $D_t^{\mathtt{v-x}}(0)$. We focus on the first part and the proof in the second part follows [63, Lemmas 3 and 5] and [16, Lemma B.4].

[4] Our proofs on the remaining quantities including V2, V3, B2, B3 do not use PSD operators.

The quantity $\mathrm{Tr}[D_t^{\mathtt{v}-\mathtt{X}}(\zeta)]$ admits the following representation by the definition of $I-\gamma_i T^{\mathtt{W}}$

$$\begin{aligned}
\mathrm{Tr}[D_t^{\mathtt{v}-\mathtt{X}}(\zeta)] &= \sum_{s=1}^{t}\prod_{i=s+1}^{t}\mathrm{Tr}\left[(I-\gamma_i T^{\mathtt{W}})\circ\gamma_s^2 B\Sigma_m\right] \\
&= \sum_{s=1}^{t} B\gamma_s^2\prod_{i=s+1}^{t}\mathrm{Tr}\Big(\mathbb{E}_{\boldsymbol{x}}[I-\gamma_i\varphi(\boldsymbol{x})\otimes\varphi(\boldsymbol{x})]\Sigma_m[I-\gamma_i\varphi(\boldsymbol{x})\otimes\varphi(\boldsymbol{x})]\Big) \\
&= B\sum_{s=1}^{t}\gamma_s^2\prod_{i=s+1}^{t}\mathrm{Tr}\Big(\Sigma_m-2\gamma_i\Sigma_m^2+\gamma_i^2\Sigma_m\mathbb{E}_{\boldsymbol{x}}\left[\varphi(\boldsymbol{x})\otimes\varphi(\boldsymbol{x})\otimes\varphi(\boldsymbol{x})\otimes\varphi(\boldsymbol{x})\right]\Big)\,.
\end{aligned}$$

Based on the above results, we have

$$\begin{aligned}
\mathrm{Tr}[D_t^{\mathtt{v}-\mathtt{X}}(0)]-\mathrm{Tr}[D_t^{\mathtt{v}-\mathtt{X}}(\zeta)] &= B\sum_{s=1}^{t}\prod_{i=s+1}^{t}\mathrm{Tr}\Big(\Sigma_m\Big[(\gamma_0^2-\gamma_s^2)I-2(\gamma_0^3-\gamma_s^2\gamma_i)\Sigma_m \\
&\qquad +(\gamma_0^4-\gamma_i^2\gamma_s^2)\mathbb{E}_{\boldsymbol{x}}\left[\varphi(\boldsymbol{x})\otimes\varphi(\boldsymbol{x})\otimes\varphi(\boldsymbol{x})\otimes\varphi(\boldsymbol{x})\right]\Big]\Big) \\
&\geqslant B\sum_{s=1}^{t}\prod_{i=s+1}^{t}\mathrm{Tr}\Big(\Sigma_m\Big[(\gamma_0^2-\gamma_s^2)I-2(\gamma_0^3-\gamma_s^2\gamma_i)\Sigma_m+(\gamma_0^4-\gamma_i^2\gamma_s^2)\Sigma_m^2\Big]\Big) \\
&= B\sum_{s=1}^{t}\prod_{i=s+1}^{t}\sum_{j=1}^{m}\Big(\lambda_j\Big[(\gamma_0^2-\gamma_s^2)-2(\gamma_0^3-\gamma_s^2\gamma_i)\lambda_j+(\gamma_0^4-\gamma_i^2\gamma_s^2)\lambda_j^2\Big]\Big) \\
&= B\sum_{s=1}^{t}\prod_{i=s+1}^{t}\sum_{j=1}^{m}\Big(\lambda_j\Big[(\gamma_0^4-\gamma_i^2\gamma_s^2)\left(\lambda_j-\frac{\gamma_0^3-\gamma_s^2\gamma_i}{\gamma_0^4-\gamma_i^2\gamma_s^2}\right)^2-\frac{\gamma_0^2\gamma_s^2(\gamma_0-\gamma_i)^2}{\gamma_0^4-\gamma_i^2\gamma_s^2}\Big]\Big)\,.
\end{aligned}$$

Accordingly, $\mathrm{Tr}[D_t^{\mathtt{v}-\mathtt{X}}(0)]-\mathrm{Tr}[D_t^{\mathtt{v}-\mathtt{X}}(\zeta)]\geqslant 0$ naturally holds when $\zeta=0$. When $\zeta\in(0,1)$, it holds if $\lambda_j\leqslant\frac{\gamma_0^3-\gamma_s^2\gamma_i-\gamma_0^2\gamma_s+\gamma_0\gamma_s\gamma_i}{\gamma_0^4-\gamma_s^2\gamma_i^2}$ with $j=1,2,\ldots,m$. This condition can be satisfied by

Case 1 (if $s=1$)**.** *In this case, $\gamma_1=\gamma_0$ and we have*

$$\lambda_j\leqslant\mathrm{Tr}(\Sigma_m)\leqslant\frac{1}{2\gamma_0}\leqslant\frac{1}{\gamma_0+\gamma_i}=\frac{\gamma_0^3-\gamma_s^2\gamma_i-\gamma_0^2\gamma_s+\gamma_0\gamma_s^2}{\gamma_0^4-\gamma_s^2\gamma_i^2}\,,\quad \textit{when } s=1\,.$$

Case 2 (if $s=2,3,\ldots$)**.** *In this case, notice*

$$\frac{\gamma_0^4-\gamma_s^2\gamma_i^2}{\gamma_0^3-\gamma_s^2\gamma_i-\gamma_0^2\gamma_s+\gamma_0\gamma_s^2}\leqslant\frac{\gamma_0^4}{\gamma_0(\gamma_0-\gamma_s)(\gamma_0^2+\gamma_s\gamma_i)}\leqslant\frac{\gamma_0^3}{(\gamma_0-\gamma_2)(\gamma_0^2+\gamma_2\gamma_3)}=\frac{1}{1-2^{-\zeta}}\,,$$

Accordingly, we have

$$\lambda_j\leqslant\mathrm{Tr}(\Sigma_m)\leqslant\frac{1-2^{-\zeta}}{\gamma_0}\leqslant\frac{\gamma_0^3-\gamma_s^2\gamma_i-\gamma_0^2\gamma_s+\gamma_0\gamma_s^2}{\gamma_0^4-\gamma_s^2\gamma_i^2}\,,$$

where the second inequality holds by Eq. (14). Accordingly, combining the above two cases, if we choose

$$\gamma_0\leqslant\frac{1}{\frac{1}{1-2^{-\zeta}}\mathrm{Tr}(\Sigma_m)}\,,\quad \text{for } \zeta\in(0,1)\,,$$

we have $\mathrm{Tr}[D_t^{\mathtt{v}-\mathtt{X}}(0)]-\mathrm{Tr}[D_t^{\mathtt{v}-\mathtt{X}}(\zeta)]\geqslant 0$.

In the next, we give the upper bound for $D_t^{\mathtt{v}-\mathtt{X}}(0)$. The proof follows [63, Lemmas 3 and 5] and [16, Lemma B.4]. We just present it here for completeness. We firstly demonstrate that $D_t^{\mathtt{v}-\mathtt{X}}(0)$ is increasing and bounded, which implies that the limit $D_\infty^{\mathtt{v}-\mathtt{X}}(0)$ exists, and then we seek for the upper bound of this limit. To be specific, $D_t^{\mathtt{v}-\mathtt{X}}(0)$ admits the following expression

$$D_t^{\mathtt{v}-\mathtt{X}}(0):=\sum_{k=1}^{t}(I-\gamma_0T^{\mathtt{W}})^{k-1}\circ\gamma_0^2B\Sigma_m=D_{t-1}^{\mathtt{v}-\mathtt{X}}(0)+(I-\gamma_0T^{\mathtt{W}})^{t-1}\circ\gamma_0^2B\Sigma_m\succcurlyeq D_{t-1}^{\mathtt{v}-\mathtt{X}}(0)\,,$$

which implies that $D_t^{\mathtt{v}-\mathtt{X}}(0)$ is increasing.

Let $A_t := (I - \gamma_0 T^{\mathtt{W}})^{t-1} \circ B\Sigma_m$, and then $A_t = (I - \gamma_0 T^{\mathtt{W}}) \circ A_{t-1}$. We have

$$\begin{aligned}
\mathrm{Tr}(A_t) &= \mathrm{Tr}[(I - \gamma_0 T^{\mathtt{W}}) \circ A_{t-1}] = \mathrm{Tr}(A_{t-1}) - 2\gamma_0 \mathrm{Tr}(\Sigma_m A_{t-1}) + \gamma_0^2 \mathrm{Tr}(S^{\mathtt{W}} \circ A_{t-1}) \\
&\leqslant \mathrm{Tr}(A_{t-1}) - 2\gamma_0 \mathrm{Tr}(\Sigma_m A_{t-1}) + \gamma_0^2 r' \mathrm{Tr}(\Sigma_m A_{t-1}) \mathrm{Tr}(\Sigma_m) \quad \text{[using Assumption 4]} \\
&\leqslant \mathrm{Tr}[(I - \gamma_0 \Sigma_m) A_{t-1}] \leqslant (1 - \gamma_0 \lambda_m) \mathrm{Tr}(A_{t-1}) \,, \quad \text{[using } \gamma_0 \leqslant \tfrac{1}{r' \mathrm{Tr}(\Sigma_m)}\text{]}
\end{aligned}$$

which implies

$$\mathrm{Tr}[D_t^{\mathtt{v}-\mathtt{X}}(0)] \leqslant \gamma_0^2 \sum_{t=0}^{\infty} \mathrm{Tr}\left((I - \gamma_0 T^{\mathtt{W}})^t \circ B\Sigma_m\right) \leqslant \mathrm{Tr}(B\Sigma_m) \sum_{t=0}^{\infty} (1 - \gamma_0 \lambda_m)^t \leqslant \frac{\gamma_0 \mathrm{Tr}(B\Sigma_m)}{\lambda_m} < \infty \,.$$

Accordingly, the monotonicity and boundedness of $\{D_t^{\mathtt{v}-\mathtt{X}}(0)\}_{t=0}^{\infty}$ implies that the limit exists, denoted as $D_\infty^{\mathtt{v}-\mathtt{X}}(0)$ with

$$D_\infty^{\mathtt{v}-\mathtt{X}}(0) = (I - \gamma_0 T^{\mathtt{W}}) \circ D_\infty^{\mathtt{v}-\mathtt{X}}(0) + \gamma_0^2 B\Sigma_m \,,$$

which implies $D_\infty^{\mathtt{v}-\mathtt{X}}(0) = \gamma_0 (T^{\mathtt{W}})^{-1} \circ B\Sigma_m$ Further, we have

$$\begin{aligned}
\widetilde{T}^{\mathtt{W}} \circ D_\infty^{\mathtt{v}-\mathtt{X}}(0) &= T^{\mathtt{W}} \circ D_\infty^{\mathtt{v}-\mathtt{X}}(0) + \gamma_0 S^{\mathtt{W}} \circ D_\infty^{\mathtt{v}-\mathtt{X}}(0) - \gamma_0 \widetilde{S}^{\mathtt{W}} \circ D_\infty^{\mathtt{v}-\mathtt{X}}(0) \quad \text{[definition of } \widetilde{T}^{\mathtt{W}}\text{]} \\
&= \gamma_0 B\Sigma_m + \gamma_0 S^{\mathtt{W}} \circ D_\infty^{\mathtt{v}-\mathtt{X}}(0) - \gamma_0 \widetilde{S}^{\mathtt{W}} \circ D_\infty^{\mathtt{v}-\mathtt{X}}(0) \\
&\preccurlyeq \gamma_0 B\Sigma_m + \gamma_0 S^{\mathtt{W}} \circ D_\infty^{\mathtt{v}-\mathtt{X}}(0) \,. \quad \text{[using } S^{\mathtt{W}} \succcurlyeq \widetilde{S}^{\mathtt{W}}\text{]}
\end{aligned} \tag{15}$$

Besides, $(\widetilde{T}^{\mathtt{W}})^{-1} \circ \Sigma_m$ can be bounded by

$$\begin{aligned}
(\widetilde{T}^{\mathtt{W}})^{-1} \circ \Sigma_m &= \gamma_0 \sum_{t=0}^{\infty} (I - \gamma_0 \widetilde{T}^{\mathtt{W}}) \circ \Sigma_m = \gamma_0 \sum_{t=0}^{\infty} (I - \gamma_0 \Sigma_m)^t \Sigma_m (I - \gamma_0 \Sigma_m)^t \\
&\preccurlyeq \gamma_0 \sum_{t=0}^{\infty} (I - \gamma_0 \Sigma_m)^t \Sigma_m = I \,. \quad \text{[using } \gamma_0 \leqslant 1/\mathrm{Tr}(\Sigma_m)\text{]}
\end{aligned} \tag{16}$$

Therefore, $D_\infty^{\mathtt{v}-\mathtt{X}}(0)$ can be further upper bounded by

$$\begin{aligned}
D_\infty^{\mathtt{v}-\mathtt{X}}(0) &\preccurlyeq \gamma_0 (\widetilde{T}^{\mathtt{W}})^{-1} \circ B\Sigma_m + \gamma_0 (\widetilde{T}^{\mathtt{W}})^{-1} \circ S^{\mathtt{W}} \circ D_\infty^{\mathtt{v}-\mathtt{X}}(0) \quad \text{[using Eq. (15)]} \\
&\preccurlyeq \gamma_0 B + \gamma_0 (\widetilde{T}^{\mathtt{W}})^{-1} \circ S^{\mathtt{W}} \circ D_\infty^{\mathtt{v}-\mathtt{X}}(0) \quad \text{[using Eq. (16)]} \\
&= \gamma_0 B \sum_{t=0}^{\infty} [\gamma_0 (\widetilde{T}^{\mathtt{W}})^{-1} \circ S^{\mathtt{W}}]^t \circ I \quad \text{[solving the recursion]} \\
&\preccurlyeq \gamma_0 B \sum_{t=0}^{\infty} \left(\gamma_0 (\widetilde{T}^{\mathtt{W}})^{-1} \circ S^{\mathtt{W}}\right)^{t-1} \circ \gamma_0 (\widetilde{T}^{\mathtt{W}})^{-1} \circ S^{\mathtt{W}} \circ I \\
&\preccurlyeq \gamma_0 B \sum_{t=0}^{\infty} \left(\gamma_0 (\widetilde{T}^{\mathtt{W}})^{-1} \circ S^{\mathtt{W}}\right)^{t-1} \circ \gamma_0 (\widetilde{T}^{\mathtt{W}})^{-1} \circ \mathrm{Tr}(\Sigma_m) \Sigma_m \quad \text{[using Assumption 4]} \\
&\preccurlyeq \gamma_0 B \sum_{t=0}^{\infty} [\gamma_0 r' \mathrm{Tr}(\Sigma_m)]^t \circ I \quad \text{[using Eq. (16)]} \\
&\preccurlyeq \frac{\gamma_0 B}{1 - \gamma_0 r' \mathrm{Tr}(\Sigma_m)} I \,. \quad \text{[using } \gamma_0 < \tfrac{1}{r' \mathrm{tr}(\Sigma_m)}\text{]}
\end{aligned} \tag{17}$$

