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Nearly optimal stochastic approximation for online principal subspace estimation

Xin Liang[1,2], Zhen-Chen Guo[3], Li Wang[4], Ren-Cang Li[4,5,*] & Wen-Wei Lin[6,7]

[1]*Yau Mathematical Sciences Center, Tsinghua University, Beijing* 100084*, China;*
[2]*Yanqi Lake Beijing Institute of Mathematical Sciences and Applications, Beijing* 101408*, China;*
[3]*Department of Mathematics, Nanjing University, Nanjing* 210093*, China;*
[4]*Department of Mathematics, University of Texas at Arlington, Arlington, TX* 76019*, USA;*
[5]*Department of Mathematics, Hong Kong Baptist University, Hong Kong, China;*
[6]*Nanjing Center for Applied Mathematics, Nanjing* 211135*, China;*
[7]*Department of Applied Mathematics, Yang Ming Chiao Tung University, Hsinchu* 300*, China*

Email: liangxinslm@tsinghua.edu.cn, guozhenchen@nju.edu.cn, li.wang@uta.edu, rcli@uta.edu, wwlin@math.nctu.edu.tw

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Abstract Principal component analysis (PCA) has been widely used in analyzing high-dimensional data. It converts a set of observed data points of possibly correlated variables into a set of linearly uncorrelated variables via an orthogonal transformation. To handle streaming data and reduce the complexities of PCA, (subspace) online PCA iterations were proposed to iteratively update the orthogonal transformation by taking one observed data point at a time. Existing works on the convergence of (subspace) online PCA iterations mostly focus on the case where the samples are almost surely uniformly bounded. In this paper, we analyze the convergence of a subspace online PCA iteration under more practical assumption and obtain a nearly optimal finite-sample error bound. Our convergence rate almost matches the minimax information lower bound. We prove that the convergence is nearly global in the sense that the subspace online PCA iteration is convergent with high probability for random initial guesses. This work also leads to a simpler proof of the recent work on analyzing online PCA for the first principal component only.

Keywords principal component analysis, principal component subspace, stochastic approximation, high-dimensional data, online algorithm, finite-sample analysis

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1 Introduction

Principal component analysis (PCA) introduced in [15, 26] is one of the most well-known and popular methods for dimensionality reduction in high-dimensional data analysis. With the volume of data continuously increases, the classical PCA suffers from two major bottlenecks: (1) the high-computational complexity, including the computing empirical covariance matrix and solving the eigen-decomposition

* Corresponding author

problem, and (2) the high storage requirement for the large covariance matrix. These issues prevent PCA from being used for solving problems with large-scale and high-dimensional data.

To reduce both the time and space complexities, Oja [24] in 1982 proposed an online PCA iteration to approximate the first principal component—the top eigenvector of the empirical covariance matrix. Computing the first principal component only is rarely adequate in real-world applications. Later in 1985, Oja and Karhunen [25] proposed a subspace online PCA iteration to approximate a principal subspace of any prescribed dimension. These methods update approximations incrementally by processing data one vector at a time as soon as it comes in such that calculating/storing the empirical covariance matrix explicitly is completely avoided and therefore result in no memory burden. In the rest of this paper, by the online PCA iteration we mean the one just for computing the first principal component whereas a subspace online PCA iteration refers to the one for computing a principal subspace.

Although the online PCA iteration [24] was proposed over 30 years ago, its convergence analysis is rather scarce until recently. Some recent works [7, 16, 27] studied the convergence of the online PCA for the first principal component from different points of view and obtained some results for the case where the samples are almost surely uniformly bounded. For such a case, De Sa et al. [10] studied a different but closely related problem, in which the angular part is equivalent to the online PCA, and obtained some convergence results. In contrast, for the distributions with sub-Gaussian tails (note that the samples of this kind of distributions may be unbounded), Li et al. [19] proved a nearly optimal convergence rate for the online PCA iteration when the initial guess is randomly chosen according to a uniform distribution and the stepsize chosen in accordance with the sample size. This result is more general than previous ones in [7, 16, 27], because it is for distributions that can possibly be unbounded, and the convergence rate is nearly optimal and nearly global.

For the subspace online PCA [25], some recent works studied the convergence for the case where the samples are almost surely uniformly bounded. In a series of papers [4, 5, 21, 22], Arora et al. studied PCA as a stochastic optimization problem and its variations via direct optimization approaches, namely using convex relaxation and adding regularizations. The subspace iteration falls into one variant of their methods. Hardt and Price [13] and Balcan et al. [6] treated the subspace iteration as a noisy power method and analyzed its convergence. Li et al. [18] investigated the convergence for the case where the initial guess follows the normal distribution. Garber et al. [12] used the shift-and-invert technique to speed up the convergence, but their analysis was only done for the top eigenvector. Allen-Zhu and Li [3] proposed a faster variant of the subspace online PCA iteration, along with their gap-dependent and gap-free convergence results. However, those works are performed under the assumption that the samples are almost surely uniformly bounded. For distributions, e.g., sub-Gaussians, that are possibly unbounded, a thorough convergence analysis of the subspace online PCA remains elusive.

In this paper, we aim to fill up the gap by establishing a nearly optimal and nearly global convergence rate for the subspace online PCA for samples of possibly unbounded distributions of sub-Gaussians. In going through the proving process in [19] for the online PCA iteration, we find that there are three major hurdles, as we will explain in detail in Subsection 4.2, that prevent their proving technique for one-dimensional case, i.e., the most significant principal component, from being straightforwardly generalized to analyze the multi-dimensional case, i.e., significant principal subspaces. To overcome these challenging difficulties, we adopt a new proving technique and apply it to a variant of subspace online PCA to fulfill the goal. The variant is mathematically equivalent to the original one in [25] except without explicit references to QR decompositions for orthogonalization, and is essentially the same as the orthogonal Oja algorithm of Abed-Meraim et al. [1]. In addition to the advantages inherited from online PCA, it leads to a computationally economical formula for the subspace online iteration. Some of the proving techniques are built by ourselves with the help of the theory of special functions of a matrix argument, which is rarely used in the statistical community. We mention in passing that our proving technique may be specialized to the online PCA for a simpler proof than that in [19] for the most significant principal component.

The rest of this paper is organized as follows. We first briefly introduce the related work in Section 2. In Section 3, we propose a variant of the subspace online PCA iteration (2.6), which will be the version to be analyzed. Our main results are stated in Section 4 together with three main theorems and discussions of the newly invented proving technique, where we compare our results for the one-dimensional case with the recent results in [19] and outline the technical differences in proofs between ours and those from [19]. Our proofs are given in Sections 5 and 6. Finally, in Section 7 we draw our conclusions. Some of the complicated calculations are deferred to Appendix A for clarity.

Notation. $\mathbb{R}^{n\times m}$ is the set of all the $n\times m$ real matrices, $\mathbb{R}^n=\mathbb{R}^{n\times 1}$ and $\mathbb{R}=\mathbb{R}^1$. I_n (or simply I if its dimension is clear from the context) is the $n\times n$ identity matrix and e_j is its j-th column (usually with dimension determined by the context). For a matrix X, $\sigma(X)$, $\|X\|_\infty$, $\|X\|_2$ and $\|X\|_{\mathrm{F}}$ are the multiset of the singular values, the ℓ_∞-operator norm, the spectral norm and the Frobenius norm of X, respectively. $\mathcal{R}(X)$ is the subspace spanned by the columns of X, $X_{(i,j)}$ is the (i,j)-th entry of X, and $X_{(k:\ell,:)}$ and $X_{(:,i:j)}$ are two submatrices of X consisting of its row k to the row ℓ and the column i to the column j, respectively. $X\circ Y$ is the Hadamard, i.e., entrywise, product of matrices (vector) X and Y of the same size.

For any vector or matrices X and Y, $X\leqslant Y$ ($X<Y$) means $X_{(i,j)}\leqslant Y_{(i,j)}$ ($X_{(i,j)}<Y_{(i,j)}$) for any i and j. $X\geqslant Y$ ($X>Y$) if $-X\leqslant -Y$ ($-X<-Y$); $X\leqslant\alpha$ ($X<\alpha$) for a scalar α means $X_{(i,j)}\leqslant\alpha$ ($X_{(i,j)}<\alpha$) for any i and j; similarly $X\geqslant\alpha$ and $X>\alpha$. For a subset or an event $\mathbb{A}$, $\mathbb{A}^{\mathrm{c}}$ is the complement set of $\mathbb{A}$. By $\sigma\{\mathbb{A}_1,\ldots,\mathbb{A}_p\}$, we denote the σ-algebra generated by the events $\mathbb{A}_1,\ldots,\mathbb{A}_p$; $\mathbb{N}=\{1,2,3,\ldots\}$. $\mathrm{E}\{\boldsymbol{X};\mathbb{A}\}:=\mathrm{E}\{\boldsymbol{X}\mathbf{1}_{\mathbb{A}}\}$ denotes the expectation of a random variable $\boldsymbol{X}$ over event $\mathbb{A}$. Note that

$$\mathrm{E}\{\boldsymbol{X};\mathbb{A}\}=\mathrm{E}\{\boldsymbol{X}\mid\mathbb{A}\}\,\mathrm{P}\{\mathbb{A}\}. \tag{1.1}$$

For a random vector or matrix $\boldsymbol{X}$, $\mathrm{E}\{\boldsymbol{X}\}:=[\mathrm{E}\{\boldsymbol{X}_{(i,j)}\}]$. Note that $\|\mathrm{E}\{\boldsymbol{X}\}\|_{\mathrm{ui}}\leqslant\mathrm{E}\{\|\boldsymbol{X}\|_{\mathrm{ui}}\}$ for $\mathrm{ui}=2,\mathrm{F}$. Write $\mathrm{cov}_\circ(\boldsymbol{X},\boldsymbol{Y}):=\mathrm{E}\{[\boldsymbol{X}-\mathrm{E}\{\boldsymbol{X}\}]\circ[\boldsymbol{Y}-\mathrm{E}\{\boldsymbol{Y}\}]\}$ and $\mathrm{var}_\circ(\boldsymbol{X}):=\mathrm{cov}_\circ(\boldsymbol{X},\boldsymbol{X})$.

Denote by $\mathbb{G}_p(\mathbb{R}^d)$ the Grassmann manifold of all the p-dimensional subspaces of $\mathbb{R}^d$. For two subspaces $\mathcal{X},\mathcal{Y}\in\mathbb{G}_p(\mathbb{R}^d)$, let $X,Y\in\mathbb{C}^{d\times p}$ be the basis matrices of $\mathcal{X}$ and $\mathcal{Y}$, respectively, i.e., $\mathcal{X}=\mathcal{R}(X)$ and $\mathcal{Y}=\mathcal{R}(Y)$, and denote by σ_j for $1\leqslant j\leqslant p$ in the nondecreasing order, i.e., $\sigma_1\leqslant\cdots\leqslant\sigma_p$, the singular values of $(X^{\mathrm{T}}X)^{-1/2}X^{\mathrm{T}}Y(Y^{\mathrm{T}}Y)^{-1/2}$. The *$p$ canonical angles $\theta_j(\mathcal{X},\mathcal{Y})$ between $\mathcal{X}$ and $\mathcal{Y}$* are defined by $0\leqslant\theta_j(\mathcal{X},\mathcal{Y}):=\arccos\sigma_j\leqslant\frac{\pi}{2}$ for $1\leqslant j\leqslant p$. They are in the non-increasing order, i.e., $\theta_1(\mathcal{X},\mathcal{Y})\geqslant\cdots\geqslant\theta_p(\mathcal{X},\mathcal{Y})$. Set $\Theta(\mathcal{X},\mathcal{Y})=\mathrm{diag}(\theta_1(\mathcal{X},\mathcal{Y}),\ldots,\theta_p(\mathcal{X},\mathcal{Y}))$. It can be seen that angles so defined are independent of the basis matrices X and Y, which are not unique. With the definition of canonical angles, $\|\sin\Theta(\mathcal{X},\mathcal{Y})\|_{\mathrm{ui}}$ for $\mathrm{ui}=2,\mathrm{F}$ are metrics on $\mathbb{G}_p(\mathbb{R}^d)$ [28, Subsection II.4].

In what follows, we sometimes place a vector or matrix in one or both arguments of $\theta_j(\cdot,\cdot)$ and $\Theta(\cdot,\cdot)$ with the understanding that it is about the subspace spanned by the vector or the columns of the matrix argument. For any $X\in\mathbb{R}^{d\times p}$, if $X_{(1:p,:)}$ is nonsingular, then we can define

$$\mathscr{T}(X):=X_{(p+1:d,:)}X_{(1:p,:)}^{-1}. \tag{1.2}$$

2 Related work

Let $\boldsymbol{X}\in\mathbb{R}^d$ be a d-dimensional random vector with the mean $\mathrm{E}\{\boldsymbol{X}\}$ and the covariance

$$\Sigma=\mathrm{E}\{(\boldsymbol{X}-\mathrm{E}\{\boldsymbol{X}\})(\boldsymbol{X}-\mathrm{E}\{\boldsymbol{X}\})^{\mathrm{T}}\}.$$

To reduce the dimension of $\boldsymbol{X}$ from d to p (usually $p\ll d$), PCA looks for a p-dimensional linear subspace that is closest to the centered random vector $\boldsymbol{X}-\mathrm{E}\{\boldsymbol{X}\}$ in the mean squared sense, through the independent and identically distributed samples $X^{(1)},\ldots,X^{(n)}$.

Without loss of generality, we assume $\mathrm{E}\{\boldsymbol{X}\}=0$. Then PCA corresponds to a stochastic optimization problem

$$\min_{\mathcal{U}\in\mathbb{G}_p(\mathbb{R}^d)}\mathrm{E}\{\|(I_d-\Pi_{\mathcal{U}})\boldsymbol{X}\|_2^2\}, \tag{2.1}$$

where $\Pi_{\mathcal{U}}$ is the orthogonal projector onto the subspace $\mathcal{U}$. Let $\Sigma=U\Lambda U^{\mathrm{T}}$ be the spectral decomposition of Σ, where

$$\Lambda=\mathrm{diag}(\lambda_1,\ldots,\lambda_d)\quad\text{with }\lambda_1\geqslant\cdots\geqslant\lambda_p\geqslant\lambda_{p+1}\geqslant\cdots\geqslant\lambda_d\geqslant 0, \tag{2.2}$$

and orthogonal $U = [u_1, \dots, u_d]$. If $\lambda_p > \lambda_{p+1}$, then the unique solution to the optimization problem (2.1), namely the p-dimensional principal subspace of Σ, is $\mathcal{U}_* = \mathcal{R}([u_1, \dots, u_p])$, the subspace spanned by $u_1, \dots, u_p$. In practice, Σ is unknown, and the sample data $\{X^{(1)}, \dots, X^{(n)}\}$ is generally used to estimate $\mathcal{U}_*$. The classical PCA does it by the spectral decomposition of the empirical covariance matrix $\widehat{\Sigma} = \frac{1}{n}\sum_{i=1}^{n} X^{(i)}(X^{(i)})^{\mathrm{T}}$. Specifically, the classical PCA uses $\widehat{\mathcal{U}}_* = \mathcal{R}([\widehat{u}_1, \dots, \widehat{u}_p])$ to estimate $\mathcal{U}_*$, where $\widehat{u}_i$ is the corresponding eigenvectors of $\widehat{\Sigma}$. In the classical PCA, obtaining the empirical covariance matrix has time complexity $\mathrm{O}(nd^2)$ and space complexity $\mathrm{O}(d^2)$. So storing and calculating a large empirical covariance matrix can be very expensive when the data are of high dimension, not to mention the cost $\mathrm{O}(d^3)$ by dense solvers or $\mathrm{O}(pnd)$ (more of $\mathrm{O}(p^2nd)$ with full reorthogonalization for robustness) by some iterative methods for computing its eigenvalues and eigenvectors [11].

To analyze the accuracy of the above estimation using a finite number of samples, an important quantity is the distance between $\mathcal{U}_*$ and $\widehat{\mathcal{U}}_*$ by their canonical angles. Vu and Lei [32, Theorem 3.1] proved that if $p(d-p)\frac{\sigma_*^2}{n}$ is bounded for some constant σ_*, then

$$\inf_{\widehat{\mathcal{U}}_* \in \mathbb{G}_p(\mathbb{R}^d)} \sup_{\boldsymbol{X} \in \mathcal{P}_0(\sigma_*^2, d)} \mathrm{E}\{\|\sin\Theta(\widehat{\mathcal{U}}_*, \mathcal{U}_*)\|_{\mathrm{F}}^2\} \geqslant cp(d-p)\frac{\sigma_*^2}{n}, \tag{2.3}$$

where $c > 0$ is an absolute constant, and $\mathcal{P}_0(\sigma_*^2, d)$ is the set of all the d-dimensional sub-Gaussian distributions for which the eigenvalues of the covariance matrix satisfy

$$\frac{\lambda_1\lambda_{p+1}}{(\lambda_p - \lambda_{p+1})^2} \leqslant \sigma_*^2. \tag{2.4}$$

Note that its left-hand side is the effective noise variance.

To reduce both the time and space complexities, Oja [24] proposed an *online PCA iteration*

$$\widetilde{u}^{(n)} = u^{(n-1)} + \beta^{(n-1)} X^{(n)}(X^{(n)})^{\mathrm{T}} u^{(n-1)}, \quad u^{(n)} = \widetilde{u}^{(n)}\|\widetilde{u}^{(n)}\|_2^{-1} \tag{2.5}$$

to approximate the first principal component, where $\beta^{(n)} > 0$ is a stepsize. Later, Oja and Karhunen [25] proposed a *subspace online PCA iteration*

$$\widetilde{U}^{(n)} = U^{(n-1)} + X^{(n)}(X^{(n)})^{\mathrm{T}} U^{(n-1)} \operatorname{diag}(\beta_1^{(n-1)}, \dots, \beta_p^{(n-1)}), \quad U^{(n)} = \widetilde{U}^{(n)} R^{(n)} \tag{2.6}$$

to approximate the principal subspace $\mathcal{U}_*$, where $\beta_i^{(n)} > 0$ for $1 \leqslant i \leqslant p$ are stepsizes, and $R^{(n)}$ is a normalization matrix to make $U^{(n)}$ have orthonormal columns. The QR decomposition is often used by almost all the existing works in the literature (see, e.g., [3, 22, 25] and the references therein). It can be seen that these methods update the approximations incrementally by processing data one vector at a time as soon as it comes in, completely avoiding the explicit calculation of the empirical covariance matrix. In the subspace online PCA, obtaining an approximate principal subspace has time complexity $\mathrm{O}(p^2d)$ and space complexity $\mathrm{O}(pd)$ per iterative step.

Recently, Li et al. [19] proved a nearly optimal convergence rate for the iteration (2.5) for the distributions with sub-Gaussian tails (note the samples of this kind of distributions may be unbounded). One of their main results reads as follows. For the initial guess $u^{(0)}$ that is randomly chosen according to a uniform distribution and the stepsize β that is chosen in accordance with the sample size n, there exists a high-probability event $\mathbb{A}_*$ with $\mathrm{P}\{\mathbb{A}_*\} \geqslant 1 - \delta$ such that

$$\mathrm{E}\{|\tan\Theta(u^{(n)}, u_*)|^2 \mid \mathbb{A}_*\} \leqslant C(d,n,\delta)\frac{\ln n}{n}\frac{1}{\lambda_1 - \lambda_2}\sum_{i=2}^{d}\frac{\lambda_1\lambda_i}{\lambda_1 - \lambda_i} \tag{2.7a}$$

$$\leqslant C(d,n,\delta)\frac{\lambda_1\lambda_2}{(\lambda_1 - \lambda_2)^2}\frac{(d-1)\ln n}{n}, \tag{2.7b}$$

where $\delta \in [0,1)$, $u_* = u_1$ is the first principal component, and $C(d,n,\delta)$ can be approximately treated as a constant because for sufficiently large d, $C(d,n,\delta)$ goes to a constant as $n \to \infty$. It can be seen that this bound matches the minimax lower bound (2.3) up to a logarithmic factor of n, and hence, *nearly* *optimal*. It is significant because a uniformly distributed initial value is nearly orthogonal to the principal component with high probability when d is large [8, Subsection 2.4], and thus such a random initial vector is not a very good initial guess to start an iteration with. This result is more general than previous ones in [7, 16, 27], because it is for distributions that can possibly be unbounded, and the convergence rate is nearly optimal and nearly global.

Unfortunately, the above significant work [19] on the online PCA iteration cannot be trivially generalized to the subspace online PCA iteration due to three major difficulties to be discussed in Subsection 4.2.