Hence, based on the above results, $D_t^{\mathtt{v}-\mathtt{X}}(0)$ can be further upper bounded by

$$
\begin{aligned}
D_t^{\mathtt{v}-\mathtt{X}}(0) &= (I-\gamma_0 T^{\mathtt{W}}) \circ D_{t-1}^{\mathtt{v}-\mathtt{X}}(0) + \gamma_0^2 B\Sigma_m \\
&= (I-\gamma_0 \widetilde{T}^{\mathtt{W}}) \circ D_{t-1}^{\mathtt{v}-\mathtt{X}}(0) + \gamma_0^2 (S^{\mathtt{W}} - \widetilde{S}^{\mathtt{W}}) \circ D_{t-1}^{\mathtt{v}-\mathtt{X}} + \gamma_0^2 B\Sigma_m \\
&\preccurlyeq (I-\gamma_0 \widetilde{T}^{\mathtt{W}}) \circ D_{t-1}^{\mathtt{v}-\mathtt{X}}(0) + \gamma_0^2 S^{\mathtt{W}} \circ D_{\infty}^{\mathtt{v}-\mathtt{X}}(0) + \gamma_0^2 B\Sigma_m \\
&\preccurlyeq (I-\gamma_0 \widetilde{T}^{\mathtt{W}}) \circ D_{t-1}^{\mathtt{v}-\mathtt{X}}(0) + \gamma_0^2 r' \mathrm{Tr}[D_{\infty}^{\mathtt{v}-\mathtt{X}}(0)] \mathrm{Tr}(\Sigma_m)\Sigma_m + \gamma_0^2 B\Sigma_m \quad \text{[using Assumption 4]} \\
&\preccurlyeq (I-\gamma_0 \widetilde{T}^{\mathtt{W}}) \circ D_{t-1}^{\mathtt{v}-\mathtt{X}}(0) + \gamma_0^2 B\Sigma_m \left(\frac{\mathrm{Tr}(\Sigma_m) r' \gamma_0}{1-\gamma_0 r' \mathrm{Tr}(\Sigma_m)} + 1 \right) \quad \text{[using Eq. (17)]} \\
&\preccurlyeq \gamma_0^2 B \left(\frac{\mathrm{Tr}(\Sigma_m) r' \gamma_0}{1-\gamma_0 r' \mathrm{Tr}(\Sigma_m)} + 1 \right) \sum_{k=0}^{\infty} (I-\gamma_0\Sigma_m)^k \Sigma_m \\
&\preccurlyeq \gamma_0 B \left(\frac{\mathrm{Tr}(\Sigma_m) r' \gamma_0}{1-\gamma_0 r' \mathrm{Tr}(\Sigma_m)} + 1 \right) I \,,
\end{aligned}
\tag{18}
$$

which concludes the proof. □

E Some useful integrals estimation

In this section, we present the estimation for the following integrals that will be needed in our proof by denoting $\kappa := 1-\zeta \in (0,1]$.

Integral 1: We consider the following integral admitting an exact estimation

$$
\int_1^t u^{-\zeta} \exp\left(-c\frac{u^{1-\zeta}-1}{1-\zeta} \right) \mathrm{d}u \leqslant t \,. \tag{19}
$$

Besides, we also calculate this integral as below: by changing the integral variable $v^\kappa := c\frac{u^{1-\zeta}-1}{1-\zeta}$ and

$$
\frac{\mathrm{d}v}{\mathrm{d}u} = u^{1-\kappa} \left(\frac{\kappa}{c}\right)^{\frac{1}{\kappa}} (u^\kappa - 1)^{\frac{\kappa-1}{\kappa}} = \frac{1}{c} u^{1-\kappa} \kappa v^{\kappa-1} \,,
$$

and then we have

$$
\begin{aligned}
\int_1^t u^{-\zeta} \exp\left(-c\frac{u^{1-\zeta}-1}{1-\zeta} \right) \mathrm{d}u &= \frac{1}{c} \int_0^{[\frac{c}{\kappa}(t^\kappa-1)]^{\frac{1}{\kappa}}} u^{-\zeta} u^{1-\kappa} \kappa v^{\kappa-1} \exp(-v^\kappa) \mathrm{d}v \\
&\leqslant \frac{1}{c} \int_0^\infty \exp(-x) \mathrm{d}x = \left(\frac{1}{c} \wedge t \right) \,,
\end{aligned}
\tag{20}
$$

where the last equality uses Eq. (19) and takes the smaller one via the notation $\wedge$. Accordingly, if we take $\zeta = 0$ in Eq. (20), we have

$$
\int_1^t \exp\left(-c\frac{u^{1-\zeta}-1}{1-\zeta} \right) \mathrm{d}u \leqslant \left(\frac{1}{c} t^\zeta \wedge t \right) \,. \tag{21}
$$

Similar to Eq. (21), we have

$$
\int_t^n \exp\left(-\widetilde{\lambda}_i \gamma_0 \frac{u^{1-\zeta}-t^{1-\zeta}}{1-\zeta} \right) \mathrm{d}u \leqslant (n-t) \wedge \frac{n^\zeta}{\widetilde{\lambda}_i \gamma_0} \,. \tag{22}
$$

Integral 2: we consider the following integral

$$\begin{aligned}
&\int_1^t u^{-\zeta}\exp\Big(-c\frac{(t+1)^{1-\zeta}-(u+1)^{1-\zeta}}{1-\zeta}\Big)\mathrm{d}u\\
&=\frac{(t+1)^{1-\kappa}}{c}\int_0^C[(t+1)(1-x)^{\frac{1}{\kappa}}-1]^{\kappa-1}(1-x)^{\frac{1-\kappa}{\kappa}}\kappa v^{\kappa-1}\exp(-v^\kappa)\mathrm{d}v \quad \text{with } x:=(\frac{v}{t+1})^\kappa\frac{\kappa}{c}\\
&\leqslant\frac{2^\zeta}{c}\int_0^\infty \kappa v^{\kappa-1}\exp(-v^\kappa)\mathrm{d}v\\
&=\left(\frac{2^\zeta}{c}\wedge t\right),
\end{aligned}\tag{23}$$

where we change the integral variable $v^\kappa := c\frac{(t+1)^{1-\zeta}-(u+1)^{1-\zeta}}{1-\zeta}$ with $\kappa := 1-\zeta$ such that

$$\mathrm{d}u=-\frac{\kappa^{1/\kappa}}{c^{1/\kappa}}(\frac{u+1}{t+1})^{1-\kappa}\left[1-(\frac{u+1}{t+1})^\kappa\right]^{1-\frac{1}{\kappa}}\mathrm{d}v=-\frac{\kappa}{c}\left[1-(\frac{v}{t+1})^\kappa\frac{\kappa}{c}\right]^{\frac{1-\kappa}{\kappa}}\left(\frac{v}{t+1}\right)^{\kappa-1}\mathrm{d}v\,,$$

with $(\frac{u+1}{t+1})^\kappa = 1-(v/(t+1))^\kappa\kappa/c$ and the upper limit of integral is $C := c^{1/\kappa}[(t+1)^\kappa-(u+1)^\kappa]^{1/\kappa}$. Due to $u=(t+1)(1-x)^{\frac{1}{\kappa}}-1\in[1,t]$, we have $(1-x)^{\frac{1}{\kappa}}\in[2/(t+1),1]$ and accordingly

$$g(x):=[(t+1)(1-x)^{\frac{1}{\kappa}}-1]^{\kappa-1}(1-x)^{\frac{1-\kappa}{\kappa}}\leqslant 2^{1-\kappa}(t+1)^{\kappa-1}\quad\text{with } x\in\left[0,1-\left(\frac{2}{t+1}\right)^\kappa\right],$$

as an increasing function of x.

Similar to Eq. (23), we have the following estimation

$$\int_1^t \gamma_0^2 u^{-2\zeta}\exp\Big(-2\widetilde{\lambda}_i\gamma_0\frac{(t+1)^{1-\zeta}-(u+1)^{1-\zeta}}{1-\zeta}\Big)\mathrm{d}u\lesssim\left(\frac{\gamma_0}{\widetilde{\lambda}_i}\wedge\gamma_0^2 t\right).\tag{24}$$

F Proofs for `Bias`

In this section, we present the error bound for `Bias`. By virtue of Minkowski inequality, we have

$$\begin{aligned}
\Big(\mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\big[\langle\bar{\eta}_n^{\mathtt{bias}},\Sigma_m\bar{\eta}_n^{\mathtt{bias}}\rangle\big]\Big)^{\frac{1}{2}}&\leqslant\Big(\underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\big[\langle\bar{\eta}_n^{\mathtt{bias}}-\bar{\eta}_n^{\mathtt{bX}},\Sigma_m(\bar{\eta}_n^{\mathtt{bias}}-\bar{\eta}_n^{\mathtt{bX}})\rangle\big]}_{\triangleq\mathtt{B1}}\Big)^{\frac{1}{2}}+\Big(\mathbb{E}_{\boldsymbol{W}}\big[\langle\bar{\eta}_n^{\mathtt{bX}},\Sigma_m\bar{\eta}_n^{\mathtt{bX}}\rangle\big]\Big)^{\frac{1}{2}}\\
&\leqslant(\mathtt{B1})^{\frac{1}{2}}+\Big(\underbrace{\mathbb{E}_{\boldsymbol{W}}\big[\langle\bar{\eta}_n^{\mathtt{bX}}-\bar{\eta}_n^{\mathtt{bXW}},\Sigma_m(\bar{\eta}_n^{\mathtt{bX}}-\bar{\eta}_n^{\mathtt{bXW}})\rangle\big]}_{\triangleq\mathtt{B2}}\Big)^{\frac{1}{2}}+\big[\underbrace{\langle\bar{\eta}_n^{\mathtt{bXW}},\widetilde{\Sigma}_m\bar{\eta}_n^{\mathtt{bXW}}\rangle}_{\triangleq\mathtt{B3}}\big]^{\frac{1}{2}}.
\end{aligned}\tag{25}$$

In the next, we give the error bounds for `B3`, `B2`, and `B1`, respectively.

F.1 Bound for `B3`

In this section, we aim to bound $\mathtt{B3} := \langle\bar{\eta}_n^{\mathtt{bXW}},\widetilde{\Sigma}_m\bar{\eta}_n^{\mathtt{bXW}}\rangle$.

Proposition 2. *Under Assumption 1, 2, 3, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta\in[0,1)$ satisfies $\gamma_0\leqslant\frac{1}{\mathrm{Tr}(\widetilde{\Sigma}_m)}$, then* `B3` *can be bounded by*

$$\mathtt{B3}\lesssim\frac{n^{\zeta-1}}{\gamma_0}\|f^*\|^2\,.$$

Proof. Due to $\gamma_0\leqslant\frac{1}{\mathrm{Tr}(\widetilde{\Sigma}_m)}$, the operator $I-\gamma_t\widetilde{\Sigma}_m$ is a contraction map for $t=1,2,\ldots,n$. Take spectral decomposition $\widetilde{\Sigma}_m=\widetilde{U}\widetilde{\Lambda}\widetilde{U}^\top$ where $\widetilde{U}$ is an orthogonal matrix and $\widetilde{\Lambda}$ is a diagonal matrix

with $(\widetilde{\Lambda})_{11} = \widetilde{\lambda}_1$ and $(\widetilde{\Lambda})_{ii} = \widetilde{\lambda}_2$ $(i = 2, 3, \ldots, m)$ as $\widetilde{\Sigma}_m$ has only two distinct eigenvalues in Lemma 1. Accordingly, we have

$$
\begin{aligned}
\langle \bar{\eta}_n^{\mathtt{bXW}}, \widetilde{\Sigma}_m \bar{\eta}_n^{\mathtt{bXW}} \rangle &= \frac{1}{n^2} \left\langle \sum_{t=0}^{n-1} \prod_{i=1}^{t} (I - \gamma_i \widetilde{\Sigma}_m) f^*, \widetilde{\Sigma}_m \sum_{t=0}^{n-1} \prod_{i=1}^{t} (I - \gamma_i \widetilde{\Sigma}_m) f^* \right\rangle \\
&= \frac{1}{n^2} \left\| \sum_{t=0}^{n-1} \prod_{i=1}^{t} (I - \gamma_i \widetilde{\Sigma}_m) \widetilde{\Sigma}_m^{\frac{1}{2}} f^* \right\|^2 \\
&\leqslant \frac{1}{n^2} \left\| \sum_{t=0}^{n-1} \prod_{i=1}^{t} (I - \gamma_i \widetilde{\Lambda}) \widetilde{\Lambda}^{\frac{1}{2}} \right\|_2^2 \|f^*\|^2 \quad \text{[using } \widetilde{\Sigma}_m = \widetilde{U} \widetilde{\Lambda} \widetilde{U}^\top \text{]} \\
&\leqslant \frac{1}{n} \max_{k=1,2} \sum_{t=0}^{n-1} \prod_{i=1}^{t} (1 - \gamma_i \widetilde{\lambda}_k)^2 \widetilde{\lambda}_k \|f^*\|^2 \\
&\leqslant \frac{1}{n} \sum_{t=0}^{n-1} \prod_{i=1}^{t} (1 - \gamma_i \widetilde{\lambda}_1)^2 \widetilde{\lambda}_1 \|f^*\|^2 + \frac{1}{n} \sum_{t=0}^{n-1} \prod_{i=1}^{t} (1 - \gamma_i \widetilde{\lambda}_2)^2 \widetilde{\lambda}_2 \|f^*\|^2 .
\end{aligned} \tag{26}
$$

Note that

$$
\begin{aligned}
\sum_{t=0}^{n-1} \prod_{i=1}^{t} (1 - \gamma_i \widetilde{\lambda}_j)^2 &\leqslant \sum_{t=0}^{n-1} \exp\left(-2\gamma_0 \widetilde{\lambda}_j \sum_{i=1}^{t} i^{-\zeta} \right) \leqslant \sum_{t=0}^{n-1} \exp\left(-2\gamma_0 \widetilde{\lambda}_j \int_1^{t+1} \frac{1}{x^\zeta} \mathrm{d}x \right) \\
&= \sum_{t=0}^{n-1} \exp\left(-2\gamma_0 \widetilde{\lambda}_j \frac{(t+1)^{1-\zeta} - 1}{1 - \zeta} \right) \\
&\leqslant 1 + \int_0^n \exp\left(-2\gamma_0 \widetilde{\lambda}_j \frac{(t+1)^{1-\zeta} - 1}{1 - \zeta} \right) \mathrm{d}x \\
&\leqslant 1 + \left(\frac{n^\zeta}{2\gamma_0 \widetilde{\lambda}_j} \wedge n \right) , \quad \text{[using Eq. (21)]}
\end{aligned} \tag{27}
$$

here according to Lemma 1, for $\widetilde{\lambda}_1$, the upper bound $\frac{n^\zeta}{2\gamma_0 \widetilde{\lambda}_1}$ is tighter than n due to $\widetilde{\lambda}_1 \sim \mathcal{O}(1)$; while this conclusion might not hold for $\widetilde{\lambda}_2$ due to $\widetilde{\lambda}_2 \sim \mathcal{O}(1/m)$. Then, taking Eq. (27) back to Eq. (26), we have

$$
\begin{aligned}
\langle \bar{\eta}_n^{\mathtt{bXW}}, \widetilde{\Sigma}_m \bar{\eta}_n^{\mathtt{bXW}} \rangle &\lesssim \frac{n^{\zeta-1}}{\gamma_0} \|f^*\|^2 + \frac{\widetilde{\lambda}_2}{n} \left(\frac{n^\zeta}{\gamma_0 \widetilde{\lambda}_2} \wedge n \right) \|f^*\|^2 \\
&\lesssim \frac{n^{\zeta-1}}{\gamma_0} \|f^*\|^2 \sim \mathcal{O}(n^{\zeta-1}) ,
\end{aligned} \tag{28}
$$

which concludes the proof. □

F.2 Bound for B2

Here we aim to bound $\mathtt{B2} := \mathbb{E}_{\boldsymbol{W}} \left[\langle \bar{\eta}_n^{\mathtt{bX}} - \bar{\eta}_n^{\mathtt{bXW}}, \Sigma_m (\bar{\eta}_n^{\mathtt{bX}} - \bar{\eta}_n^{\mathtt{bXW}}) \rangle \right] = \mathbb{E}_{\boldsymbol{W}} \left[\langle \bar{\alpha}_n^{\mathtt{W}}, \widetilde{\Sigma}_m \bar{\alpha}_n^{\mathtt{W}} \rangle \right] + \mathbb{E}_{\boldsymbol{W}} \left[\langle \bar{\alpha}_n^{\mathtt{W}}, (\Sigma_m - \widetilde{\Sigma}_m) \bar{\alpha}_n^{\mathtt{W}} \rangle \right]$, where

$$
\alpha_t^{\mathtt{W}} := \eta_t^{\mathtt{bX}} - \eta_t^{\mathtt{bXW}} = (I - \gamma_t \Sigma_m)(\eta_{t-1}^{\mathtt{bX}} - \eta_{t-1}^{\mathtt{bXW}}) + \gamma_t (\widetilde{\Sigma}_m - \Sigma_m) \eta_{t-1}^{\mathtt{bXW}} , \tag{29}
$$

with $\alpha_0^{\mathtt{W}} = 0$. Here $\alpha_t^{\mathtt{W}}$ can be further formulated as

$$
\alpha_t^{\mathtt{W}} = \sum_{k=1}^{t} \gamma_k \prod_{j=k+1}^{t} (I - \gamma_j \Sigma_m)(\widetilde{\Sigma}_m - \Sigma_m) \prod_{s=1}^{k-1} (I - \gamma_s \widetilde{\Sigma}_m) f^* , \tag{30}
$$

where we use the recursion

$$
A_t := (I - \gamma_t \Sigma_m) A_{t-1} + B_t = \sum_{s=1}^{t} \prod_{i=s+1}^{t} (I - \gamma_i \Sigma_m) B_s .
$$

Accordingly, B2 admits

$$\texttt{B2} = \mathbb{E}_{\boldsymbol{W}}\left[\langle \bar{\alpha}_n^{\texttt{W}}, \Sigma_m \bar{\alpha}_n^{\texttt{W}}\rangle\right] = \frac{1}{n^2}\mathbb{E}_{\boldsymbol{W}}\left\langle \sum_{t=0}^{n-1}\alpha_t^{\texttt{W}}, \Sigma_m \sum_{t=0}^{n-1}\alpha_t^{\texttt{W}}\right\rangle = \frac{1}{n^2}\mathbb{E}_{\boldsymbol{W}}\left\|\Sigma_m^{\frac{1}{2}}\sum_{t=0}^{n-1}\alpha_t^{\texttt{W}}\right\|^2, \tag{31}$$

and we have the following error bound for B2.

Proposition 3. *Under Assumption 1, 2, 3, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0,1)$ satisfies*

$$\gamma_0 \leqslant \min\left\{\frac{1}{\mathrm{Tr}(\Sigma_m)}, \frac{1}{\mathrm{Tr}(\widetilde{\Sigma}_m)}\right\},$$

then B2 *can be bounded by*

$$\texttt{B2} \lesssim \frac{\|f^*\|^2}{\gamma_0} n^{\zeta-1}.$$

Remark: In our paper, we require $I - \gamma_t\Sigma_m$ $(t = 1, 2, \ldots m)$ to be a contraction map. Though $\mathrm{Tr}(\Sigma_m)$ is a random variable, it is with a sub-exponential $\mathcal{O}(1)$ norm, that means, the condition $\gamma_0 < 1/\mathrm{Tr}(\Sigma_m)$ can be equivalently substituted by $\gamma_0 < 1/[c\mathrm{Tr}(\widetilde{\Sigma}_m)]$ for some large c (independent of n, m, d) with exponentially high probability. This is also used for estimating other quantities.

Before we present the error bounds for B2, we need the following lemma.

Lemma 6. *Under Assumption 1, 2, 3, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0,1)$ satisfies*

$$\gamma_0 \leqslant \min\left\{\frac{1}{\mathrm{Tr}(\Sigma_m)}, \frac{1}{\mathrm{Tr}(\widetilde{\Sigma}_m)}\right\},$$

denote $\Upsilon_i := \sum_{t=0}^{n-1}\sum_{k=1}^{t}\gamma_k(\widetilde{\lambda}_i - \lambda_i)\lambda_i^{\frac{1}{2}}\prod_{j=k+1}^{t}(1-\gamma_j\lambda_i)\prod_{s=1}^{k-1}(1-\gamma_s\widetilde{\lambda}_i)$, $\forall i \in [m]$, we have

$$\Upsilon_i \lesssim \lambda_i^{\frac{1}{2}}\left(\frac{n^\zeta}{\gamma_0\lambda_i} \wedge n\right), \quad \text{if } \lambda_i \neq 0; \quad \text{and } \Upsilon_i = 0, \quad \text{if } \lambda_i = 0.$$

Proof. Following the derivation in Appendix E, we consider the index i with $\lambda_i \neq 0$ such that

$$\begin{aligned}
\Upsilon_i &:= \sum_{t=0}^{n-1}\sum_{k=1}^{t}\gamma_k(\widetilde{\lambda}_i - \lambda_i)\lambda_i^{\frac{1}{2}}\prod_{j=k+1}^{t}(1-\gamma_j\lambda_i)\prod_{s=1}^{k-1}(1-\gamma_s\widetilde{\lambda}_i) \\
&\leqslant \sum_{t=0}^{n-1}(\widetilde{\lambda}_i - \lambda_i)\lambda_i^{\frac{1}{2}}\sum_{k=1}^{t}\gamma_k\exp\big(-\sum_{j=k+1}^{t}\gamma_j\lambda_i\big)\exp\big(-\sum_{s=1}^{k-1}\gamma_s\widetilde{\lambda}_i\big) \\
&\leqslant \sum_{t=0}^{n-1}(\widetilde{\lambda}_i - \lambda_i)\lambda_i^{\frac{1}{2}}\sum_{k=1}^{t}\gamma_k\exp\left(-\lambda_i\int_{k+1}^{t+1}\frac{\gamma_0}{x^\zeta}\mathrm{d}x\right)\exp\left(-\widetilde{\lambda}_i\int_1^k\frac{\gamma_0}{x^\zeta}\mathrm{d}x\right) \\
&= \sum_{t=0}^{n-1}(\widetilde{\lambda}_i - \lambda_i)\lambda_i^{\frac{1}{2}}\sum_{k=1}^{t}\gamma_0 k^{-\zeta}\exp\left(-\lambda_i\gamma_0\frac{(t+1)^{1-\zeta}-(k+1)^{1-\zeta}}{1-\zeta}\right)\exp\left(-\widetilde{\lambda}_i\gamma_0\frac{k^{1-\zeta}-1}{1-\zeta}\right) \\
&\lesssim \sum_{t=0}^{n-1}\gamma_0(\widetilde{\lambda}_i - \lambda_i)\lambda_i^{\frac{1}{2}}\Bigg[\int_1^t u^{-\zeta}\exp\left(-\gamma_0\frac{\lambda_i(t+1)^{1-\zeta}-\lambda_i u^{1-\zeta}+\widetilde{\lambda}_i u^{1-\zeta}-\widetilde{\lambda}_i}{1-\zeta}\right)\mathrm{d}u \\
&\qquad + t^{-\zeta}\exp\left(-\widetilde{\lambda}_i\gamma_0\frac{t^{1-\zeta}-1}{1-\zeta}\right)\Bigg],
\end{aligned} \tag{32}$$

Denote $\kappa := 1 - \zeta$ and

$$v^\kappa := \gamma_0\frac{\lambda_i(t+1)^{1-\zeta}-\lambda_i u^{1-\zeta}+\widetilde{\lambda}_i u^{1-\zeta}-\widetilde{\lambda}_i}{1-\zeta},$$

by changing the integral variable u to v, we have

$$\frac{\mathrm{d}u}{\mathrm{d}v} = \frac{u^{1-\kappa}}{\widetilde{\lambda}_i - \lambda_i}\left(\frac{\gamma_0}{\kappa}\right)^{-1/\kappa}[(\widetilde{\lambda}_i - \lambda_i)u^\kappa + \lambda_i(t+1)^\kappa - \widetilde{\lambda}_i] = \frac{u^{1-\kappa}}{\widetilde{\lambda}_i - \lambda_i}\frac{\kappa}{\gamma_0}v^{\kappa-1}\,,$$

Accordingly, Eq. (32) can be upper bounded by

$$\begin{aligned}
\Upsilon_i &\lesssim \sum_{t=0}^{n-1}\gamma_0(\widetilde{\lambda}_i - \lambda_i)\lambda_i^{\frac{1}{2}}\Bigg[\int_1^t u^{-\zeta}\exp\bigg(-\gamma_0\frac{\lambda_i(t+1)^{1-\zeta} - \lambda_i u^{1-\zeta} + \widetilde{\lambda}_i u^{1-\zeta} - \widetilde{\lambda}_i}{1-\zeta}\bigg)\mathrm{d}u \\
&\qquad + t^{-\zeta}\exp\bigg(-\widetilde{\lambda}_i\gamma_0\frac{t^{1-\zeta}-1}{1-\zeta}\bigg)\Bigg] \\
&\leqslant \sum_{t=0}^{n-1}\gamma_0(\widetilde{\lambda}_i - \lambda_i)\lambda_i^{\frac{1}{2}}\left[\int_{c_1^{\frac{1}{\kappa}}}^{c_2^{\frac{1}{\kappa}}} u^{-\zeta}\exp(-v^\kappa)\frac{1}{\widetilde{\lambda}_i - \lambda_i}u^{1-\kappa}\frac{\kappa}{\gamma_0}v^{\kappa-1}\mathrm{d}v + t^{-\zeta}\exp\bigg(-\widetilde{\lambda}_i\gamma_0\frac{t^{1-\zeta}-1}{1-\zeta}\bigg)\right] \\
&= \sum_{t=0}^{n-1}\left[\lambda_i^{\frac{1}{2}}\int_{c_1}^{c_2}\exp(-x)\mathrm{d}x + \gamma_0(\widetilde{\lambda}_i - \lambda_i)\lambda_i^{\frac{1}{2}}t^{-\zeta}\exp\bigg(-\widetilde{\lambda}_i\gamma_0\frac{t^{1-\zeta}-1}{1-\zeta}\bigg)\right] \\
&\lesssim \lambda_i^{\frac{1}{2}}\int_0^n \exp\bigg(-\lambda_i\gamma_0\frac{(u+1)^{1-\zeta}-1}{1-\zeta}\bigg)\mathrm{d}u \\
&\leqslant \lambda_i^{\frac{1}{2}}\left(\frac{n^\zeta}{\gamma_0\lambda_i}\wedge n\right), \quad \text{[using Eq. (22)]}
\end{aligned}$$

where $c_1 := \frac{\gamma_0}{\kappa}\lambda_i[(t+1)^\kappa - 1]$ and $c_2 := \frac{\gamma_0}{\kappa}\widetilde{\lambda}_i[t^\kappa - 1]$. Finally, we conclude the proof. □

In the next, we are ready to present the error bounds for B2.