3 Efficient subspace online PCA

Let $X^{(n)} \in \mathbb{R}^d$ for $n = 1, 2, \dots$ be independent and identically distributed samples of $\boldsymbol{X}$. As $\{X^{(1)}, \dots, X^{(n)}\}$ comes in a sequential order, the subspace online PCA iteration (2.6) of Oja and Karhunen [25] is used to compute the principal subspace of dimension p. Differing from (2.6), our proposed subspace online PCA has the following changes:

(1) a fixed stepsize $\beta_i^{(n)} = \beta > 0$, $\forall\, n$, $i = 1, \dots, p$, is used;

(2) the normalization matrix to make $U^{(n)}$ have orthonormal columns is explicitly given by

$$R^{(n)} = [(\widetilde{U}^{(n)})^{\mathrm{T}} \widetilde{U}^{(n)}]^{-1/2}. \tag{3.1}$$

With the changes, our subspace online PCA iteration becomes

$$\widetilde{U}^{(n)} = U^{(n-1)} + \beta X^{(n)} (X^{(n)})^{\mathrm{T}} U^{(n-1)}, \quad U^{(n)} = \widetilde{U}^{(n)} [(\widetilde{U}^{(n)})^{\mathrm{T}} \widetilde{U}^{(n)}]^{-1/2}. \tag{3.2}$$

It can be verified that $U^{(n)}$ have orthonormal columns. This variant is equivalent to (2.6) in the sense that both $U^{(n)}$ here and the one there have the same column space. It turns out that the matrix square root and the inverse in (3.1) can be done analytically as in Lemma 3.1 below, leading to a simple and computationally economical formula for $U^{(n)}$ of (3.2).

An equivalence of Lemma 3.1 was implied in [1], although not explicitly and rigorously stated, to the analytically transform iteration formula (3.2). For that reason, we credit the lemma to [1], but provide a proof for completeness because of some missing details in the derivation in [1].

Lemma 3.1 (See [1]). *Let $V \in \mathbb{R}^{d \times p}$ with $V^{\mathrm{T}} V = I_p$, $0 \neq x \in \mathbb{R}^d$ and $0 < \beta \in \mathbb{R}$, and let*

$$W := V + \beta x x^{\mathrm{T}} V = (I_d + \beta x x^{\mathrm{T}}) V, \quad V_+ := W (W^{\mathrm{T}} W)^{-1/2}.$$

If $V^{\mathrm{T}} x \neq 0$, then

$$V_+ = V + \beta \tilde{\alpha} x z^{\mathrm{T}} - \frac{1 - \tilde{\alpha}}{\gamma^2} V z z^{\mathrm{T}},$$

where $z = V^{\mathrm{T}} x$, $\gamma = \|z\|_2$, $\tilde{z} = z/\gamma$, $\alpha = \beta(2 + \beta \|x\|_2^2)\gamma^2$ and $\tilde{\alpha} = (1 + \alpha)^{-1/2}$. In particular, $V_+^{\mathrm{T}} V_+ = I_p$.

Proof. We have

$$W^{\mathrm{T}} W = V^{\mathrm{T}} [I_d + \beta x x^{\mathrm{T}}]^2 V = I_p + \alpha \tilde{z} \tilde{z}^{\mathrm{T}}.$$

Let $Z_\perp \in \mathbb{R}^{p \times (p-1)}$ such that $[\tilde{z}, Z_\perp]^{\mathrm{T}} [\tilde{z}, Z_\perp] = I_p$. The eigen-decomposition of $W^{\mathrm{T}} W$ is

$$W^{\mathrm{T}} W = [\tilde{z}, Z_\perp] \begin{bmatrix} 1 + \alpha & \\ & I_{p-1} \end{bmatrix} [\tilde{z}, Z_\perp]^{\mathrm{T}},$$

which yields

$$(W^{\mathrm{T}} W)^{-1/2} = [\tilde{z}, Z_\perp] \begin{bmatrix} (1 + \alpha)^{-1/2} & \\ & I_{p-1} \end{bmatrix} [\tilde{z}, Z_\perp]^{\mathrm{T}} = I_p - [1 - (1 + \alpha)^{-1/2}] \tilde{z} \tilde{z}^{\mathrm{T}}.$$

Therefore,

$$
\begin{aligned}
V_+ &= (V + \beta x x^{\mathrm{T}} V)\{I_p - [1 - (1+\alpha)^{-1/2}]\tilde{z}\tilde{z}^{\mathrm{T}}\} \\
&= V + \beta x x^{\mathrm{T}} V - [1 - (1+\alpha)^{-1/2}](V + \beta x x^{\mathrm{T}} V)\tilde{z}\tilde{z}^{\mathrm{T}} \ (\text{use } x^{\mathrm{T}} V = z^{\mathrm{T}} = \gamma \tilde{z}^{\mathrm{T}}) \\
&= V + \beta\gamma x \tilde{z}^{\mathrm{T}} - [1 - (1+\alpha)^{-1/2}] V \tilde{z}\tilde{z}^{\mathrm{T}} - [1 - (1+\alpha)^{-1/2}]\beta\gamma x \tilde{z}^{\mathrm{T}} \\
&= V + (1+\alpha)^{-1/2}\beta x z^{\mathrm{T}} - \frac{1 - (1+\alpha)^{-1/2}}{\gamma^2} V z z^{\mathrm{T}},
\end{aligned}
$$

as expected, knowing $\tilde{\alpha} = (1+\alpha)^{-1/2}$. □

To apply this lemma to transform (3.2), we perform substitutions, i.e.,

$$
\widetilde{U}^{(n)} \leftarrow W, \quad U^{(n-1)} \leftarrow V, \quad U^{(n)} \leftarrow V_+, \quad X^{(n)} \leftarrow x, \quad Z^{(n)} \leftarrow z
$$

to obtain

$$
U^{(n)} = U^{(n-1)} + \beta(1+\alpha^{(n)})^{-1/2} X^{(n)} (Z^{(n)})^{\mathrm{T}} - [1 - (1+\alpha^{(n)})^{-1/2}] \frac{U^{(n-1)} Z^{(n)} (Z^{(n)})^{\mathrm{T}}}{\|Z^{(n)}\|_2^2},
$$

where $\alpha^{(n)} = \beta(2+\beta(X^{(n)})^{\mathrm{T}} X^{(n)}) \|Z^{(n)}\|_2^2$ and $Z^{(n)} = (U^{(n-1)})^{\mathrm{T}} X^{(n)}$. Finally, we outline in Algorithm 1 the subspace online PCA algorithm derived from (3.2). This is essentially the same as the orthogonal Oja algorithm (see [1]) and will be the one we are going to analyze. Computationally, it has the advantages of not involving any explicit orthogonalization by the Gram-Schmidt process or the matrix square root, but only in terms of matrix-vector multiplications. This formulation is numerically stable and computationally fast. At convergence, it is expected that

$$
U^{(n)} \to U_* := U \begin{bmatrix} I_p \\ 0 \end{bmatrix} = [u_1, u_2, \ldots, u_p]
$$

in the sense that $\|\sin\Theta(U^{(n)}, U_*)\|_{\mathrm{ui}} \to 0$ as $n \to \infty$. The rest of this paper is devoted to analyzing its convergence, with the help of the next lemma.

Algorithm 1 Subspace online PCA

```
1: Choose U^(0) ∈ R^{d×p} with (U^(0))^T U^(0) = I, and choose the stepsize β > 0.
2: for n = 1, 2, ... until convergence do
3:    Take an X's sample X^(n);
4:    Z^(n) = (U^(n−1))^T X^(n), α^(n) = β(2 + β(X^(n))^T X^(n))(Z^(n))^T Z^(n), α̃^(n) = (1 + α^(n))^(−1/2);
5:    U^(n) = U^(n−1) + β α̃^(n) X^(n) (Z^(n))^T − (1 − α̃^(n)) / ((Z^(n))^T Z^(n)) · U^(n−1) Z^(n) (Z^(n))^T.
6: end for
```

Lemma 3.2. *For $V \in \mathbb{R}^{d\times p}$ with nonsingular $V_{(1:p,:)}$, we see that for* $\mathrm{ui} = 2, \mathrm{F}$,

$$
\left\| \tan\Theta\left(V, \begin{bmatrix} I_p \\ 0 \end{bmatrix}\right) \right\|_{\mathrm{ui}} = \|\mathscr{T}(V)\|_{\mathrm{ui}}, \tag{3.3}
$$

where $\mathscr{T}(V)$ is defined as in (1.2).

Proof. Let $Y = \left[\begin{smallmatrix} I_p \\ 0 \end{smallmatrix}\right] \in \mathbb{R}^{d\times p}$. It can be seen that the singular values $\sigma_j = \cos\theta_j(V, Y)$ of

$$
[I + \mathscr{T}(V)^{\mathrm{T}} \mathscr{T}(V)]^{-1/2} \begin{bmatrix} I \\ \mathscr{T}(V) \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} I \\ 0 \end{bmatrix} = [I + \mathscr{T}(V)^{\mathrm{T}} \mathscr{T}(V)]^{-1/2}
$$

and the singular values τ_j of $\mathscr{T}(V)$ are related by

$$
\tau_j = \frac{\sqrt{1 - \sigma_j^2}}{\sigma_j} = \tan\theta_j(V, Y),
$$

where $j = 1, \ldots, p$. Hence, the identity (3.3) holds. □

Notations introduced in this section, except those in Lemma 3.1, will be adopted throughout the rest of this paper.