Proof of Proposition 3. According to Eq. (31), we need estimation for $\left\|\Sigma_m^{\frac{1}{2}}\sum_{t=0}^{n-1}\alpha_t^{\mathtt{W}}\right\|_2$ for estimating B2. By spectrum decomposition, we have $\prod_{j=k+1}^t(I-\gamma_j\Sigma_m) = U\left(\prod_{j=k+1}^t(I-\gamma_j\Lambda)\right)U^\top$ and $\prod_{s=1}^{k-1}(I-\gamma_s\widetilde{\Sigma}_m) = \widetilde{U}\prod_{s=1}^{k-1}(I-\gamma_s\widetilde{\Lambda})\widetilde{U}^\top$. Then we have

$$\begin{aligned}
\left\|\Sigma_m^{1/2}\sum_{t=0}^{n-1}\alpha_t^{\mathtt{W}}\right\|_2 &= \left\|\sum_{t=0}^{n-1}\sum_{k=1}^{t}\gamma_k\prod_{j=k+1}^{t}(I-\gamma_j\Sigma_m)(\widetilde{\Sigma}_m - \Sigma_m)\prod_{s=1}^{k-1}(I-\gamma_s\widetilde{\Sigma}_m)\Sigma_m^{\frac{1}{2}}f^*\right\|_2 \\
&= \left\|\sum_{t=0}^{n-1}\sum_{k=1}^{t}\gamma_k\prod_{j=k+1}^{t}(I-\gamma_j\Lambda_m)(\widetilde{\Lambda}_m - \Lambda_m)\prod_{s=1}^{k-1}(I-\gamma_s\widetilde{\Lambda}_m)\Lambda_m^{\frac{1}{2}}f^*\right\|_2 \\
&\leqslant \max_{i\in\{1,2,\ldots,m\}}\sum_{t=0}^{n-1}\sum_{k=1}^{t}\gamma_k(\widetilde{\lambda}_i - \lambda_i)\lambda_i^{\frac{1}{2}}\prod_{j=k+1}^{t}(1-\gamma_j\lambda_i)\prod_{s=1}^{k-1}(1-\gamma_s\widetilde{\lambda}_i)\|f^*\|\,,
\end{aligned} \tag{33}$$

where the second equality holds by $\|\boldsymbol{AB}\|_2 = \|\boldsymbol{BA}\|_2$ for any two PSD matrices.

By Lemma 6, we have

$$\begin{aligned}
\mathtt{B2} &= \frac{1}{n^2}\mathbb{E}_{\boldsymbol{W}}\left\|\Sigma_m^{\frac{1}{2}}\sum_{t=0}^{n-1}\alpha_t^{\mathtt{W}}\right\|^2 = \frac{1}{n^2}\mathbb{E}_{\boldsymbol{W}}\left\|\max_{i\in\{1,2,\ldots,m\}}\Upsilon_i\right\|^2 \lesssim \frac{1}{n^2}\mathbb{E}_{\boldsymbol{W}}\left[\lambda_i^{\frac{1}{2}}\left(\frac{n^\zeta}{\gamma_0\lambda_i}\wedge n\right)\right]^2\|f^*\|^2 \\
&:= \|f^*\|^2\mathbb{E}_{\boldsymbol{W}}\left[\frac{n^{2(1-\zeta)}}{\gamma_0^2\lambda_{i^*}}\wedge\lambda_{i^*}\right] = \|f^*\|^2\begin{cases}\mathbb{E}_{\boldsymbol{W}}\left[\dfrac{n^{2(1-\zeta)}}{\gamma_0^2\lambda_{i^*}}\right], & \text{if } \lambda_{i^*}\geqslant\frac{n^{\zeta-1}}{\gamma_0} \\ \mathbb{E}_{\boldsymbol{W}}[\lambda_{i^*}], & \text{if } \lambda_{i^*}\leqslant\frac{n^{\zeta-1}}{\gamma_0}\,.\end{cases} \\
&\lesssim \frac{\|f^*\|^2}{\gamma_0}n^{\zeta-1}\,.
\end{aligned} \tag{34}$$

□

F.3 Bound for B1

Here we aim to bound $\texttt{B1} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\left[\langle \bar{\eta}_n^{\texttt{bias}} - \bar{\eta}_n^{\texttt{bX}}, \Sigma_m(\bar{\eta}_n^{\texttt{bias}} - \bar{\eta}_n^{\texttt{bX}})\rangle\right]$. Define $\alpha_t^{\texttt{X}} := \eta_t^{\texttt{bias}} - \eta_t^{\texttt{bX}}$, we have

$$\alpha_t^{\texttt{X}} = [I - \gamma_t \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\alpha_{t-1}^{\texttt{X}} + \gamma_t[\Sigma_m - \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\eta_{t-1}^{\texttt{bX}}\,, \tag{35}$$

with $\alpha_0^{\texttt{X}} = 0$ and $\eta_{t-1}^{\texttt{bX}} = \prod_{j=1}^{t-1}(I - \gamma_j \Sigma_m) f^*$. Accordingly, we have

$$\texttt{B1} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\left[\langle \bar{\eta}_n^{\texttt{bias}} - \bar{\eta}_n^{\texttt{bX}}, \Sigma_m(\bar{\eta}_n^{\texttt{bias}} - \bar{\eta}_n^{\texttt{bX}})\rangle\right] = \mathbb{E}_{\boldsymbol{W}}\left(\mathbb{E}_{\boldsymbol{X}}[\langle \bar{\alpha}_n^{\texttt{X}}, \Sigma_m \bar{\alpha}_n^{\texttt{X}}\rangle]\right)\,.$$

Proposition 4. *Under Assumption 1, 2, 3, 4 with $r' \geqslant 1$, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0, 1)$ satisfies*

$$\gamma_0 < \min\left\{\frac{1}{r'\mathrm{Tr}(\Sigma_m)}, \frac{1}{c'\mathrm{Tr}(\Sigma_m)}\right\}\,,$$

where the constant c' is defined in Eq. (14)*. Then* B1 *can be bounded by*

$$\texttt{B1} \lesssim \frac{\gamma_0 r' n^{\zeta-1}}{\sqrt{\mathbb{E}[1 - \gamma_0 r' \mathrm{Tr}(\Sigma_m)]^4}}\|f^*\|^2 \sim \mathcal{O}\left(n^{\zeta-1}\right)\,.$$

To prove Proposition 4, we need a lemma on stochastic recursions based on $\mathbb{E}[\alpha_t^{\texttt{X}}|\alpha_{t-1}^{\texttt{X}}] = (I - \gamma_t \Sigma_m)\alpha_{t-1}^{\texttt{X}}$, that shares the similar proof fashion with [29, Lemma 1] and [31, Lemma 11].

Lemma 7. *Under Assumption 1, 2, 3, 4 with $r' \geqslant 1$, denoting $H_{t-1} := [\Sigma_m - \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\eta_{t-1}^{\texttt{bX}}$, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0, 1)$ satisfies*

$$\gamma_0 < \frac{1}{r'\mathrm{Tr}(\Sigma_m)}\,,$$

we have

$$\mathbb{E}_{\boldsymbol{X}}[\langle \bar{\alpha}_n^{\texttt{X}}, \Sigma_m \bar{\alpha}_n^{\texttt{X}}\rangle] \leqslant \frac{1}{2n[1 - \gamma_0 r' \mathrm{Tr}(\Sigma_m)]}\left(\sum_{k=1}^{n-1}\mathbb{E}\|\alpha_k^{\texttt{X}}\|^2(\frac{1}{\gamma_{k+1}} - \frac{1}{\gamma_k}) + 2\sum_{t=0}^{n-1}\gamma_{t+1}\mathbb{E}_{\boldsymbol{X}}\|H_t\|^2\right)\,.$$

Remark: We require $\|\Sigma_m\|_2 \neq \frac{1}{r'\gamma_0}$ to avoid the denominator to be zero, which naturally holds as the probability measure of the continuous random variable $\|\Sigma_m\|_2$ at a point is zero.

Proof. According to the definition of $\alpha_t^{\texttt{X}}$ in Eq. (35), define $H_{t-1} := [\Sigma_m - \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\eta_{t-1}^{\texttt{bX}}$, we have

$$\begin{aligned}
\|\alpha_t^{\texttt{X}}\|^2 &= \|\alpha_{t-1}^{\texttt{X}} - \gamma_t([\varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\alpha_{t-1}^{\texttt{W}} - H_{t-1})\|^2 \\
&= \|\alpha_{t-1}^{\texttt{X}}\|^2 + \gamma_t^2\|H_{t-1} - [\varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\alpha_{t-1}^{\texttt{X}}\|^2 + 2\gamma_t\langle \alpha_{t-1}^{\texttt{W}}, H_{t-1} - [\varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\alpha_{t-1}^{\texttt{X}}\rangle \\
&\leqslant \|\alpha_{t-1}^{\texttt{X}}\|^2 + 2\gamma_t^2\left(\|H_{t-1}\|^2 + \|[\varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\alpha_{t-1}^{\texttt{X}}\|^2\right) + 2\gamma_t\langle \alpha_{t-1}^{\texttt{X}}, H_{t-1} - [\varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\alpha_{t-1}^{\texttt{X}}\rangle\,,
\end{aligned}$$

which implies (by taking the conditional expectation)

$$\begin{aligned}
\mathbb{E}_{\boldsymbol{X}}[\|\alpha_t^{\texttt{W}}\|^2|\alpha_{t-1}^{\texttt{W}}] &\leqslant \|\alpha_{t-1}^{\texttt{X}}\|^2 + 2\gamma_t^2\|H_{t-1}\|^2 + 2\gamma_t^2\langle \alpha_{t-1}^{\texttt{X}}, \mathbb{E}_{\boldsymbol{X}}[\varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\alpha_{t-1}^{\texttt{X}}\rangle \\
&\quad - 2\gamma_t\langle \alpha_{t-1}^{\texttt{X}}, \Sigma_m \alpha_{t-1}^{\texttt{X}}\rangle \\
&\leqslant \|\alpha_{t-1}^{\texttt{X}}\|^2 + 2\gamma_t^2\|H_{t-1}\|^2 + 2\gamma_t^2 r'\mathrm{Tr}(\Sigma_m)\langle \alpha_{t-1}^{\texttt{X}}, \Sigma_m \alpha_{t-1}^{\texttt{X}}\rangle - 2\gamma_t\langle \alpha_{t-1}^{\texttt{X}}, \Sigma_m \alpha_{t-1}^{\texttt{X}}\rangle \\
&= \|\alpha_{t-1}^{\texttt{X}}\|^2 + 2\gamma_t^2\|H_{t-1}\|^2 - 2\gamma_t[1 - \gamma_t r'\mathrm{Tr}(\Sigma_m)]\langle \alpha_{t-1}^{\texttt{X}}, \Sigma_m \alpha_{t-1}^{\texttt{X}}\rangle\,.
\end{aligned} \tag{36}$$

where the first inequality holds by $\mathbb{E}_{\boldsymbol{X}}[H_{t-1}] = 0$, and the second inequality satisfies by Assumption 4.

By taking the expectation of Eq. (36), we have

$$\mathbb{E}_{\boldsymbol{X}}[\|\alpha_t^{\texttt{X}}\|^2] \leqslant \mathbb{E}_{\boldsymbol{X}}[\|\alpha_{t-1}^{\texttt{X}}\|^2] + 2\gamma_t^2\mathbb{E}_{\boldsymbol{X}}[\|H_{t-1}\|^2] - 2\gamma_t[1 - \gamma_t r'\mathrm{Tr}(\Sigma_m)]\mathbb{E}_{\boldsymbol{X}}\langle \alpha_{t-1}^{\texttt{X}}, \Sigma_m \alpha_{t-1}^{\texttt{X}}\rangle\,,$$

which indicates that

$$\begin{aligned}\mathbb{E}_{\boldsymbol{X}}\left[\langle \bar{\alpha}_n^{\mathtt{X}}, \Sigma_m \bar{\alpha}_n^{\mathtt{X}}\rangle\right]\rangle &\leqslant \frac{1}{n}\sum_{t=0}^{n-1}\mathbb{E}_{\boldsymbol{X}}\langle \alpha_t^{\mathtt{W}}, \Sigma_m \alpha_t^{\mathtt{W}}\rangle \leqslant \frac{1}{2n[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]}\left(\sum_{k=1}^{n-1}\mathbb{E}_{\boldsymbol{X}}\|\alpha_k^{\mathtt{X}}\|^2(\frac{1}{\gamma_{k+1}}-\frac{1}{\gamma_k})\right.\\ &\left.+\frac{1}{2\gamma_1}\mathbb{E}_{\boldsymbol{X}}\|\alpha_0^{\mathtt{X}}\|^2-\frac{1}{2\gamma_t}\mathbb{E}_{\boldsymbol{X}}\|\alpha_t^{\mathtt{X}}\|^2+\sum_{t=0}^{n-1}\gamma_{t+1}\mathbb{E}_{\boldsymbol{X}}\|H_t\|^2\right)\\ &\leqslant \frac{1}{2n[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]}\left(\sum_{k=1}^{n-1}\mathbb{E}_{\boldsymbol{X}}\|\alpha_k^{\mathtt{X}}\|^2(\frac{1}{\gamma_{k+1}}-\frac{1}{\gamma_k})+2\sum_{t=0}^{n-1}\gamma_{t+1}\mathbb{E}_{\boldsymbol{X}}\|H_t\|^2\right),\end{aligned}$$

due to $\alpha_0^{\mathtt{W}}=0$. □

In the next, we present the error bounds for two respective terms in Lemma 7.

Lemma 8. *Based on the definition of $\alpha_t^{\mathtt{X}}$ in Eq.* (37)*, under Assumption 1, 2, 3, 4 with $r'\geqslant 1$, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta\in[0,1)$ satisfies*

$$\gamma_0 < \min\left\{\frac{1}{r'\mathrm{Tr}(\Sigma_m)}, \frac{1}{c'\mathrm{Tr}(\Sigma_m)}\right\},$$

where the constant c' is defined in Eq. (14)*. Then, we have*

$$\sum_{k=1}^{n-1}\mathbb{E}\|\alpha_k^{\mathtt{X}}\|^2(\frac{1}{\gamma_{k+1}}-\frac{1}{\gamma_k}) \lesssim \frac{\gamma_0 r'\mathrm{Tr}(\Sigma_m)}{1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)}(n^{\zeta}-1)\|f^*\|^2.$$

Proof. Based on the definition of $\alpha_t^{\mathtt{X}}$ in Eq. (35), it can be reformulated as

$$\begin{aligned}\alpha_t^{\mathtt{X}} &= [I-\gamma_t\varphi(\boldsymbol{x}_t)\otimes\varphi(\boldsymbol{x}_t)]\alpha_{t-1}^{\mathtt{X}}+\gamma_t[\Sigma_m-\varphi(\boldsymbol{x}_t)\otimes\varphi(\boldsymbol{x}_t)]\prod_{j=1}^{k-1}(I-\gamma_j\Sigma_m)f^*\\ &= \sum_{s=1}^{t}\gamma_s\prod_{i=s+1}^{t}[I-\gamma_i\varphi(\boldsymbol{x}_i)\otimes\varphi(\boldsymbol{x}_i)][\Sigma_m-\varphi(\boldsymbol{x}_s)\otimes\varphi(\boldsymbol{x}_s)]\prod_{j=1}^{s-1}(I-\gamma_j\Sigma_m)f^*.\end{aligned} \tag{37}$$

and accordingly

$$\begin{aligned}C_t^{\mathtt{b}-\mathtt{X}} &:= \mathbb{E}_{\boldsymbol{X}}[\alpha_t^{\mathtt{X}}\otimes\alpha_t^{\mathtt{X}}] = (I-\gamma_t T^{\mathtt{W}})\circ C_{t-1}^{\mathtt{b}-\mathtt{X}}+\gamma_t^2(S^{\mathtt{W}}-\widetilde{S}^{\mathtt{W}})\circ[\eta_{t-1}^{\mathtt{bX}}\otimes\eta_{t-1}^{\mathtt{bX}}]\\ &\preccurlyeq (I-\gamma_t T^{\mathtt{W}})\circ C_{t-1}^{\mathtt{b}-\mathtt{X}}+\gamma_t^2 S^{\mathtt{W}}\circ[\eta_{t-1}^{\mathtt{bX}}\otimes\eta_{t-1}^{\mathtt{bX}}]\\ &\preccurlyeq (I-\gamma_t T^{\mathtt{W}})\circ C_{t-1}^{\mathtt{b}-\mathtt{X}}+\gamma_t^2 r'\mathrm{Tr}\left[\prod_{s=1}^{t-1}(I-\gamma_s\Sigma_m)^2\Sigma_m\right]\Sigma_m(f^*\otimes f^*) \quad \text{[using Assumption 4]}\\ &\preccurlyeq (I-\gamma_t T^{\mathtt{W}})\circ C_{t-1}^{\mathtt{b}-\mathtt{X}}+\gamma_t^2 r'\mathrm{Tr}(\Sigma_m)\Sigma_m(f^*\otimes f^*) \quad \text{[using } \exp(-2\lambda_i\gamma_0\tfrac{t^{1-\zeta}-1}{1-\zeta})\leqslant 1\text{]}\\ &= r'\mathrm{Tr}(\Sigma_m)\sum_{s=1}^{t}\prod_{i=s+1}^{t}\left(I-\gamma_i T^{\mathtt{W}}\right)\circ\gamma_s^2\Sigma_m(f^*\otimes f^*)\\ &\preccurlyeq \frac{\gamma_0 r'\mathrm{Tr}(\Sigma_m)}{1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)}(f^*\otimes f^*). \quad \text{[using Lemma 5]}\end{aligned} \tag{38}$$

Accordingly, we have

$$\begin{aligned}\sum_{t=1}^{n-1}\mathbb{E}_{\boldsymbol{X}}\|\alpha_t^{\mathtt{X}}\|^2(\frac{1}{\gamma_{t+1}}-\frac{1}{\gamma_t}) &= \sum_{t=1}^{n-1}\|C_t^{\mathtt{b}-\mathtt{X}}\|_2\left(\frac{1}{\gamma_{t+1}}-\frac{1}{\gamma_t}\right) \quad \text{[using Eq. (38)]}\\ &\leqslant \sum_{t=1}^{n-1}\frac{\gamma_0 r'\mathrm{Tr}(\Sigma_m)}{1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)}[(t+1)^{\zeta}-t^{\zeta}]\|f^*\|^2\\ &\lesssim \frac{\gamma_0 r'\mathrm{Tr}(\Sigma_m)}{1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)}(n^{\zeta}-1)\|f^*\|^2,\end{aligned}$$

which concludes the proof. □

Lemma 9. *Denote $H_{t-1} := [\Sigma_m - \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\eta_{t-1}^{\mathtt{bX}}$, Assumption 1, 2, 3, 4 with $r' \geqslant 1$, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0,1)$ satisfies*

$$\gamma_0 \leqslant \frac{1}{\mathrm{Tr}(\Sigma_m)}\,,$$

we have

$$\sum_{t=0}^{n-1} \gamma_{t+1} \mathbb{E}_{\boldsymbol{X}} \|H_t\|^2 \leqslant \frac{1}{2}\|f^*\|^2 r' \mathrm{Tr}(\Sigma_m)\,.$$

Proof.

$$\begin{aligned}
\sum_{t=0}^{n-1} \gamma_{t+1} \mathbb{E}_{\boldsymbol{X}} \|H_t\|^2 &= \sum_{t=0}^{n-1} \gamma_{t+1} \left\langle f^*, \prod_{j=1}^{t-1}(I - \gamma_j \Sigma_m) \mathbb{E}_{\boldsymbol{X}}[\Sigma_m - \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]^2 \prod_{j=1}^{t-1}(I - \gamma_j \Sigma_m) f^* \right\rangle \\
&\leqslant \sum_{t=0}^{n-1} \gamma_{t+1} \left\langle f^*, r' \mathrm{Tr}(\Sigma_m) \Big[\prod_{j=1}^{t-1}(I - \gamma_j \Sigma_m)\Big]^2 \Sigma_m f^* \right\rangle \quad \text{[using Assumption 4]} \\
&\leqslant \|f^*\|^2 r' \mathrm{Tr}(\Sigma_m) \left\| \sum_{t=0}^{n-1} \gamma_{t+1} \Big[\prod_{j=1}^{t-1}(I - \gamma_j \Sigma_m)\Big]^2 \Sigma_m \right\|_2 \\
&= \|f^*\|^2 r' \mathrm{Tr}(\Sigma_m) \max_{i \in \{1,2,\ldots,m\}} \sum_{t=0}^{n-1} \gamma_{t+1} \prod_{j=1}^{t-1}(1 - \gamma_j \lambda_i)^2 \lambda_i \\
&\leqslant \|f^*\|^2 r' \mathrm{Tr}(\Sigma_m) \max_{i \in \{1,2,\ldots,m\}} \gamma_0 \lambda_i \int_0^n u^{-\zeta} \exp\left(-2\gamma_0 \lambda_i \frac{u^{1-\zeta} - 1}{1-\zeta}\right) \mathrm{d}u \\
&\leqslant \frac{1}{2}\|f^*\|^2 r' \mathrm{Tr}(\Sigma_m)\,, \quad \text{[using Eq. (20)]}
\end{aligned}$$

which concludes the proof. □

Based on the above results, we are ready to prove Proposition 4.

Proof. According to Lemma 8, we have

$$\begin{aligned}
\mathbb{E}_{\boldsymbol{W}} \frac{\sum_{k=1}^{n-1} \mathbb{E}\|\alpha_k^{\mathtt{X}}\|^2 (\frac{1}{\gamma_{k+1}} - \frac{1}{\gamma_k})}{2n[1 - \gamma_0 r' \mathrm{Tr}(\Sigma_m)]} &\lesssim \mathbb{E}_{\boldsymbol{W}} \frac{\gamma_0 r' \mathrm{Tr}(\Sigma_m)}{2n[1 - \gamma_0 r' \mathrm{Tr}(\Sigma_m)]^2}(n^\zeta - 1)\|f^*\|^2 \\
&\leqslant \gamma_0 r' n^{\zeta - 1} \sqrt{\mathbb{E}[\mathrm{Tr}(\Sigma_m)]^2} \frac{1}{\sqrt{\mathbb{E}[1 - \gamma_0 r' \mathrm{Tr}(\Sigma_m)]^4}} \|f^*\|^2 \\
&\lesssim \frac{\gamma_0 r' n^{\zeta - 1}}{\sqrt{\mathbb{E}[1 - \gamma_0 r' \mathrm{Tr}(\Sigma_m)]^4}} \|f^*\|^2 \\
&\sim \mathcal{O}(n^{\zeta - 1})\,,
\end{aligned}$$

where the second inequality holds by Cauchy-Schwarz inequality and the last inequality holds by Lemma 2 with

$$\frac{1}{\mathbb{E}[1 - \gamma_0 r' \mathrm{tr}(\Sigma_m)]^4} \leqslant \frac{1}{[1 - \gamma_0 r' \mathbb{E}\mathrm{tr}(\Sigma_m)]^4} = \frac{1}{[1 - \gamma_0 r' \mathrm{tr}(\widetilde{\Sigma}_m)]^4} \sim \mathcal{O}(1)\,. \tag{39}$$

According to Lemma 9, we have

$$\begin{aligned}
\mathbb{E}_{\boldsymbol{W}} \frac{2\sum_{t=0}^{n-1}\gamma_{t+1}\mathbb{E}_{\boldsymbol{X}}\|H_t\|^2}{2n[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]} &\leqslant \mathbb{E}_{\boldsymbol{W}} \frac{r'\mathrm{Tr}(\Sigma_m)}{2n[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]}\|f^*\|^2 \\
&\lesssim \frac{r'}{n}\sqrt{\mathbb{E}[\mathrm{Tr}(\Sigma_m)]^2}\frac{1}{\sqrt{\mathbb{E}[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]^2}}\|f^*\|^2 \\
&\lesssim \frac{r'}{n\sqrt{\mathbb{E}[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]^2}}\|f^*\|^2 \quad \text{[using Lemma 2]} \\
&\sim \mathcal{O}\left(\frac{1}{n}\right).
\end{aligned}$$

Accordingly, combining the above two equations, we have

$$\begin{aligned}
\mathtt{B1} := \mathbb{E}_{\boldsymbol{W}}\mathbb{E}_{\boldsymbol{X}}[\langle \bar{\alpha}_n^{\mathtt{X}}, \Sigma_m \bar{\alpha}_n^{\mathtt{X}}\rangle] &\leqslant \frac{1}{2n[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]}\mathbb{E}_{\boldsymbol{W}}\left(\sum_{k=1}^{n-1}\mathbb{E}\|\alpha_k^{\mathtt{X}}\|^2\left(\frac{1}{\gamma_{k+1}}-\frac{1}{\gamma_k}\right)+2\sum_{t=0}^{n-1}\gamma_{t+1}\mathbb{E}_{\boldsymbol{X}}\|H_t\|^2\right) \\
&\lesssim \frac{\gamma_0 r' n^{\zeta-1}}{\sqrt{\mathbb{E}[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]^4}}\|f^*\|^2,
\end{aligned}$$

which concludes the proof. □

F.4 Proof of Theorem 1

Proof. Combining the above results for three terms B1, B2, B3, if

$$\gamma_0 < \min\left\{\frac{1}{\mathrm{Tr}(\widetilde{\Sigma}_m)}, \frac{1}{r'\mathrm{Tr}(\Sigma_m)}, \frac{1}{c'\mathrm{Tr}(\Sigma_m)}\right\} \sim \mathcal{O}(1), \tag{40}$$

where the constant c is defined in Eq. (14). Then the Bias can be upper bounded by

$$\begin{aligned}
\mathtt{Bias} &\leqslant \left(\sqrt{\mathtt{B1}}+\sqrt{\mathtt{B2}}+\sqrt{\mathtt{B3}}\right)^2 \leqslant 3(\mathtt{B1}+\mathtt{B2}+\mathtt{B3}) \\
&\lesssim \frac{\gamma_0 r' n^{\zeta-1}}{\sqrt{\mathbb{E}[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]^4}}\|f^*\|^2 \\
&\lesssim \gamma_0 r' n^{\zeta-1}\|f^*\|^2,
\end{aligned}$$

where the last inequality holds by Eq. (39).

□

G Proof for Variance

In this section, we present the error bound for Variance. Recall the definition of $\eta_t^{\mathtt{vX}}$ in Eq. (8) and $\eta_t^{\mathtt{vXW}}$ in Eq. (9), and

$$\bar{\eta}_n^{\mathtt{vX}} := \frac{1}{n}\sum_{t=0}^{n-1}\bar{\eta}_t^{\mathtt{vX}}, \qquad \bar{\eta}_n^{\mathtt{vXW}} := \frac{1}{n}\sum_{t=0}^{n-1}\bar{\eta}_t^{\mathtt{vXW}},$$

by virtue of Minkowski inequality, Variance can be further decomposed as

$$\begin{aligned}
\left(\mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\left[\langle \bar{\eta}_n^{\mathtt{var}}, \Sigma_m \bar{\eta}_n^{\mathtt{var}}\rangle\right]\right)^{\frac{1}{2}} &\leqslant \Big(\underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\left[\langle \bar{\eta}_n^{\mathtt{var}}-\bar{\eta}_n^{\mathtt{vX}}, \Sigma_m(\bar{\eta}_n^{\mathtt{var}}-\bar{\eta}_n^{\mathtt{vX}})\rangle\right]}_{\triangleq \mathtt{V1}}\Big)^{\frac{1}{2}} + \left(\mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\left[\langle \bar{\eta}_n^{\mathtt{vX}}, \Sigma_m \bar{\eta}_n^{\mathtt{vX}}\rangle\right]\right)^{\frac{1}{2}} \\
&\leqslant (\mathtt{V1})^{\frac{1}{2}} + \Big(\underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\left[\langle \bar{\eta}_n^{\mathtt{vX}}-\bar{\eta}_n^{\mathtt{vXW}}, \Sigma_m(\bar{\eta}_n^{\mathtt{vX}}-\bar{\eta}_n^{\mathtt{vXW}})\rangle\right]}_{\triangleq \mathtt{V2}}\Big)^{\frac{1}{2}} + \Big[\underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle \bar{\eta}_n^{\mathtt{vXW}}, \Sigma_m \bar{\eta}_n^{\mathtt{vXW}}\rangle}_{\triangleq \mathtt{V3}}\Big]^{\frac{1}{2}}.
\end{aligned} \tag{41}$$

Accordingly, the Variance can be decomposed as Variance $\lesssim$ V1 + V2 + V3, and in the next we give the error bounds for them, respectively.