4 Main results

For convenience, we first review our setting. Let $\boldsymbol{X} = [\boldsymbol{X}_1, \boldsymbol{X}_2, \ldots, \boldsymbol{X}_d]^{\mathrm{T}}$ be a random vector in $\mathbb{R}^d$. Assume $\mathrm{E}\{\boldsymbol{X}\} = 0$. Its covariance matrix $\Sigma := \mathrm{E}\{\boldsymbol{X}\boldsymbol{X}^{\mathrm{T}}\}$ has the spectral decomposition

$$\Sigma = U\Lambda U^{\mathrm{T}} \quad \text{with } U = [u_1, u_2, \ldots, u_d], \quad \Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_d), \tag{4.1}$$

where $U \in \mathbb{R}^{d\times d}$ is orthogonal, and λ_i for $1 \leqslant i \leqslant d$ are the eigenvalues of Σ, arranged for convenience in the non-increasing order. Assume

$$\lambda_1 \geqslant \cdots \geqslant \lambda_p > \lambda_{p+1} \geqslant \cdots \geqslant \lambda_d > 0. \tag{4.2}$$

Given $\{X^{(1)}, \ldots, X^{(n)}\}$ in a sequential order, the proposed subspace online PCA iteration (3.2) is used to compute the principal subspace $U^{(n)}$ of dimension p to estimate

$$\mathcal{U}_* = \mathcal{R}(U_{(:,1:p)}) = \mathcal{R}([u_1, u_2, \ldots, u_p]). \tag{4.3}$$

Our major result on the convergence rate of the subspace online PCA iteration in Algorithm 1 states as follows: if the initial guess $U^{(0)}$ is randomly chosen to satisfy that $\mathcal{R}(U^{(0)})$ is uniformly sampled from $\mathbb{G}_p(\mathbb{R}^d)$, and the stepsize $\beta_i^{(n)}$ is chosen the same for $1 \leqslant i \leqslant p$ and in accordance with the sample size n, then there exists a high-probability event $\mathbb{H}_*$ with $\mathrm{P}\{\mathbb{H}_*\} \geqslant 1 - 2\delta^{p^2}$ such that

$$\mathrm{E}\{\|\tan\Theta(U^{(n)}, U_*)\|_{\mathrm{F}}^2 \mid \mathbb{H}_*\} \leqslant C(d,n,\delta)\frac{\ln n}{n}\frac{1}{\lambda_p - \lambda_{p+1}}\sum_{j=1}^{p}\sum_{i=p+1}^{d}\frac{\lambda_j\lambda_i}{\lambda_j - \lambda_i} \tag{4.4a}$$

$$\leqslant C(d,n,\delta)\frac{\lambda_p\lambda_{p+1}}{(\lambda_p - \lambda_{p+1})^2}\frac{p(d-p)\ln n}{n}, \tag{4.4b}$$

where the constant $C(d,n,\delta) \to 24\psi^4/(1-\delta^{p^2})$ as $d \to \infty$ and $n \to \infty$, and ψ is $\boldsymbol{X}$'s Orlicz-ψ_2 norm (see Definition 4.1 below). This also matches the minimax lower bound (2.3) up to a logarithmic factor of n, and hence is *nearly optimal* and *nearly global* for the subspace online PCA, in the same way as (2.7) of Li et al. [19] for the vector online PCA. Both are valid for any sub-Gaussian distribution.

Comparing (4.4) and (2.7), we find that (2.7) becomes the special case of our results (4.4) in the case of $p = 1$. Unfortunately, the proving technique in [19] used for the one-dimensional case ($p = 1$) is not generalizable to the multi-dimensional case ($p > 1$). More details will be forthcoming in Subsection 4.2.

We also note that the factor in our result is

$$\frac{\lambda_p\lambda_{p+1}}{(\lambda_p - \lambda_{p+1})^2} \quad \text{vs.} \quad \frac{\lambda_1\lambda_{p+1}}{(\lambda_p - \lambda_{p+1})^2}.$$

The second quantity appeared in (2.4). The first quantity is always smaller but both are of the similar order if λ_1 and λ_p are of the similar order. However, their magnitude can differ greatly when $\lambda_p \ll \lambda_1$.

4.1 Three main theorems

In this subsection, we state our three main theorems of the paper for the multi-dimensional case and (4.4) is a consequence of them. Before that, we will introduce necessary definitions and assumptions. We point out that any statement we will make is meant to hold *almost surely*.

We are concerned with random variables/vectors that have a sub-Gaussian distribution. To that end, we need to introduce the Orlicz ψ_α-norm of a random variable/vector. More details can be found in [30].

Definition 4.1. The *Orlicz ψ_α-norm* of a random variable $\boldsymbol{X} \in \mathbb{R}$ is defined as

$$\|\boldsymbol{X}\|_{\psi_\alpha} := \inf\left\{\xi > 0 : \mathrm{E}\left\{\exp\left(\left|\frac{\boldsymbol{X}}{\xi}\right|^\alpha\right)\right\} \leqslant 2\right\},$$

and the *Orlicz ψ_α-norm* of a random vector $\boldsymbol{X} \in \mathbb{R}^d$ is defined as

$$\|\boldsymbol{X}\|_{\psi_\alpha} := \sup_{\|v\|_2=1} \|v^{\mathrm{T}}\boldsymbol{X}\|_{\psi_\alpha}.$$

We say that the random variable/vector $\boldsymbol{X}$ follows a *sub-Gaussian distribution* if $\|\boldsymbol{X}\|_{\psi_2} < \infty$.

By definition, any bounded random variable/vector follows a sub-Gaussian distribution. To prepare our convergence analysis, we make a few assumptions.

Assumption 4.2. *$\boldsymbol{X} = [\boldsymbol{X}_1, \boldsymbol{X}_2, \ldots, \boldsymbol{X}_d]^{\mathrm{T}} \in \mathbb{R}^d$ is a random vector.*
(A-1) $\mathrm{E}\{\boldsymbol{X}\} = 0$, *and* $\Sigma := \mathrm{E}\{\boldsymbol{X}\boldsymbol{X}^{\mathrm{T}}\}$ *has the spectral decomposition* (4.1) *satisfying* (4.2);
(A-2) $\psi := \|\Sigma^{-1/2}\boldsymbol{X}\|_{\psi_2} < \infty$.

The principal subspace $\mathcal{U}_*$ in (4.3) is uniquely determined under Assumption 4.2(A-1). On the other hand, Assumption 4.2(A-2) ensures that all the 1-dimensional marginals of $\boldsymbol{X}$ have sub-Gaussian tails, or equivalently, $\boldsymbol{X}$ follows a sub-Gaussian distribution. This is also an assumption that is used in [19].

In what follows, we will state our main results under the assumption and leave their proofs to Sections 5 and 6 because of their high complexity. To that end, first we introduce some quantities as follows:

- the eigenvalue gap $\gamma := \lambda_p - \lambda_{p+1}$,
- the sum of the top i eigenvalues $\eta_i := \lambda_1 + \cdots + \lambda_i$, $i = 1, \ldots, d$,
- the dominance of the top i eigenvalues $\mu_i := \frac{\eta_i}{\eta_d} \in [\frac{i}{d}, 1]$,
- for $s > 0$ and the stepsize $\beta < 1$ such that $\beta\gamma < 1$, the integer function

$$N_s(\beta) := \min\{n \in \mathbb{N} : (1-\beta\gamma)^n \leqslant \beta^s\} = \left\lceil \frac{s \ln \beta}{\ln(1-\beta\gamma)} \right\rceil, \tag{4.5}$$

where $\lceil\cdot\rceil$ is the ceiling function taking the smallest integer that is no smaller than its argument, and finally,

- for $0 < \varepsilon < 1/7$, the integer function

$$M(\varepsilon) := \min\{m \in \mathbb{N} : \beta^{7\varepsilon/2-1/2} \leqslant \beta^{(1-2^{1-m})(3\varepsilon-1/2)}\} = 2 + \left\lceil \frac{\ln \frac{1/2-3\varepsilon}{\varepsilon}}{\ln 2} \right\rceil \geqslant 2.$$

In practice, it is always desirable to use a good initial guess in an iterative method whenever there is one available because it positively affects computational efficiency in reducing the number of iterations required to achieve an approximation within a prescribed tolerance. On the other hand, when there is not one known, a randomly chosen initial guess is often taken. Our first main result in Theorem 4.3 covers the case where a somewhat good initial subspace $U^{(0)}$ is available whereas our second main result in Theorem 4.5 is about using a randomly chosen initial subspace.

Theorem 4.3. *Given $\varepsilon \in (0, 1/7)$, $\omega \in (0, 1)$ and $\phi > 0$, κ and β satisfy*

$$\begin{aligned} &\kappa > 6^{[M(\varepsilon)-1]/2} \max\{\sqrt{2}, 2(\sqrt{2}-1)^{1/2}\phi\lambda_1^{-1/2}\omega^{1/2}\}, \\ &0 < \beta < \min\left\{1, \left(\frac{1}{8\kappa\eta_p}\right)^{\frac{2}{1-4\varepsilon}}, \left(\frac{\gamma}{130\kappa^2\eta_p^2}\right)^{\frac{1}{\varepsilon}}\right\}. \end{aligned} \tag{4.6}$$

Let $U^{(n)}$ for $n = 1, 2, \ldots$ be the approximations of U_* generated by Algorithm 1. *Under Assumption* 4.2*, if*

$$\|\tan\Theta(U^{(0)}, U_*)\|_2^2 \leqslant \phi^2 d - 1 \tag{4.7}$$

and

$$(\sqrt{2}+1)\lambda_1 d\beta^{1-7\varepsilon} \leqslant \omega, \quad K > N_{3/2-37\varepsilon/4}(\beta), \tag{4.8}$$

then there exist absolute constants[1)] C_ψ, C_ν *and* $C_\circ$ *and a high-probability event* $\mathbb{H}$ *with*

$$\mathrm{P}\{\mathbb{H}\} \geqslant 1 - K[(2+\mathrm{e})d + p + 1]\exp(-C_{\nu\psi}\beta^{-\varepsilon}) \tag{4.9}$$

such that for any $n \in [N_{3/2-37\varepsilon/4}(\beta), K]$,

$$\begin{aligned}\mathrm{E}\{\|\tan\Theta(U^{(n)}, U_*)\|_{\mathrm{F}}^2; \mathbb{H}\} \leqslant (1-\beta\gamma)^{2(n-1)}p\phi^2 d + \frac{32\psi^4\beta}{2-\lambda_1\beta}\varphi(p,d;\Lambda) \\ + C_\circ\kappa^4\mu_p^{-2}\eta_p^2\gamma^{-1}p\sqrt{d-p}\,\beta^{3/2-7\varepsilon},\end{aligned} \tag{4.10}$$

where $\mathrm{e} = \exp(1)$ *is Euler's number,* $C_{\nu\psi} = \max\{C_\nu\mu_p, C_\psi\min\{\psi^{-1}, \psi^{-2}\}\}$ *and*

$$\varphi(p,d;\Lambda) := \sum_{j=1}^{p}\sum_{i=p+1}^{d}\frac{\lambda_j\lambda_i}{\lambda_j-\lambda_i} \in \left[\frac{p(d-p)\lambda_1\lambda_d}{\lambda_1-\lambda_d}, \frac{p(d-p)\lambda_p\lambda_{p+1}}{\lambda_p-\lambda_{p+1}}\right]. \tag{4.11}$$

Remark 4.4. (1) Although an interval is presented in (4.11) to bound $\varphi(p,d;\Lambda)$, there are more informative ones under additional assumptions on the random vector $\boldsymbol{X}$. For example, in some of the past works [3–5, 7, 16, 21, 22, 27], it is assumed $\sum_{i=1}^{d}\lambda_i = \mathrm{E}\{\|\boldsymbol{X}\|_2^2\} \leqslant c$ for some constant c, independent of the dimension d. Then

$$\varphi(p,d;\Lambda) = \sum_{j=1}^{p}\sum_{i=p+1}^{d}\frac{\lambda_j\lambda_i}{\lambda_j-\lambda_i} \leqslant \frac{1}{\lambda_p-\lambda_{p+1}}\sum_{j=1}^{p}\sum_{i=p+1}^{d}\lambda_j\lambda_i \leqslant \frac{1}{\gamma}\left(\sum_{j=1}^{p}\lambda_j\right)\left(c - \sum_{i=1}^{p}\lambda_i\right) \leqslant \frac{c^2}{4\gamma}. \tag{4.12}$$

As a result, the second term on the right-hand side of (4.10) is of $O(\beta)$. Under the same assumption, after a careful check (of Appendix A.2), the third term can be ensured of $O(\beta)$, too, by making $7\varepsilon \leqslant 1/2$. Both terms do not go to 0 as $n \to \infty$, as we would like to ideally have. Nonetheless, we argue that it does not diminish the usefulness of the error bound. Here is the reason. Like in any iterative method, the ultimate goal is to drive the approximation error down to a prescribed level. Since the terms are of $O(\beta)$, given a prescribed error tolerance, we can always take the stepsize β in the same order of the tolerance to yield an eventual approximation to the subspace within the desired error level.

(2) Theorem 4.3 involves a set of pre-chosen constant parameters: ϵ, ω, ϕ, κ and β subject to the inequalities in (4.6) so that $K[(2+\mathrm{e})d+p+1]\exp(-C_{\nu\psi}\beta^{-\varepsilon})$ is sufficiently tiny to make $\mathbb{H}$ a high-probability event. For that reason n is limited to no bigger than K. Ideally, the event $\mathbb{H}$ should exist with high probability for all sufficiently large n. According to our proof, the theorem remains valid with simply setting K to n:

$$n > N_{3/2-37\varepsilon/4}(\beta), \quad \mathrm{P}(\mathbb{H}) \geqslant 1 - n[(2+\mathrm{e})d+p+1]\exp(-C_{\nu\psi}\beta^{-\varepsilon}), \tag{4.9$'$}$$

everything else being equal. This means that with any given constant parameters, there is no guarantee that $\mathbb{H}$ is still a high-probability event if n is too large. While this is not ideal, we argue that if the number n of samples or some rough range of it is known, we can always optimize these constant parameters, by making β small enough, so that $n[(2+\mathrm{e})d+p+1]\exp(-C_{\nu\psi}\beta^{-\varepsilon})$ is still tiny to render a high-probability event $\mathbb{H}$. For example, in Theorem 4.5, we specify what is needed on the constant parameters. We point out in passing that the results in [19] for the vector online PCA also require that the number n of samples be bounded from above.

One subtlety in bounding $\mathrm{P}(\mathbb{H})$ from below as in (4.9$'$) is that now the event $\mathbb{H}$ depends on n. Theorem 4.2 as stated with the preset K ensures one high-probability event $\mathbb{H}$ for all $n \in [N_{3/2-37\varepsilon/4}(\beta), K]$. From the practical point of view, the number of samples is always finite, i.e., such a K does exist, and one might have some idea about what it is. When we do, the constant parameters can be judiciously chosen to ensure $K[(2+\mathrm{e})d+p+1]\exp(-C_{\nu\psi}\beta^{-\varepsilon})$ tiny.

(3) This remark applies to Theorem 4.5 later as well.

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1) We attach each with a subscript for the convenience of indicating their associations. They do not change as the values of the subscript variables vary, by which we mean *absolute constants*. Later in (5.6), we explicitly bound these absolute constants.

Theorem 4.3 assumes a somewhat accurate initial subspace $U^{(0)}$, i.e., satisfying (4.7) which is not very restrictive because $\phi^2 d - 1$ can be very big for huge d. As we mentioned earlier, often we do not have a good initial subspace, in which case, we may simply resort to a randomly selected $U^{(0)}$.

Consider the uniform distribution on $\mathbb{G}_p(\mathbb{R}^d)$, the one with the Haar invariant probability measure (see [9, Subsection 1.4] and [17, Subsection 4.6]). We are interested in a randomly selected $U^{(0)}$ such that

$$\mathcal{R}(U^{(0)}) \text{ is uniformly sampled from } \mathbb{G}_p(\mathbb{R}^d). \tag{4.13}$$

The reader is referred to [9, Subsection 2.2] on how to generate such a uniform distribution on $\mathbb{G}_p(\mathbb{R}^d)$.

Theorem 4.5. *Under Assumption* 4.2*, for sufficiently large d and any β satisfying* (4.6) *with*

$$\kappa = 6^{[M(\varepsilon)-1]/2} \max\{2C_p, \sqrt{2}\},$$

and

$$p < (d+1)/2, \quad \varepsilon \in (0, 1/7), \quad \delta \in (0, 2^{-1/p^2}), \quad K > N_{3/2-37\varepsilon/4}(\beta),$$

where C_p is a constant only dependent on p, if (4.13) *holds, and*

$$d\beta^{1-3\varepsilon} \leqslant \delta^2, \quad K[(2+\mathrm{e})d + p + 1]\exp(-C_{\nu\psi}\beta^{-\varepsilon}) \leqslant \delta^{p^2},$$

then there exists a high-probability event $\mathbb{H}_*$ with $\mathrm{P}\{\mathbb{H}_*\} \geqslant 1 - 2\delta^{p^2}$ such that

$$\begin{aligned} \mathrm{E}\{\|\tan\Theta(U^{(n)}, U_*)\|_{\mathrm{F}}^2; \mathbb{H}_*\} \leqslant (1-\beta\gamma)^{2(n-1)} p\, C_p^2 \delta^{-2} d + \frac{32\psi^4\beta}{2-\lambda_1\beta}\varphi(p, d; \Lambda) \\ + C_\circ \kappa^4 \mu_p^{-2} \eta_p^2 \gamma^{-1} p \sqrt{d-p}\,\beta^{3/2-7\varepsilon} \end{aligned} \tag{4.14}$$

for any $n \in [N_{3/2-37\varepsilon/4}(\beta), K]$, where $\varphi(p, d; \Lambda)$ is as in (4.11)*.*

Our third main result is about picking a nearly optimal stepsize β for the nearly optimal convergence rate, and assume that the sample size is reasonably large and fixed at N_*. The idea is to pick a good β to balance the terms on the right-hand side of (4.14) subject to $N_* \geqslant N_{3/2}(\beta)$ (and thus we also need a large enough number of samples). The nearly optimal stepsize β is

$$\beta = \beta_* := \frac{3\ln N_*}{2\gamma N_*}, \tag{4.15}$$

which is consistent with the choice in [19] for $p = 1$.

Theorem 4.6. *Under Assumption* 4.2*, for sufficiently large $d \geqslant 2p$ and a sufficiently large number N_* of samples, $\varepsilon \in (0, 1/7)$, $\delta \in (0, 2^{-1/p^2})$ satisfying*

$$d\beta_*^{1-3\varepsilon} \leqslant \delta^2, \quad N_*[(2+\mathrm{e})d + p + 1]\exp(-C_{\nu\psi}\beta_*^{-\varepsilon}) \leqslant \delta^{p^2}, \tag{4.16}$$

where β_* is given by (4.15)*, if* (4.13) *holds, then there exists a high-probability event $\mathbb{H}_*$ with $\mathrm{P}\{\mathbb{H}_*\} \geqslant 1 - 2\delta^{p^2}$ such that*

$$\mathrm{E}\{\|\tan\Theta(U^{(N_*)}, U_*)\|_{\mathrm{F}}^2; \mathbb{H}_*\} \leqslant C_*(d, N_*, \delta)\frac{\varphi(p, d; \Lambda)}{\lambda_p - \lambda_{p+1}}\frac{\ln N_*}{N_*}, \tag{4.17}$$

where the constant $C_*(d, N_*, \delta) \to 24\psi^4$ as $d \to \infty$, $N_* \to \infty$, and $\varphi(p, d; \Lambda)$ is as in (4.11)*.*

In Theorems 4.3, 4.5 and 4.6, the conclusions are stated in term of the expectation of $\|\tan\Theta(U^{(n)}, U_*)\|_{\mathrm{F}}^2$ over some high-probability event. These expectations can be turned into conditional expectations, thanks to the relation (1.1). In fact, (4.4) is a consequence of (4.17) and (1.1).

4.2 Discussions of new proving techniques

Our three theorems in the previous subsection, namely Theorems 4.3, 4.5 and 4.6, are the analogs for $p > 1$ of Li et al.'s three theorems [19, Theorems 1–3] which are for $p = 1$ only. Naturally, we know how our results are when applied to the case $p = 1$ and our proofs would stand against those in [19]. We choose to compare our results with those in [19] because Li et al. [19] dealt with sub-Gaussian samples whereas other existing works in the literature studied the vector/subspace online PCA for bounded samples only. In what follows, we will do a fairly detailed comparison. Before we do that, let us state their theorems (in our notation).

Theorem 4.7 (See [19, Theorem 1]). *Under Assumption* 4.2 *and* $p = 1$*, suppose that there exists a constant* $\phi > 1$ *such that* $\tan\Theta(U^{(0)}, U_*) \leqslant \phi^2 d$*. Let*

$$\widehat{N}^{\rm o}(\beta,\phi) := \min\{n\in\mathbb{N} : (1-\beta\gamma)^n \leqslant [4\phi^2 d]^{-1}\} = \left\lceil \frac{-\ln[4\phi^2 d]}{\ln(1-\beta\gamma)}\right\rceil,$$

$$\widehat{N}_s(\beta) := \min\{n\in\mathbb{N} : (1-\beta\gamma)^n \leqslant [\lambda_1^2\gamma^{-1}\beta]^s\} = \left\lceil \frac{s\ln[\lambda_1^2\gamma^{-1}\beta]}{\ln(1-\beta\gamma)}\right\rceil.$$