G.1 Bound for V3

In this section, we aim to bound $\mathtt{V3} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle \bar{\eta}_n^{\mathtt{vXW}}, \Sigma_m \bar{\eta}_n^{\mathtt{vXW}}\rangle$. Note that $\mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\eta_t^{\mathtt{vXW}} | \eta_{t-1}^{\mathtt{vXW}}] = (I - \gamma_t \widetilde{\Sigma}_m)\eta_{t-1}^{\mathtt{vXW}}$, similar to Appendix F.2 for B2, we have the following expression for V3

$$
\begin{aligned}
\mathtt{V3} &:= \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle \bar{\eta}_n^{\mathtt{vXW}}, \Sigma_m \bar{\eta}_n^{\mathtt{vXW}}\rangle = \mathbb{E}_{\boldsymbol{W}}[\mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}\langle \Sigma_m, \bar{\eta}_n^{\mathtt{vXW}} \otimes \bar{\eta}_n^{\mathtt{vXW}}\rangle] \\
&= \frac{1}{n^2}\mathbb{E}_{\boldsymbol{W}}\left(\left\langle \Sigma_m, \sum_{0\leqslant k\leqslant t\leqslant n-1} \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\eta_t^{\mathtt{vXW}} \otimes \eta_k^{\mathtt{vXW}}] + \sum_{0\leqslant k< t\leqslant n-1} \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\eta_t^{\mathtt{vXW}} \otimes \eta_k^{\mathtt{vXW}}]\right\rangle\right) \\
&\leqslant \frac{1}{n^2}\mathbb{E}_{\boldsymbol{W}}\left(\left\langle \Sigma_m, \sum_{0\leqslant k\leqslant t\leqslant n-1} \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\eta_t^{\mathtt{vXW}} \otimes \eta_k^{\mathtt{vXW}}] + \sum_{0\leqslant k\leqslant t\leqslant n-1} \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\eta_t^{\mathtt{vXW}} \otimes \eta_k^{\mathtt{vXW}}]\right\rangle\right) \\
&= \frac{2}{n^2}\sum_{t=0}^{n-1}\sum_{k=t}^{n-1}\mathbb{E}_{\boldsymbol{W}}\left\langle \prod_{j=t}^{k-1}(I-\gamma_j\widetilde{\Sigma}_m)\Sigma_m, \underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\eta_t^{\mathtt{vXW}} \otimes \eta_t^{\mathtt{vXW}}]}_{:=C_t^{\mathtt{vXW}}}\right\rangle ,
\end{aligned}
\tag{42}
$$

and thus we have the following error bound for V3.

Proposition 5. *Under Assumption 1, 3, 5 with $\tau > 0$, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0,1)$ satisfies $\gamma_0 \leqslant \frac{1}{\mathrm{Tr}(\widetilde{\Sigma}_m)}$, then* V3 *can be bounded by*

$$
\mathtt{V3} \lesssim \begin{cases} \gamma_0\tau^2\dfrac{m}{n^{1-\zeta}}, & \text{if } m \leqslant n \\ \gamma_0\tau^2\left(n^{\zeta-1} + \dfrac{n}{m}\right), & \text{if } m > n\,. \end{cases}
$$

To prove Proposition 5, we need the following lemma.

Lemma 10. *Denote $C_t^{\mathtt{vXW}} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\eta_t^{\mathtt{vXW}} \otimes \eta_t^{\mathtt{vXW}}]$, under Assumptions 1, 3, 5 with $\tau > 0$, if $\gamma_0 \leqslant 1/\mathrm{Tr}(\widetilde{\Sigma}_m)$, we have*

$$
C_t^{\mathtt{vXW}} \preccurlyeq \tau^2 \sum_{k=1}^{t}\gamma_k^2 \prod_{j=k+1}^{t}(I-\gamma_j\widetilde{\Sigma}_m)^2\Sigma_m\,.
$$

Proof. Recall the definition of $\eta_t^{\mathtt{vXW}}$ in Eq. (9), it can be further represented as

$$
\eta_t^{\mathtt{vXW}} = (I-\gamma_t\widetilde{\Sigma}_m)\eta_{t-1}^{\mathtt{vXW}} + \gamma_t\varepsilon_k\varphi(\boldsymbol{x}_k) = \sum_{k=1}^{t}\prod_{j=k+1}^{t}(I-\gamma_j\widetilde{\Sigma}_m)\gamma_k\varepsilon_k\varphi(\boldsymbol{x}_k) \quad \text{with } \eta_0^{\mathtt{vXW}} = 0\,.
$$

Accordingly, $C_t^{\mathtt{vXW}}$ admits (with $C_0^{\mathtt{vXW}} = 0$)

$$
C_t^{\mathtt{vXW}} = \sum_{k=1}^{t}\prod_{j=k+1}^{t}(I-\gamma_j\widetilde{\Sigma}_m)^2\gamma_k^2\Xi \preccurlyeq \tau^2\sum_{k=1}^{t}\gamma_k^2\prod_{j=k+1}^{t}(I-\gamma_j\widetilde{\Sigma}_m)^2\Sigma_m \quad \text{[using Assumption 5]}
$$

where we use $\mathbb{E}[\varepsilon_i\varepsilon_j] = 0$ for $i \neq j$. □

In the next, we are ready to bound V3 in Proposition 5.

Proof of Proposition 5. Note that $\widetilde{\lambda}_1 \sim \mathcal{O}(1)$ and $\widetilde{\lambda}_2 \sim \mathcal{O}(1/m)$ in Lemma 2, we take the upper bound of the integral in Eq. (22) to $\frac{n^\zeta}{\widetilde{\lambda}_1\gamma_0}$ for $\widetilde{\lambda}_1$. However, according to the order of $\widetilde{\lambda}_2$, if $\widetilde{\lambda}_2 \lesssim 1/n$, the exact upper bound is tight. Based on this, we first consider that $m \leqslant n$ case such that $\widetilde{\lambda}_2 \gtrsim 1/n$,

and then focus on the $m \geqslant n$ case. Taking $\frac{n^\zeta}{\widetilde{\lambda}_i \gamma_0}$ in Eq. (22) and $\frac{\gamma_0}{\widetilde{\lambda}_i}$ in Eq. (24), we have

$$
\begin{aligned}
\mathtt{V3} &:= \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}} \langle \bar{\eta}_n^{\mathtt{vXW}}, \Sigma_m \bar{\eta}_n^{\mathtt{vXW}} \rangle = \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}} \langle \Sigma_m, \bar{\eta}_n^{\mathtt{vXW}} \otimes \bar{\eta}_n^{\mathtt{vXW}} \rangle \\
&\leqslant \frac{2}{n^2} \sum_{t=0}^{n-1} \sum_{k=t}^{n-1} \mathbb{E}_{\boldsymbol{W}} \left\langle \prod_{j=t}^{k-1} (I - \gamma_j \widetilde{\Sigma}_m) \Sigma_m, \underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}} [\bar{\eta}_t^{\mathtt{vXW}} \otimes \bar{\eta}_t^{\mathtt{vXW}}]}_{:= C_t^{\mathtt{vXW}}} \right\rangle \quad \text{[using Eq. (42)]} \\
&\leqslant \frac{2\tau^2}{n^2} \sum_{t=0}^{n-1} \sum_{k=t}^{n-1} \mathbb{E}_{\boldsymbol{W}} \left\langle \prod_{j=t}^{k-1} (I - \gamma_j \widetilde{\Sigma}_m) \Sigma_m, \sum_{s=1}^{t} \gamma_s^2 \prod_{j=s+1}^{t} (I - \gamma_j \widetilde{\Sigma}_m)^2 \Sigma_m \right\rangle \quad \text{[using Lemma 10]} \\
&\leqslant \frac{2\tau^2}{n^2} \sum_{t=0}^{n-1} \sum_{k=t}^{n-1} \left\| \prod_{j=t}^{k-1} (I - \gamma_j \widetilde{\Sigma}_m) \widetilde{\Sigma}_m \sum_{s=1}^{t} \gamma_s^2 \prod_{j=s+1}^{t} (I - \gamma_j \widetilde{\Sigma}_m)^2 \right\|_2 \operatorname{Tr}\left(\mathbb{E}_{\boldsymbol{W}} [\Sigma_m^2 \widetilde{\Sigma}_m^{-1}] \right) \\
&\lesssim \frac{2\tau^2}{n^2} \sum_{t=0}^{n-1} \sum_{k=t}^{n-1} \max_{i \in \{1,2,\ldots,m\}} \left\| \prod_{j=t}^{k-1} (1 - \gamma_j \widetilde{\lambda}_i) \widetilde{\lambda}_i \sum_{s=1}^{t} \gamma_s^2 \prod_{j=s+1}^{t} (1 - \gamma_j \widetilde{\lambda}_i)^2 \right\|_2 \quad \text{[using Lemma 4]} \\
&\leqslant \frac{2\tau^2}{n^2} \sum_{t=0}^{n-1} \sum_{k=t}^{n-1} \max_{i \in \{1,2,\ldots,m\}} \left\| \widetilde{\lambda}_i \exp\left(-\widetilde{\lambda}_i \gamma_0 \frac{k^{1-\zeta} - t^{1-\zeta}}{1-\zeta} \right) \sum_{s=1}^{t} \gamma_s^2 \exp\left(-2\widetilde{\lambda}_i \gamma_0 \frac{(t+1)^{1-\zeta} - (s+1)^{1-\zeta}}{1-\zeta} \right) \right\|_2 \\
&\lesssim \frac{\tau^2}{n^2} \sum_{t=0}^{n-1} \max_{i \in \{1,2,\ldots,m\}} \left[\widetilde{\lambda}_i \frac{n^\zeta}{\widetilde{\lambda}_i \gamma_0} \left(\frac{\gamma_0}{\widetilde{\lambda}_i} + \gamma_t^2 \right) \right] \quad \text{[using Eqs. (22), (24)]} \\
&\leqslant \frac{\tau^2}{n^2} \left[n^{1+\zeta} m + n^\zeta \operatorname{Tr}(\widetilde{\Sigma}_m) \gamma_0 \int_0^n t^{-2\zeta} \mathrm{d}t \right] \\
&\lesssim \gamma_0 \tau^2 \frac{m}{n^{1-\zeta}}, \quad \text{[using Lemma 2]}
\end{aligned}
\tag{43}
$$

where the last equality holds that $\int_0^n t^{-2\zeta} \mathrm{d}t \leqslant n$ for any $\zeta \in [0, 1)$.

If $\widetilde{\lambda}_2 \lesssim 1/n$, that means, $m > n$ in the over-parameterized regime, we have

$$
\begin{aligned}
\mathtt{V3} &\lesssim \frac{2\tau^2}{n^2} \sum_{t=0}^{n-1} \left[\widetilde{\lambda}_1 \frac{n^\zeta}{\widetilde{\lambda}_1 \gamma_0} \left(\frac{\gamma_0}{\widetilde{\lambda}_1} + \gamma_t^2 \right) + \widetilde{\lambda}_2 (n-t) t \right] \\
&\lesssim \frac{\gamma_0 \tau^2}{n^2} \left(n^{1+\zeta} + \widetilde{\lambda}_2 \frac{n(n-1)(n+1)}{6} \right) \quad \text{[since } \lambda_1 \sim \mathcal{O}(1)\text{]} \\
&\lesssim \gamma_0 \tau^2 \left(n^{\zeta-1} + \frac{n}{m} \right),
\end{aligned}
$$

which concludes the proof.

□

G.2 Bound for V2

Here we aim to bound V2

$$
\mathtt{V2} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}} \left[\langle \bar{\eta}_n^{\mathtt{vX}} - \bar{\eta}_n^{\mathtt{vXW}}, \Sigma_m (\bar{\eta}_n^{\mathtt{vX}} - \bar{\eta}_n^{\mathtt{vXW}}) \rangle \right].
$$

Recall the definition of $\eta_t^{\mathtt{vX}}$ and $\eta_t^{\mathtt{vXW}}$ in Eqs. (8) and (9), we have

$$
\eta_t^{\mathtt{vXW}} = (I - \gamma_t \widetilde{\Sigma}_m) \eta_{t-1}^{\mathtt{vXW}} + \gamma_t \varepsilon_k \varphi(\boldsymbol{x}_k) = \sum_{k=1}^{t} \prod_{j=k+1}^{t} (I - \gamma_j \widetilde{\Sigma}_m) \gamma_k \varepsilon_k \varphi(\boldsymbol{x}_k) \quad \text{with } \eta_0^{\mathtt{vXW}} = 0,
$$

and accordingly, we define

$$
\begin{aligned}
\alpha_t^{\mathtt{vX-W}} &:= \eta_t^{\mathtt{vX}} - \eta_t^{\mathtt{vXW}} = (I - \gamma_t \Sigma_m) \alpha_{t-1}^{\mathtt{vX-W}} + \gamma_t (\widetilde{\Sigma}_m - \Sigma_m) \eta_{t-1}^{\mathtt{vXW}}, \quad \text{with } \alpha_0^{\mathtt{vX-W}} = 0 \\
&= \sum_{s=1}^{t} \prod_{i=s+1}^{t} (I - \gamma_i \Sigma_m) \gamma_s (\widetilde{\Sigma}_m - \Sigma_m) \sum_{k=1}^{s-1} \prod_{j=k+1}^{s-1} (I - \gamma_j \widetilde{\Sigma}_m) \gamma_k \varepsilon_k \varphi(\boldsymbol{x}_k).
\end{aligned}
$$

Proposition 6. *Under Assumptions 1, 3, 5 with $\tau > 0$, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0,1)$ satisfies*

$$\gamma_0 \leqslant \frac{1}{\mathrm{Tr}(\Sigma_m)}\,, \tag{44}$$

then V2 *can be bounded by*

$$\mathtt{V2} \lesssim \begin{cases} \gamma_0 \tau^2 \dfrac{m}{n^{1-\zeta}}, & \text{if } m \leqslant n \\ \gamma_0 \tau^2, & \text{if } m > n\,. \end{cases}$$

To prove Proposition 6, we need the following lemma.

Lemma 11. *Denote $C_t^{\mathtt{vX-W}} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\alpha_t^{\mathtt{vX-W}} \otimes \alpha_t^{\mathtt{vX-W}}]$, under Assumptions 1, 3, 5 with $\tau > 0$, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0,1)$ satisfies*

$$\gamma_0 \leqslant \min\left\{\frac{1}{\mathrm{Tr}(\Sigma_m)}, \frac{1}{\mathrm{Tr}(\widetilde{\Sigma}_m)}\right\}\,,$$

we have

$$\|C_t^{\mathtt{vX-W}}\|_2 \lesssim \tau^2 \gamma_0^2 \left(\gamma_0 \|\Sigma_m\|_2 + 1\right)\left(\gamma_0 \|\widetilde{\Sigma}_m\|_2 + 1\right)\,.$$

Proof. According to the definition of $C_t^{\mathtt{vX-W}}$, it admits the following expression

$$\begin{aligned}
C_t^{\mathtt{vX-W}} &= \sum_{s=1}^{t} \prod_{i=s+1}^{t} (I - \gamma_i \Sigma_m) \gamma_s^2 (\widetilde{\Sigma}_m - \Sigma_m) \sum_{k=1}^{s-1} \prod_{j=k+1}^{s-1} (I - \gamma_j \widetilde{\Sigma}_m)^2 \gamma_k^2 \Xi (\widetilde{\Sigma}_m - \Sigma_m)(I - \gamma_i \Sigma_m) \\
&\preccurlyeq \sum_{s=1}^{t} \prod_{i=s+1}^{t} (I - \gamma_i \Sigma_m) \gamma_s^2 (\widetilde{\Sigma}_m - \Sigma_m) \sum_{k=1}^{s-1} \prod_{j=k+1}^{s-1} (I - \gamma_j \widetilde{\Sigma}_m)^2 \gamma_k^2 \Xi (\widetilde{\Sigma}_m - \Sigma_m)(I - \gamma_i \Sigma_m) \\
&\preccurlyeq \tau^2 \sum_{s=1}^{t} \prod_{i=s+1}^{t} (I - \gamma_i \Sigma_m) \gamma_s^2 (\widetilde{\Sigma}_m - \Sigma_m) \sum_{k=1}^{s-1} \prod_{j=k+1}^{s-1} (I - \gamma_j \widetilde{\Sigma}_m)^2 \gamma_k^2 \Sigma_m (\widetilde{\Sigma}_m - \Sigma_m)(I - \gamma_i \Sigma_m)\,,
\end{aligned}$$

where the first equality holds by $\mathbb{E}[\varepsilon_i \varepsilon_j] = 0$ for $i \neq j$ and the second inequality holds by Assumption 5.