Then for any $\varepsilon \in (0, 1/8)$*, the stepsize* $\beta > 0$ *satisfying* $d[\lambda_1^2\gamma^{-1}\beta]^{1-2\varepsilon} \leqslant b_1\phi^{-2}$*, and for any* $t > 1$*, there exists an event* $\mathbb{H}$ *with*

$$\mathrm{P}\{\mathbb{H}\} \geqslant 1 - 2(d+2)\widehat{N}^{\rm o}(\beta,\phi)\exp(-C_0[\lambda_1^2\gamma^{-1}\beta]^{-2\varepsilon}) - 4d\widehat{N}_t(\beta)\exp(-C_1[\lambda_1^2\gamma^{-1}\beta]^{-2\varepsilon}),$$

such that for any $n \in [\widehat{N}_1(\beta) + \widehat{N}^{\rm o}(\beta,\phi), \widehat{N}_t(\beta)]$*,*

$$\mathrm{E}\{\tan^2\Theta(U^{(n)}, U_*); \mathbb{H}\} \leqslant (1-\beta\gamma)^{2[n-\widehat{N}^{\rm o}(\beta,\phi)]} + C_2\beta\varphi(1,d;\Lambda) + C_2\sum_{i=2}^{d}\frac{\lambda_1-\lambda_2}{\lambda_1-\lambda_i}[\lambda_1^2\gamma^{-1}\beta]^{3/2-4\varepsilon}, \quad (4.18)$$

where $b_1 \in (0, \ln^2, 2/16)$*, and* C_0*,* C_1 *and* C_2 *are absolute constants.*

We can see that Theorem 4.3 for $p = 1$ is essentially the same as Theorem 4.7. In fact, since $(1-\beta\gamma)^{1-\widehat{N}^{\rm o}(\beta,\phi)} \leqslant 4\phi^2 d \leqslant (1-\beta\gamma)^{-\widehat{N}^{\rm o}(\beta,\phi)}$, the upper bounds by (4.10) for $p = 1$ and by (4.18) are comparable in the sense that they are in the same order in d, β and δ. Naturally one may try to generalize the proving technique in [19] which is for the one-dimensional case ($p = 1$) to handle the multi-dimensional case ($p > 1$). Indeed, we tried but did not succeed, due to the reason that we believe there are insurmountable obstacles. In fact, one of the key steps in proof works for $p = 1$ but does not seem to work for $p > 1$. Next, we explain these obstacles in details.

The basic structure of the proof in [19] is to split the Grassmann manifold $\mathbb{G}_p(\mathbb{R}^d)$, from where the initial guess comes, into two regions: the *cold region* and the *warm region*. Roughly speaking, an approximation $U^{(n)}$ in the warm region means that $\|\tan\Theta(U^{(n)}, U_*)\|_{\rm F}$ is small while in the cold region it means that $\|\tan\Theta(U^{(n)}, U_*)\|_{\rm F}$ is not that small. U_* sits at the "*center*" of the warm region which is wrapped around by the cold region. The proof is divided into two cases: the first case is when the initial guess is in the warm region and the other one is when it is in the cold region. For the first case, they proved that the algorithm will produce a sequence convergent to the principal subspace (which is actually the most significant principal component because it is for $p = 1$) with high probability. For the second case, they first proved that the algorithm will produce a sequence of approximations that, after a finite number of iterations, will fall into the warm region with high probability, and then use the conclusion proved for the first case to conclude the proof due to the Markov property.

For our situation $p > 1$, we still structure our proof in the same way, i.e., dividing the whole proof into two cases: $U^{(0)}$ coming from the *cold region* or the *warm region*. The proof in [19] for the warm region case can be carried over with a little extra effort, as we will see later, but it was not possible for us to use a similar argument in [19] to obtain the job done for the cold region case. Three major difficulties are as follows.

(1) In [19], essentially $\|\cot\Theta(U^{(n)}, U_*)\|_{\rm F}$ was used to track the behavior of a martingale along with the power iteration. Note that $\cot\Theta(U^{(n)}, U_*)$ is $p \times p$. Thus it is a scalar when $p = 1$, perfectly well-conditioned if treated as a matrix, but for $p > 1$, it is a genuine matrix and, in fact, an inverse of a

random matrix in the proof. The first difficulty is how to estimate the inverse because it may not even exist.

(2) We tried to separate the flow of $U^{(n)}$ into two subflows: the ill-conditioned flow and the well-conditioned flow, and estimate the related quantities separately. Here, the ill-conditioned flow at each step represents the subspace generated by the singular vectors of $\cot\Theta(U^{(n)}, U_*)$ whose corresponding singular values are tiny, while the well-conditioned flow at each step represents the subspace generated by the other singular vectors, of which the inverse (restricted to this subspace) is well conditioned. Unfortunately, tracking the two flows can be an impossible task because, due to the randomness, some elements in the ill-conditioned flow could jump to the well-conditioned flow during the iteration and vice versa.

(3) The third one is to build a martingale to go along with a proper power iteration, or equivalently, to find the Doob decomposition of the process, because the recursion formula of the main part of the inverse—the drift in the Doob decomposition, even if limited to the well-conditioned flow—is not a linear operator, which makes it impossible to build a proper power iteration.

In the end, to deal with the cold region, we give up the idea of estimating $\|\cot\Theta(U^{(n)}, U_*)\|_{\mathrm{F}}$. Instead, we invent another method: cutting the cold region into many layers, each wrapped around by another with the innermost one around the warm region. We prove the initial guess in any layer will produce a sequence of approximations that will fall into its inner neighbor layer (or the warm region if the layer is innermost) in a finite number of iterations with high probability. Therefore eventually, any initial guess in the cold region will lead to an approximation in the warm region within a finite number of iterations with high probability, returning to the case of initial guesses coming from the warm region because of the Markov property. This enables us to completely avoid the difficulties mentioned above. This technique works for $p = 1$, too, and it can result in a simpler proof for the online PCA than that in [19].

The other two main theorems of Li et al. [19, Theorems 2 and 3] are stated as follows.

Theorem 4.8 (See [19, Theorem 2]). *Under Assumption* 4.2 *and* $p = 1$*, suppose that* $U^{(0)}$ *is uniformly sampled from the unit sphere. Then for any* $\varepsilon \in (0, 1/8)$*, the stepsize* $\beta > 0$ *and* $\delta > 0$ *satisfying*

$$d[\lambda_1^2\gamma^{-1}\beta]^{1-2\varepsilon} \leqslant b_2\delta^2, \quad 4d\widehat{N}_2(\beta)\exp(-C_3[\lambda_1^2\gamma^{-1}\beta]^{-2\varepsilon}) \leqslant \delta,$$

there exists an event $\mathbb{H}_*$ *with* $\mathrm{P}\{\mathbb{H}_*\} \geqslant 1 - 2\delta$ *such that for any* $n \in [\widehat{N}_2(\beta), \widehat{N}_3(\beta)]$,

$$\mathrm{E}\{\tan^2\Theta(U^{(n)}, U_*); \mathbb{H}_*\} \leqslant C_4(1-\beta\gamma)^{2n}\delta^{-4}d^2 + C_4\beta\varphi(1, d; \Lambda) + C_4\sum_{i=2}^{d}\frac{\lambda_1 - \lambda_2}{\lambda_1 - \lambda_i}[\lambda_1^2\gamma^{-1}\beta]^{3/2-4\varepsilon}, \quad (4.19)$$

where b_2*,* C_3 *and* C_4 *are absolute constants.*

Theorem 4.9 (See [19, Theorem 3]). *Under Assumption* 4.2 *and* $p = 1$*, suppose that* $U^{(0)}$ *is uniformly sampled from the unit sphere and let* $\beta_* = \frac{2\ln N_*}{\gamma N}$*. Then for any* $\varepsilon \in (0, 1/8)$*,* $N_* \geqslant 1$ *and* $\delta > 0$ *satisfying*

$$d[\lambda_1^2\gamma^{-1}\beta_*]^{1-2\varepsilon} \leqslant b_3\delta^2, \quad 4d\widehat{N}_2(\beta_*)\exp(-C_6[\lambda_1^2\gamma^{-1}\beta_*]^{-2\varepsilon}) \leqslant \delta,$$

there exists an event $\mathbb{H}_*$ *with* $\mathrm{P}\{\mathbb{H}_*\} \geqslant 1 - 2\delta$ *such that*

$$\mathrm{E}\{\tan^2\Theta(U^{(N_*)}, U_*); \mathbb{H}_*\} \leqslant C_*(d, N_*, \delta)\frac{\varphi(1, d; \Lambda)}{\lambda_1 - \lambda_2}\frac{\ln N_*}{N_*}, \quad (4.20)$$

where the constant $C_*(d, N_*, \delta) \to C_5$ *as* $d \to \infty$*,* $N_* \to \infty$*, and* b_3*,* C_5 *and* C_6 *are absolute constants.*

Our Theorems 4.5 and 4.6 when applied to the case $p = 1$ do not exactly yield Theorems 4.8 and 4.9, respectively. But the resulting conditions and upper bounds have the same orders in constant parameters d, β and δ, and the coefficients of β and $\frac{\ln N_*}{N}$ in the upper bounds are comparable. Note that the first term on the right-hand side of (4.14) is proportional to d, not d^2 as in (4.19), and hence ours is tighter for high-dimensional data.

Our proofs for Theorems 4.5 and 4.6 are nearly the same as those in [19] for Theorems 4.8 and 4.9 owing to the fact that the difficult estimates have already been taken care of by either Theorem 4.3

or Theorem 4.7. But still there are some extras for $p > 1$, namely, the need to estimate the marginal probability for the uniform distribution on the Grassmann manifold of dimension higher than 1. We are not aware of anything like that in the literature, and thus have to build it ourselves with the help of the theory of special functions of a matrix argument, rarely used in the statistical community.

It may also be worth pointing out that all the absolute constants, except C_p which has an explicit expression in (6.3) and C_ψ, in our theorems will be explicitly bounded as in (5.6), whereas those in Theorems 4.7–4.9 are not.

5 Proof of Theorem 4.3

We start by building a substantial amount of preparation material in Subsections 5.1–5.3 before we prove the theorem in Subsection 5.4. In Subsection 5.1, we set the stage and introduce the matrix $T^{(n)}$ to serve the role of $\tan\Theta(U^{(n)}, U_*)$ associated with the n-th approximation. In particular, we have $\|T^{(n)}\|_{\rm ui} = \|\tan\Theta(U^{(n)}, U_*)\|_{\rm ui}$. In Subsection 5.2, we present incremental estimates for one iterative step of the subspace online PCA in Lemmas 5.2 and 5.3. These estimates allow us to associate one iterative step with a quasi-power iterative step by an operator $\mathcal{L}$ defined at the beginning of Subsection 5.3, and then further we relate $T^{(n)}$ to $\mathcal{L}^n T^{(0)}$ by showing $T^{(n)} - \mathcal{L}^n T^{(0)}$ is bounded with high probability in Lemma 5.4. This lemma is very critical to our proofs. It leads to Lemma 5.5 which says that $\|T^{(n)}\|_2$ stagedly decreases and Lemma 5.6 in which the expectation of $T^{(n)}$ is estimated. Finally, we are ready to prove Theorem 4.3 in Subsection 5.4. Figure 1 shows a pictorial description of our proving process.

5.1 Simplification

Without loss of generality, we may assume that the covariance matrix Σ is diagonal. Otherwise, we can perform a (constant) orthogonal transformation as follows. Recall the spectral decomposition $\Sigma = U\Lambda U^{\rm T}$ in (4.1). Instead of the random vector $\boldsymbol{X}$, we equivalently consider $\boldsymbol{Y} \equiv [\boldsymbol{Y}_1, \boldsymbol{Y}_2, \ldots, \boldsymbol{Y}_n]^{\rm T} =: U^{\rm T}\boldsymbol{X}$. Accordingly, perform the same orthogonal transformation on all the involved quantities:

$$Y^{(n)} = U^{\rm T} X^{(n)}, \quad V^{(n)} = U^{\rm T} U^{(n)}, \quad V_* = U^{\rm T} U_* = \begin{bmatrix} I_p \\ 0 \end{bmatrix}. \tag{5.1}$$

As a consequence, we have equivalent versions of Algorithm 1 and Theorems 4.3, 4.5 and 4.6. Firstly, because

$$(V^{(n-1)})^{\rm T} Y^{(n)} = (U^{(n-1)})^{\rm T} X^{(n)} = Z^{(n)}, \quad (Y^{(n)})^{\rm T} Y^{(n)} = (X^{(n)})^{\rm T} X^{(n)},$$

the equivalent version of Algorithm 1 is obtained by symbolically replacing all the letters X and U by Y and V, respectively, while keeping their respective superscripts. If the algorithm converges, it is expected that $\mathcal{R}(V^{(n)}) \to \mathcal{R}(V_*)$. Secondly, noting

$$\|\Sigma^{-1/2}\boldsymbol{X}\|_{\psi_2} = \|U\Lambda^{-1/2}U^{\rm T}\boldsymbol{X}\|_{\psi_2} = \|\Lambda^{-1/2}\boldsymbol{Y}\|_{\psi_2},$$

we can restate Assumption 4.2 equivalently as

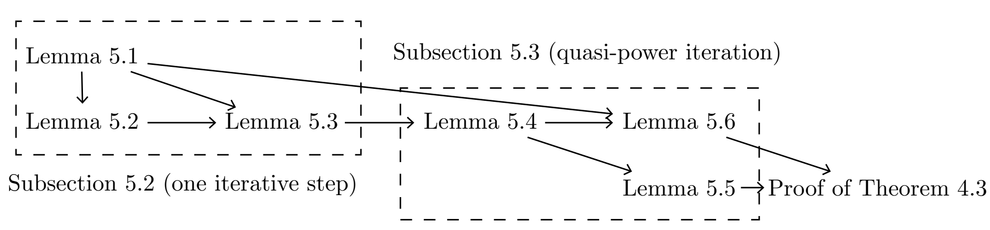

Figure 1 Proving process for Theorem 4.3

(A-1′) $\mathrm{E}\{\boldsymbol{Y}\}=0$ and $\mathrm{E}\{\boldsymbol{Y}\boldsymbol{Y}^{\mathrm{T}}\}=\Lambda=\mathrm{diag}(\lambda_1,\ldots,\lambda_d)$ with (4.2);
(A-2′) $\psi:=\|\Lambda^{-1/2}\boldsymbol{Y}\|_{\psi_2}<\infty$.
Thirdly, all the canonical angles between two subspaces are invariant under the orthogonal transformation. Therefore, the equivalent versions of Theorems 4.3, 4.5 and 4.6 for $\boldsymbol{Y}$ can be simply obtained by replacing all letters X and U by Y and V, respectively, while keeping their respective superscripts.

In what follows, we assume that Σ is diagonal. In the rest of this section, we prove the mentioned equivalent version of Theorem 4.3. Likewise in the next section, we prove the equivalent versions of Theorems 4.5 and 4.6.

To facilitate our proof, we introduce new notations for two particular submatrices of any $V\in\mathbb{R}^{d\times p}$:

$$\bar{V}=V_{(1:p,:)},\quad \underline{V}=V_{(p+1:d,:)}. \tag{5.2}$$

In particular, $\mathscr{T}(V)=\underline{V}\bar{V}^{-1}$ for the operator $\mathscr{T}$ defined in (1.2), provided that $\bar{V}$ is nonsingular. Set

$$\bar{\Lambda}=\mathrm{diag}(\lambda_1,\ldots,\lambda_p),\quad \underline{\Lambda}=\mathrm{diag}(\lambda_{p+1},\ldots,\lambda_d). \tag{5.3}$$

Although the assignments to $\bar{\Lambda}$ and $\underline{\Lambda}$ are not consistent with the extractions defined by (5.2), they do not seem to cause confusions in our later presentations.

For $\kappa>1$, define $\mathbb{S}(\kappa):=\{V\in\mathbb{R}^{d\times p}:\sigma(\bar{V})\subset[\frac{1}{\kappa},1]\}$, where $\sigma(\bar{V})$ is the set of the singular values of $\bar{V}$. It can be verified that

$$V\in\mathbb{S}(\kappa)\Leftrightarrow\|\mathscr{T}(V)\|_2\leqslant\sqrt{\kappa^2-1}. \tag{5.4}$$

For the sequence $V^{(n)}$, define

$$N_{\mathrm{out}}\{\mathbb{S}(\kappa)\}:=\min\{n:V^{(n)}\notin\mathbb{S}(\kappa)\},\quad N_{\mathrm{in}}\{\mathbb{S}(\kappa)\}:=\min\{n:V^{(n)}\in\mathbb{S}(\kappa)\}.$$

$N_{\mathrm{out}}\{\mathbb{S}(\kappa)\}$ is the first step of the iterative process at which $V^{(n)}$ jumps from $\mathbb{S}(\kappa)$ to its outside, and $N_{\mathrm{in}}\{\mathbb{S}(\kappa)\}$ is the first step of the iterative process at which $V^{(n)}$ jumps from the outside to $\mathbb{S}(\kappa)$. Write

$$\widetilde{\lambda}_i:=\lambda_i\beta^{-2\varepsilon},\quad \widetilde{\eta}_i:=\widetilde{\lambda}_1+\cdots+\widetilde{\lambda}_i=\eta_i\beta^{-2\varepsilon},$$

and define

$$N_{\mathrm{qb}}\{\Lambda\}:=\max\{n\geqslant1:\|Z^{(n)}\|_2\leqslant\widetilde{\eta}_p^{1/2},|Y_i^{(n)}|\leqslant\widetilde{\lambda}_i^{1/2},i=1,\ldots n\}+1, \tag{5.5}$$

where $Z^{(n)}=(U^{(n-1)})^{\mathrm{T}}X^{(n)}$ is as defined in Algorithm 1. $N_{\mathrm{qb}}\{\Lambda\}$ is the first step of the iterative process at which either $|Y_i^{(n)}|>\widetilde{\lambda}_i^{1/2}$ for some i or the norm of $Z^{(n)}$ exceeds $\widetilde{\eta}_p^{1/2}$. For $n<N_{\mathrm{qb}}\{\Lambda\}$, we have

$$\|Y^{(n)}\|_2\leqslant\widetilde{\eta}_d^{1/2}=\nu^{1/2}\widetilde{\eta}_p^{1/2},\quad \|Z^{(n)}\|_2\leqslant\widetilde{\eta}_p^{1/2}\quad\text{with }\nu=1/\mu_p.$$

For convenience, we introduce $T^{(n)}=\mathscr{T}(V^{(n)})$, and let $\mathbb{F}_n=\sigma\{Y^{(1)},\ldots,Y^{(n)}\}$ be the σ-algebra filtration, i.e., the information known by step n. Also, since in this section, ε and β are fixed, we suppress the dependency information of $M(\varepsilon)$ on ε and $N_s(\beta)$ on β to simply write M for $M(\varepsilon)$ and N_s for $N_s(\beta)$.

Lastly, we discuss some of the important implications of the conditions:

$$0<\beta<\min\left\{1,\left(\frac{1}{8\kappa\eta_p}\right)^{\frac{2}{1-4\varepsilon}},\left(\frac{\gamma}{130\kappa^2\eta_p^2}\right)^{\frac{1}{\varepsilon}}\right\}, \tag{4.6}$$

$$(\sqrt{2}+1)\lambda_1 d\beta^{1-7\varepsilon}\leqslant\omega,\quad K>N_{3/2-37\varepsilon/4}(\beta) \tag{4.8}$$

of Theorem 4.3. They guarantee that
(β-1) $\beta<1$;
(β-2) $\beta\gamma\leqslant\beta\widetilde{\eta}_p\leqslant\nu\beta\widetilde{\eta}_p=\beta\widetilde{\eta}_d\leqslant d\beta\widetilde{\lambda}_1=d\lambda_1\beta^{1-2\varepsilon}\leqslant(\sqrt{2}-1)\omega\leqslant\sqrt{2}-1$.
Set

$$C_V=\frac{5}{2}+\frac{7}{2}(\nu\widetilde{\eta}_p\beta)+\frac{15}{8}(\nu\widetilde{\eta}_p\beta)^2+\frac{3}{8}(\nu\widetilde{\eta}_p\beta)^3\leqslant\frac{16+13\sqrt{2}}{8}\approx4.298, \tag{5.6a}$$

$$C_\Delta = 2 + \frac{1}{2}(\nu\widetilde{\eta}_p\beta) + C_V\widetilde{\eta}_p\beta \leqslant \frac{22+7\sqrt{2}}{8} \approx 3.987, \tag{5.6b}$$

$$C_T = C_V + 2C_\Delta + 2C_\Delta C_V\widetilde{\eta}_p\beta \leqslant \frac{251+122\sqrt{2}}{16} \approx 26.471, \tag{5.6c}$$

$$C_\kappa = \frac{(3-\sqrt{2})C_\Delta^2}{64(C_T+2C_\Delta)^2} \leqslant \frac{565+171\sqrt{2}}{21504} \approx 0.038, \tag{5.6d}$$

$$C_\nu = 4\sqrt{2}C_T C_\kappa \leqslant \frac{223702+183539\sqrt{2}}{86016} \approx 5.618, \tag{5.6e}$$

$$\begin{aligned} C_\circ &= \frac{29+8\sqrt{2}}{16(3-\sqrt{2})} + \frac{4C_T}{(3-\sqrt{2})C_\Delta}\beta^{3\varepsilon} + [C_T + \frac{29+8\sqrt{2}}{32}]\beta^{1/2-3\varepsilon} \\ &\quad + \frac{3C_T^2}{2(3-\sqrt{2})C_\Delta^2}\beta^{1/2+3\varepsilon} + \frac{2C_T}{C_\Delta}\beta^{1-3\varepsilon} + \frac{C_T^2}{2C_\Delta^2}\beta^{3/2-3\varepsilon} \\ &\leqslant \frac{2582968+1645155\sqrt{2}}{14336} \approx 342.464. \end{aligned} \tag{5.6f}$$

The condition (4.6) also guarantees that

(β-3) $2C_\Delta\widetilde{\eta}_p\beta^{1/2}\kappa = 2C_\Delta\eta_p\beta^{1/2-2\varepsilon}\kappa \leqslant \frac{2C_\Delta}{8} < 1$, and thus $2C_\Delta\widetilde{\eta}_p\beta\kappa < 1$;

(β-4) $4\sqrt{2}C_T\kappa^2\widetilde{\eta}_p^2\gamma^{-1}\beta^{5\varepsilon} \leqslant 1$, and thus $4\sqrt{2}C_T\kappa^2\widetilde{\eta}_p^2\gamma^{-1}\beta^{1/2+\chi} \leqslant 1$ for $\chi \in [-1/2+5\varepsilon, 0]$.