Accordingly, $\|C_t^{\mathtt{vX-W}}\|_2$ can be upper bounded by

$$\begin{aligned}
\|C_t^{\mathtt{vX-W}}\|_2 &\leqslant \tau^2 \sum_{s=1}^{t} \gamma_s^2 \left\| \prod_{i=s+1}^{t} (I - \gamma_i \Sigma_m)^2 \Sigma_m (\widetilde{\Sigma}_m - \Sigma_m)^2 \sum_{k=1}^{s-1} \gamma_k^2 \prod_{j=k+1}^{s-1} (I - \gamma_j \widetilde{\Sigma}_m)^2 \right\|_2 \\
&\leqslant \tau^2 \sum_{s=1}^{t} \gamma_s^2 \left\| \prod_{i=s+1}^{t} (I - \gamma_i \Sigma_m)^2 \Sigma_m \right\|_2 \left\| \sum_{k=1}^{s-1} \gamma_k^2 \prod_{j=k+1}^{s-1} (I - \gamma_j \widetilde{\Sigma}_m)^2 \widetilde{\Sigma}_m \right\|_2 \left\| \widetilde{\Sigma}_m - 2\Sigma_m + \widetilde{\Sigma}_m^{-1} \Sigma_m^2 \right\|_2 \\
&\lesssim \tau^2 \sum_{s=1}^{t} \max_{q \in \{1,2,\ldots,m\}} \gamma_s^2 \exp\left(-2\lambda_q \sum_{i=s+1}^{t} \gamma_i\right) \lambda_q \sum_{k=1}^{s-1} \gamma_k^2 \max_{p \in \{1,2\}} \exp\left(-2\widetilde{\lambda}_p \sum_{j=k+1}^{s-1} \gamma_j\right) \widetilde{\lambda}_p \\
&\qquad \left\| \widetilde{\Sigma}_m - 2\Sigma_m + \widetilde{\Sigma}_m^{-1} \Sigma_m^2 \right\|_2\,.
\end{aligned}$$

Similar to Eq. (23), we have the following estimation

$$\begin{aligned}
\sum_{k=1}^{s-1} \gamma_k^2 \prod_{j=k+1}^{s-1} (1 - \gamma_j \widetilde{\lambda}_p)^2 &\leqslant \sum_{k=1}^{s-1} \gamma_k^2 \exp\left(-2\widetilde{\lambda}_p \sum_{j=k+1}^{s-1} \gamma_j\right) \\
&\leqslant \gamma_{s-1}^2 + \gamma_0^2 \int_1^{s-1} u^{-2\zeta} \exp\left(-2\widetilde{\lambda}_p \gamma_0 \frac{s^{1-\zeta} - (u+1)^{1-\zeta}}{1-\zeta}\right) \mathrm{d}u \\
&\leqslant \gamma_0^2 + \left(\frac{\gamma_0}{\widetilde{\lambda}_p} \wedge \gamma_0^2 s\right)\,,
\end{aligned}$$

which implies

$$\max_{p=1,2} \widetilde{\lambda}_p \sum_{k=1}^{s-1} \gamma_k^2 \prod_{j=k+1}^{s-1} (1-\gamma_j \widetilde{\lambda}_p)^2 \leqslant \gamma_0^2 \widetilde{\lambda}_1 + \gamma_0 \leqslant \gamma_0^2 \widetilde{\Sigma}_m + \gamma_0 \,. \tag{45}$$

Similar to Eq. (23), we have the following estimation

$$\begin{aligned}
\sum_{s=1}^{t} \gamma_s^2 \exp\left(-2\lambda_q \sum_{i=s+1}^{t} \gamma_i\right) &\leqslant \sum_{s=1}^{t} \gamma_s^2 \exp\left(-2\lambda_q \gamma_0 \frac{(t+1)^{1-\zeta} - (s+1)^{1-\zeta}}{1-\zeta}\right) \\
&\leqslant \gamma_t^2 + \gamma_0^2 \int_1^t u^{-2\zeta} \exp\left(-2\lambda_q \gamma_0 \frac{(t+1)^{1-\zeta} - (u+1)^{1-\zeta}}{1-\zeta}\right) \mathrm{d}u \\
&\leqslant \gamma_0^2 + \left(\frac{\gamma_0}{\lambda_q} \wedge \gamma_0^2 t\right) ,
\end{aligned}$$

which implies

$$\max_{q \in \{1,2,\ldots,m\}} \sum_{s=1}^{t} \gamma_s^2 \lambda_q \exp\left(-2\lambda_q \sum_{i=s+1}^{t} \gamma_i\right) = \gamma_0^2 \|\Sigma_m\|_2 + \gamma_0 \,. \tag{46}$$

Combining the above two equations (45) and (46), we have

$$\|C_t^{\mathtt{vX-W}}\|_2 \lesssim \tau^2 \gamma_0^2 \left(\gamma_0 \|\Sigma_m\|_2 + 1\right) \left(\gamma_0 \|\widetilde{\Sigma}_m\|_2 + 1\right) .$$

□

Proof of Proposition 6. By virtue of $\mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\alpha_t^{\mathtt{vX-W}} | \alpha_{t-1}^{\mathtt{vX-W}}] = (I - \gamma_t \Sigma_m) \alpha_{t-1}^{\mathtt{vX-W}}$ and Lemma 11, $\mathtt{V2}$ can be bounded by

$$\begin{aligned}
\mathtt{V2} &= \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\left[\langle \bar{\eta}_n^{\mathtt{vX}} - \bar{\eta}_n^{\mathtt{vXW}}, \Sigma_m (\bar{\eta}_n^{\mathtt{vX}} - \bar{\eta}_n^{\mathtt{vXW}}) \rangle\right] = \mathbb{E}_{\boldsymbol{W}} \langle \Sigma_m, \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\bar{\alpha}_n^{\mathtt{vX-W}} \otimes \bar{\alpha}_n^{\mathtt{vX-W}}] \rangle \\
&\leqslant \frac{2}{n^2} \sum_{t=0}^{n-1} \sum_{k=t}^{n-1} \mathbb{E}_{\boldsymbol{W}} \left\langle \prod_{j=t}^{k-1} (I - \gamma_j \Sigma_m) \Sigma_m, \underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\eta_t^{\mathtt{vX-W}} \otimes \eta_t^{\mathtt{vX-W}}]}_{:= C_t^{\mathtt{vX-W}}} \right\rangle \\
&\lesssim \frac{\tau^2 \gamma_0^2}{n^2} \|\widetilde{\Sigma}_m\|_2 \mathbb{E}_{\boldsymbol{W}} \left(\left\| \widetilde{\Sigma}_m - 2\Sigma_m + \widetilde{\Sigma}_m^{-1} \Sigma_m^2 \right\|_2 [\|\Sigma_m\|_2 \gamma_0 + 1] \operatorname{Tr}\left[\sum_{t=0}^{n-1} \sum_{k=t}^{n-1} \prod_{j=t}^{k-1} (I - \gamma_j \Sigma_m) \Sigma_m \right] \right) \\
&\lesssim \frac{\tau^2 \gamma_0^2}{n^2} \|\widetilde{\Sigma}_m\|_2 \mathbb{E}_{\boldsymbol{W}} \left[\|\Sigma_m\|_2 \left\| \widetilde{\Sigma}_m - 2\Sigma_m + \widetilde{\Sigma}_m^{-1} \Sigma_m^2 \right\|_2 \sum_{i=1}^{m} \sum_{t=0}^{n-1} \lambda_i \left(\frac{n^\zeta}{\lambda_i \gamma_0} \wedge (n-t) \right) \right] . \quad \text{[using Eq. (22)]}
\end{aligned}$$

In the $m \leqslant n$ case, we choose $n^\zeta / (\lambda_i \gamma_0)$, and thus

$$\begin{aligned}
\mathtt{V2} &\lesssim \frac{\tau^2 m \gamma_0^2}{n^2} \|\widetilde{\Sigma}_m\|_2 \mathbb{E}_{\boldsymbol{W}} \left[\|\Sigma_m\|_2 \left\| \widetilde{\Sigma}_m - 2\Sigma_m + \widetilde{\Sigma}_m^{-1} \Sigma_m^2 \right\|_2 \right] \frac{n^{1+\zeta}}{\gamma_0} \\
&\leqslant \tau^2 \gamma_0 \frac{m \|\widetilde{\Sigma}_m\|_2}{n^{1-\zeta}} \sqrt{\mathbb{E}_{\boldsymbol{W}} \|\Sigma_m\|_2^2} \sqrt{\mathbb{E}_{\boldsymbol{W}} \left\| \widetilde{\Sigma}_m - 2\Sigma_m + \widetilde{\Sigma}_m^{-1} \Sigma_m^2 \right\|_2^2} \quad \text{[using Cauchy–Schwarz inequality]} \\
&\lesssim \tau^2 \gamma_0 \frac{m}{n^{1-\zeta}} . \quad \text{[using Lemma 2 and 4]}
\end{aligned}$$

If $m > n$, we have

$$\begin{aligned}
\mathtt{V2} &\lesssim \frac{2\tau^2 \gamma_0^2}{n^2} \|\widetilde{\Sigma}_m\|_2 \mathbb{E}_{\boldsymbol{W}} \left([\operatorname{Tr}(\Sigma_m)]^2 \left\| \widetilde{\Sigma}_m - 2\Sigma_m + \widetilde{\Sigma}_m^{-1} \Sigma_m^2 \right\|_2 \right) \sum_{t=0}^{n-1} t \\
&\leqslant \tau^2 \gamma_0 \|\widetilde{\Sigma}_m\|_2 \sqrt{\mathbb{E}_{\boldsymbol{W}} [\operatorname{Tr}(\Sigma_m)]^2} \sqrt{\mathbb{E}_{\boldsymbol{W}} \left\| \widetilde{\Sigma}_m - 2\Sigma_m + \widetilde{\Sigma}_m^{-1} \Sigma_m^2 \right\|_2^2} \\
&\lesssim \tau^2 \gamma_0 , \quad \text{[using Lemmas 2 and 4]}
\end{aligned}$$

which concludes the proof. □

G.3 Bound for V1

Here we aim to bound V1

$$\texttt{V1} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\left[\langle \bar{\eta}_n^{\texttt{var}} - \bar{\eta}_n^{\texttt{vX}}, \Sigma_m(\bar{\eta}_n^{\texttt{var}} - \bar{\eta}_n^{\texttt{vX}})\rangle\right].$$

Recall the definition of $\eta_t^{\texttt{var}}$ in Eq. (6) and $\eta_t^{\texttt{vX}}$ in Eq. (8), we define

$$\begin{aligned}
\alpha_t^{\texttt{v-X}} &:= \eta_t^{\texttt{var}} - \eta_t^{\texttt{vX}} = [I - \gamma_t\varphi(\boldsymbol{x}_t)\otimes\varphi(\boldsymbol{x}_t)]\alpha_{t-1}^{\texttt{v-X}} + \gamma_t[\Sigma_m - \varphi(\boldsymbol{x}_t)\otimes\varphi(\boldsymbol{x}_t)]\eta_{t-1}^{\texttt{vX}}, \quad \text{with } \alpha_0^{\texttt{v-X}} = 0.\\
&= [I - \gamma_t\varphi(\boldsymbol{x}_t)\otimes\varphi(\boldsymbol{x}_t)]\alpha_{t-1}^{\texttt{v-X}} + \gamma_t[\Sigma_m - \varphi(\boldsymbol{x}_t)\otimes\varphi(\boldsymbol{x}_t)]\sum_{k=1}^{t-1}\prod_{j=k+1}^{t-1}(I-\gamma_j\Sigma_m)\gamma_k\varepsilon_k\varphi(\boldsymbol{x}_k)\\
&= \sum_{s=1}^{t}\prod_{i=s+1}^{t}\gamma_s[I-\gamma_i\varphi(\boldsymbol{x}_i)\otimes\varphi(\boldsymbol{x}_i)][\Sigma_m - \varphi(\boldsymbol{x}_t)\otimes\varphi(\boldsymbol{x}_t)]\sum_{k=1}^{s-1}\prod_{j=k+1}^{s-1}(I-\gamma_j\Sigma_m)\gamma_k\varepsilon_k\varphi(\boldsymbol{x}_k),
\end{aligned}$$

and thus the error bound for V1 is given by the following proposition.

Proposition 7. *Under Assumption 1, 2, 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*

$$\gamma_0 < \min\left\{\frac{1}{r'\mathrm{Tr}(\Sigma_m)}, \frac{1}{2\mathrm{Tr}(\Sigma_m)}\right\},$$

then V1 *can be bounded by*

$$\texttt{V1} \lesssim \frac{\tau^2 r'\gamma_0^2}{\sqrt{\mathbb{E}[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]^2}}\begin{cases}\dfrac{m}{n^{1-\zeta}}, & \text{if } m \leqslant n\\ 1, & \text{if } m > n.\end{cases}$$

To prove Proposition 7, we need the following lemma. Define $C_t^{\texttt{v-X}} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\alpha_t^{\texttt{v-X}}\otimes\alpha_t^{\texttt{v-X}}]$, we have the following lemma that is useful to bound $C_t^{\texttt{v-X}}$.

Lemma 12. *Denote $C_t^{\texttt{v-X}} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\alpha_t^{\texttt{v-X}}\otimes\alpha_t^{\texttt{v-X}}]$, under Assumptions 1, 2, 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*

$$\gamma_0 < \min\left\{\frac{1}{r'\mathrm{Tr}(\Sigma_m)}, \frac{1}{c'\mathrm{Tr}(\Sigma_m)}\right\},$$

where c' is defined in Eq. (14)*. Then, we have*

$$C_t^{\texttt{v-X}} \preccurlyeq \frac{\gamma_0^2 r'\tau^2[\mathrm{Tr}(\Sigma_m) + \gamma_0\mathrm{Tr}(\Sigma_m^2)]}{1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)} I.$$

Proof. According to the definition of $C_t^{\texttt{v-X}}$, it admits the following expression

$$\begin{aligned}
C_t^{\texttt{v-X}} &= \sum_{s=1}^{t}\prod_{i=s+1}^{t}\gamma_s^2\mathbb{E}_{\boldsymbol{x}}[I-\gamma_i\varphi(\boldsymbol{x}_i)\otimes\varphi(\boldsymbol{x}_i)]^2\mathbb{E}_{\boldsymbol{x}}[\Sigma_m - \varphi(\boldsymbol{x}_t)\otimes\varphi(\boldsymbol{x}_t)]^2\sum_{k=1}^{s-1}\prod_{j=k+1}^{s-1}(I-\gamma_j\Sigma_m)^2\gamma_k^2\Xi\\
&= (I-\gamma_t T^{\texttt{W}})\circ C_{t-1}^{\texttt{v-X}} + \gamma_t^2(S^{\texttt{W}} - \widetilde{S}^{\texttt{W}})\circ\sum_{k=1}^{t-1}\prod_{j=k+1}^{t-1}(I-\gamma_j\Sigma_m)^2\gamma_k^2\Xi \quad \text{[using PSD operators]}\\
&\preccurlyeq (I-\gamma_t T^{\texttt{W}})\circ C_{t-1}^{\texttt{v-X}} + \gamma_t^2 S^{\texttt{W}}\circ\sum_{k=1}^{t-1}\prod_{j=k+1}^{t-1}(I-\gamma_j\Sigma_m)^2\gamma_k^2\Xi \quad \text{[using } S^{\texttt{W}} \succcurlyeq \widetilde{S}^{\texttt{W}}\text{]}\\
&\preccurlyeq (I-\gamma_t T^{\texttt{W}})\circ C_{t-1}^{\texttt{v-X}} + \tau^2\gamma_t^2 S^{\texttt{W}}\circ\sum_{k=1}^{t-1}\prod_{j=k+1}^{t-1}(I-\gamma_j\Sigma_m)^2\gamma_k^2\Sigma_m \quad \text{[using Assumption 5]}\\
&\preccurlyeq (I-\gamma_t T^{\texttt{W}})\circ C_{t-1}^{\texttt{v-X}} + \tau^2\gamma_t^2 r'\mathrm{Tr}\left[\sum_{k=1}^{t-1}\prod_{j=k+1}^{t-1}(I-\gamma_j\Sigma_m)^2\gamma_k^2\Sigma_m^2\right]\Sigma_m. \quad \text{[using Assumption 4]}
\end{aligned} \tag{47}$$

Similar to Eq. (23), we have the following estimation

$$\begin{aligned}
\mathrm{Tr}\left[\sum_{k=1}^{t-1}\prod_{j=k+1}^{t-1}(I-\gamma_j\Sigma_m)^2\Sigma_m^2\gamma_k^2\right] &= \sum_{i=1}^{m}\lambda_i^2\sum_{k=1}^{t-1}\gamma_k^2\prod_{j=k+1}^{t-1}(1-\gamma_j\lambda_i)^2 \leqslant \sum_{i=1}^{m}\lambda_i^2\sum_{k=1}^{t-1}\gamma_k^2\exp\left(-2\lambda_i\sum_{j=k+1}^{s-1}\gamma_j\right)\\
&\leqslant \gamma_0^2\sum_{i=1}^{m}\lambda_i^2\left[1+\int_1^{t-1}u^{-2\zeta}\exp\left(-2\lambda_i\gamma_0\frac{t^{1-\zeta}-(u+1)^{1-\zeta}}{1-\zeta}\right)\mathrm{d}u\right]\\
&\leqslant \gamma_0^2\mathrm{Tr}(\Sigma_m^2)+\sum_{i=1}^{m}\lambda_i^2\left(\frac{\gamma_0}{\lambda_i}\wedge\gamma_0^2 t\right) \quad \text{[using Eq. (24)]}\\
&\leqslant \gamma_0^2\mathrm{Tr}(\Sigma_m^2)+\gamma_0\mathrm{Tr}(\Sigma_m)\,,
\end{aligned}$$

where we use the error bound $\frac{\gamma_0}{\lambda_i}$ instead of the exact one $\gamma_0^2 t$ for tight estimation.

Taking the above equation back to Eq. (47), we have

$$\begin{aligned}
C_t^{\mathtt{v-X}} &\preccurlyeq (I-\gamma_t T^{\mathtt{W}})\circ C_{t-1}^{\mathtt{v-X}}+\gamma_t^2\tau^2 r'\gamma_0[\mathrm{Tr}(\Sigma_m)+\gamma_0\mathrm{Tr}(\Sigma_m^2)]\Sigma_m\\
&\preccurlyeq \tau^2 r'\gamma_0[\mathrm{Tr}(\Sigma_m)+\gamma_0\mathrm{Tr}(\Sigma_m^2)]\sum_{s=1}^{t}\prod_{i=s+1}^{t}(I-\gamma_i T^{\mathtt{W}})\circ\gamma_s^2\Sigma_m\\
&\preccurlyeq \frac{\gamma_0^2 r'\tau^2[\mathrm{Tr}(\Sigma_m)+\gamma_0\mathrm{Tr}(\Sigma_m^2)]}{1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)}I\,, \quad \text{[using Lemma 5]}
\end{aligned}$$

which concludes the proof. □

Proof of Proposition 7. Accordingly, by virtue of $\mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\alpha_t^{\mathtt{v-X}}|\alpha_{t-1}^{\mathtt{v-X}}] = (I-\gamma_t\Sigma_m)\alpha_{t-1}^{\mathtt{v-X}}$ and Lemma 12, $\mathtt{V1}$ can be bounded by

$$\begin{aligned}
\mathtt{V1} &= \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\left[\langle\bar{\eta}_n^{\mathtt{var}}-\bar{\eta}_n^{\mathtt{v-X}},\Sigma_m(\bar{\eta}_n^{\mathtt{var}}-\bar{\eta}_n^{\mathtt{v-X}})\rangle\right] = \mathbb{E}_{\boldsymbol{W}}\langle\Sigma_m,\mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\bar{\alpha}_n^{\mathtt{v-X}}\otimes\bar{\alpha}_n^{\mathtt{v-X}}]\rangle\\
&\leqslant \frac{2}{n^2}\sum_{t=0}^{n-1}\sum_{k=t}^{n-1}\mathbb{E}_{\boldsymbol{W}}\left\langle\prod_{j=t}^{k-1}(I-\gamma_j\Sigma_m)\Sigma_m,\underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{\varepsilon}}[\eta_t^{\mathtt{v-X}}\otimes\eta_t^{\mathtt{v-X}}]}_{:=C_t^{\mathtt{v-X}}}\right\rangle\\
&\lesssim \frac{\tau^2\gamma_0^2 r'}{n^2}\mathbb{E}_{\boldsymbol{W}}\left[\frac{[\mathrm{Tr}(\Sigma_m)+\gamma_0\mathrm{Tr}(\Sigma_m^2)]}{1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)}\sum_{i=1}^{m}\sum_{t=0}^{n-1}\lambda_i\left(\frac{n^\zeta}{\lambda_i\gamma_0}\wedge(n-t)\right)\right]\,, \quad \text{[using Lemma 12]}
\end{aligned}$$

where the last inequality follows the integral estimation in Eq. (22).

For $m\leqslant n$, we use $\frac{n^\zeta}{\lambda_i\gamma_0}$, and thus

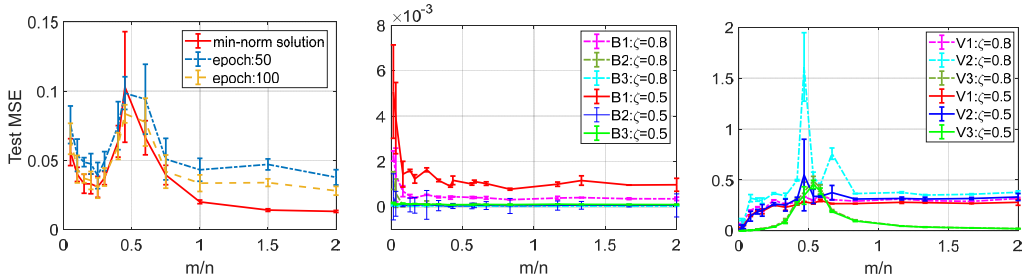
$$\mathtt{V1}\lesssim\frac{\tau^2\gamma_0 r' m}{n^{1-\zeta}}\mathbb{E}_{\boldsymbol{W}}\left[\frac{[\mathrm{Tr}(\Sigma_m)+\gamma_0\mathrm{Tr}(\Sigma_m^2)]}{1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)}\right]\lesssim\frac{\tau^2 r'\gamma_0}{\sqrt{\mathbb{E}[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]^2}}\frac{m}{n^{1-\zeta}}\,,$$

where we use the Cauchy–Schwarz inequality and $\mathrm{Tr}(\Sigma_m)$ as a nonnegative sub-exponential random variable with the sub-exponential norm $\mathcal{O}(1)$ in Lemma 2.

For $m>n$, take $n-t$ and Eq. (39), we have

$$\mathtt{V1}\lesssim\tau^2\gamma_0^2 r'\mathbb{E}_{\boldsymbol{W}}\left[\frac{[\mathrm{Tr}(\Sigma_m)+\gamma_0\mathrm{Tr}(\Sigma_m^2)]}{1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)}\right]\lesssim\frac{\tau^2 r'\gamma_0^2}{\sqrt{\mathbb{E}[1-\gamma_0 r'\mathrm{Tr}(\Sigma_m)]^2}}\sim\mathcal{O}(1)\,.$$

□



(a) a synthetic regression dataset (b) `Bias` (c) `Variance`

Figure 3: Normalized MSE (mean±std.) of RF regression with different epochs on a synthetic regression dataset across the Gaussian kernel in (a); trends of `Bias` and `Variance` under different step-size are empirically given in (b) and (c), respectively.

G.4 Proof of Theorem 2

Proof. Combining the above results for three terms `V1`, `V2`, `V3`, we can directly obtain the result for `Variance`.

$$
\begin{aligned}
\texttt{Variance} &\leqslant \left(\sqrt{\texttt{V1}}+\sqrt{\texttt{V2}}+\sqrt{\texttt{V3}}\right)^2 \leqslant 3(\texttt{V1}+\texttt{V2}+\texttt{V3}) \\
&\lesssim \frac{\gamma_0 r' \tau^2}{\sqrt{\mathbb{E}[1-\gamma_0 r' \mathrm{Tr}(\Sigma_m)]^2}} \begin{cases} mn^{\zeta-1}, & \text{if } m \leqslant n \\ 1+n^{\zeta-1}+\dfrac{n}{m}, & \text{if } m > n \end{cases} \\
&\lesssim \gamma_0 r' \tau^2 \begin{cases} mn^{\zeta-1}, & \text{if } m \leqslant n \\ 1+n^{\zeta-1}+\dfrac{n}{m}, & \text{if } m > n \end{cases} \\
&\sim \begin{cases} \mathcal{O}\left(mn^{\zeta-1}\right), & \text{if } m \leqslant n \\ \mathcal{O}\left(1+n^{\zeta-1}+\dfrac{n}{m}\right), & \text{if } m > n \end{cases}
\end{aligned}
$$

where we use Eq. (39) for the third inequality. □

H More experiments

In this section, we provide additional experimental results to support our theory.

H.1 Results on a regression dataset

We conduct the RF regression via averaged SGD and minimum solution under different initialization schemes and different epochs on a synthetic regression dataset across the Gaussian kernel.

data generation: Apart from the commonly used MNIST in the double descent topic [13, 53], we also add a synthetic regression dataset via normalized MSE in Figure 3(a) for fully supporting our work. The data are generated from a normal Gaussian distribution with the training data ranging from $n = 10$ to $n = 400$, the test data being 200, and the feature dimension $d = 50$. The label is generated by $y = f_\rho(\boldsymbol{x}) + \epsilon$, where the ϵ is a Gaussian noise with the variance 0.01. The target function f^* is generated by a Laplace kernel $k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{x}'\|_2}{d}\right)$, to ensure $f^* \in \mathcal{H}$. To be specific, for any a data point $\boldsymbol{x} \in \mathbb{R}^d$, its target function is $f^*(\boldsymbol{x}) = [k(\boldsymbol{x}, \boldsymbol{x}_1), k(\boldsymbol{x}, \boldsymbol{x}_2), \cdots, k(\boldsymbol{x}, \boldsymbol{x}_n)]\boldsymbol{w}$, where $\boldsymbol{w} \in \mathbb{R}^n$ is a standard random Gaussian vector as a sign. We remark that the reason why we do not choose the Gaussian kernel as the target function is to avoid the data and model induced by a same (type) kernel.

experimental settings: We follow Figure 2(a) with the same experiment settings, i.e., conducting RF regression via averaged SGD and minimum-norm solution under the Gaussian kernel. In our experiment, the initial step-size is set to $\gamma_0 = 1$ with $\zeta = 0.5$. Nevertheless, we take *constant*

initialization (i.e., set the initialization point as a constant vector) and *different epochs* (i.e., 50 and 100) for broad comparison.

Fig. 3(a) shows that, first, under this regression dataset with *constant initialization*, we still observe a phase transition between the two sides of the interpolation threshold at $2m = n$ when min-norm solution and averaged SGD are employed, which leads to the double descent phenomenon. Second, averaged SGD with more epochs result in a better generalization performance, but is still slightly inferior to that with min-norm solution. We need remark that, when employing gradient descent, under mild conditions, the solution converges to the minimum norm solution, as suggested by [4]. Nevertheless, whether this result holds for SGD is unclear, depending on the choice of the ground truth, step-size, etc [64, 65]. Studying the property of converged solution is indeed beyond the scope of this paper.

H.2 Different step-size on Bias and Variance

Following Section 5.2, we also evaluate our error bounds for `Bias` and `Variance` under different step-sizes on the MNIST dataset. Figure 3(b) on bias and 3(c) on variance coincides with the results of Section 5.2: monotonically decreasing bias and unimodal variance (phase transition of `V3` and non-decreasing `V1` and `V2`) under different step-size. We remark that, the estimated error bounds are normalized for better illustration, and accordingly we cannot directly compare the value of these components under different step-size.