5.2 Increments by one iterative step

Lemma 5.1. *For any fixed integer $K \geqslant 1$,*

$$\mathrm{P}\{N_{\mathrm{qb}}\{\Lambda\} > K\} \geqslant 1 - K(\mathrm{e}d+p+1)\exp(-C_\psi\min\{\psi^{-1},\psi^{-2}\}\beta^{-2\varepsilon}),$$

where C_ψ is an absolute constant.

Proof. Since $\{N_{\mathrm{qb}}\{\Lambda\} \leqslant K\} \subset \bigcup_{n\leqslant K}(\{\|Z^{(n)}\|_2 \geqslant \widetilde{\eta}_p^{1/2}\} \cup \bigcup_{i=1}^d\{|e_i^{\mathrm{T}}Y^{(n)}| \geqslant \widetilde{\lambda}_i^{1/2}\})$, we know

$$\mathrm{P}\{N_{\mathrm{qb}}\{\Lambda\} \leqslant K\} \leqslant \sum_{n\leqslant K}\left(\mathrm{P}\{\|Z^{(n)}\|_2 \geqslant \widetilde{\eta}_p^{1/2}\} + \sum_{1\leqslant i\leqslant d}\mathrm{P}\{|e_i^{\mathrm{T}}Y^{(n)}| \geqslant \widetilde{\lambda}_i^{1/2}\}\right). \tag{5.7}$$

First,

$$\begin{aligned} \mathrm{P}\{|e_i^{\mathrm{T}}Y^{(n)}| \geqslant \widetilde{\lambda}_i^{1/2}\} &= \mathrm{P}\left\{\left|\frac{(\Lambda^{1/2}e_i)^{\mathrm{T}}}{\|\Lambda^{1/2}e_i\|_2}\Lambda^{-1/2}Y^{(n)}\right| \geqslant \frac{\widetilde{\lambda}_i^{1/2}}{\|\Lambda^{1/2}e_i\|_2}\right\} \\ &\leqslant \exp\left(1 - \frac{C_{\psi,i}\frac{\widetilde{\lambda}_i}{e_i^{\mathrm{T}}\Lambda e_i}}{\|\frac{(\Lambda^{1/2}e_i)^{\mathrm{T}}}{\|\Lambda^{1/2}e_i\|_2}\Lambda^{-1/2}Y^{(n)}\|_{\psi_2}}\right) \text{ (by [31, (5.10)])} \\ &\leqslant \exp\left(1 - \frac{C_{\psi,i}\widetilde{\lambda}_i}{\|\Lambda^{-1/2}Y^{(n)}\|_{\psi_2}\lambda_i}\right) = \exp(1 - C_{\psi,i}\psi^{-1}\beta^{-2\varepsilon}), \end{aligned} \tag{5.8}$$

where $C_{\psi,i}$, $i=1,\ldots,d$ are absolute constants [31, (5.10)]. Next, we claim

$$\mathrm{P}\{\|Z^{(n)}\|_2 \geqslant \widetilde{\eta}_p^{1/2}\} \leqslant (p+1)\exp(-C_{\psi,d+1}\psi^{-2}\beta^{-2\varepsilon}) \tag{5.9}$$

to be proven in the next paragraph. Together, (5.7)–(5.9) yield

$$\begin{aligned} \mathrm{P}\{N_{\mathrm{qb}}\{\Lambda\} \leqslant K\} &= \sum_{n\leqslant K}\sum_{1\leqslant i\leqslant d}\exp(1 - C_{\psi,i}\psi^{-1}\beta^{-2\varepsilon}) + \sum_{n\leqslant K}(p+1)\exp(-C_{\psi,d+1}\psi^{-2}\beta^{-2\varepsilon}) \\ &\leqslant K(\mathrm{e}d+p+1)\exp(-C_\psi\min\{\psi^{-1},\psi^{-2}\}\beta^{-2\varepsilon}), \end{aligned}$$

where $C_\psi = \min_{1\leqslant i\leqslant d+1}C_{\psi,i}$. Finally, use $\mathrm{P}\{N_{\mathrm{qb}}\{\Lambda\} > K\} = 1 - \mathrm{P}\{N_{\mathrm{qb}}\{\Lambda\} \leqslant K\}$ to complete the proof.

It remains to prove (5.9). To avoid the cluttered superscripts, we drop the superscript "$\cdot^{(n-1)}$" on V, and drop the superscript "$\cdot^{(n)}$" on Y and Z. Consider

$$W := \begin{bmatrix} 0 & Z \\ Z^{\mathrm{T}} & 0 \end{bmatrix} = \begin{bmatrix} & V^{\mathrm{T}}Y \\ Y^{\mathrm{T}}V & \end{bmatrix} = \sum_{k=1}^{d} Y_k \begin{bmatrix} & & & v_{k1} \\ & & & \vdots \\ & & & v_{kp} \\ v_{k1} & \cdots & v_{kp} & 0 \end{bmatrix} =: \sum_{k=1}^{d} Y_k W_k,$$

where v_{ij} is the (i,j)-th entry of V and Y_k is the k-th entry of Y. By the matrix version of master tail bound [29, Theorem 3.6], for any $\alpha > 0$, we have

$$\mathrm{P}\{\|Z\|_2 \geqslant \alpha\} = \mathrm{P}\{\lambda_{\max}(W) \geqslant \alpha\} \leqslant \inf_{\theta>0} \mathrm{e}^{-\theta\alpha}\, \mathrm{trace}\exp\left(\sum_{k=1}^{d} \ln \mathrm{E}\{\exp(\theta Y_k W_k)\}\right).$$

Y is sub-Gaussian and $\mathrm{E}\{Y\} = 0$, so is Y_k. Moreover,

$$\|Y_k\|_{\psi_2} = \|e_k^{\mathrm{T}}\Lambda^{1/2}\|_2 \left\| \frac{e_k^{\mathrm{T}}\Lambda^{1/2}}{\|e_k^{\mathrm{T}}\Lambda^{1/2}\|_2} \Lambda^{-1/2} Y \right\|_{\psi_2} \leqslant \lambda_k^{1/2} \|\Lambda^{-1/2}Y\|_{\psi_2} = \lambda_k^{1/2}\psi.$$

Also, by [31, (5.12)],

$$\mathrm{E}\{\exp(\theta W_k Y_k)\} \leqslant \exp(C_{\psi,d+k}\theta^2 W_k \circ W_k \|Y_k\|_{\psi_2}^2) \leqslant \exp(c_{\psi,k}\theta^2\lambda_k\psi^2 W_k \circ W_k),$$

where $c_{\psi,k}$, $k = 1,\ldots,d$ are absolute constants. Therefore, writing $[4C_{\psi,d+1}]^{-1} = \max_{1\leqslant k\leqslant d} c_{\psi,k}$ and $W_\psi := \sum_{k=1}^{d} \lambda_k W_k \circ W_k$ with the spectral decomposition $W_\psi = V_\psi \Lambda_\psi V_\psi^{\mathrm{T}}$, we have

$$\begin{aligned}
\mathrm{trace}\exp\left(\sum_{k=1}^{d} \ln \mathrm{E}\{\exp(\theta Y_k W_k)\}\right) &\leqslant \mathrm{trace}\exp\left(\sum_{k=1}^{d} c_{\psi,k}\theta^2\lambda_k\psi^2 W_k \circ W_k\right) \\
&\leqslant \mathrm{trace}\exp([4C_{\psi,d+1}]^{-1}\theta^2\psi^2 W_\psi) \\
&= \mathrm{trace}\exp([4C_{\psi,d+1}]^{-1}\theta^2\psi^2 V_\psi\Lambda_\psi V_\psi^{\mathrm{T}}) \\
&= \mathrm{trace}(V_\psi \exp([4C_{\psi,d+1}]^{-1}\theta^2\psi^2\Lambda_\psi) V_\psi^{\mathrm{T}}) \\
&= \mathrm{trace}\exp([4C_{\psi,d+1}]^{-1}\theta^2\psi^2\Lambda_\psi) \\
&\leqslant (p+1)\exp([4C_{\psi,d+1}]^{-1}\theta^2\psi^2\lambda_{\max}(\Lambda_\psi)) \\
&= (p+1)\exp([4C_{\psi,d+1}]^{-1}\theta^2\psi^2\lambda_{\max}(W_\psi)).
\end{aligned}$$

Note that

$$W_\psi = \begin{bmatrix} 0 & \cdots & 0 & \sum_{k=1}^{d}\lambda_k v_{k1}^2 \\ \vdots & & \vdots & \vdots \\ 0 & \cdots & 0 & \sum_{k=1}^{d}\lambda_k v_{kp}^2 \\ \sum_{k=1}^{d}\lambda_k v_{k1}^2 & \cdots & \sum_{k=1}^{d}\lambda_k v_{kp}^2 & 0 \end{bmatrix} = \begin{bmatrix} 0 & \cdots & 0 & e_1^{\mathrm{T}}V^{\mathrm{T}}\Lambda V e_1 \\ \vdots & & \vdots & \vdots \\ 0 & \cdots & 0 & e_p^{\mathrm{T}}V^{\mathrm{T}}\Lambda V e_p \\ e_1^{\mathrm{T}}V^{\mathrm{T}}\Lambda V e_1 & \cdots & e_p^{\mathrm{T}}V^{\mathrm{T}}\Lambda V e_p & 0 \end{bmatrix},$$

and thus

$$\lambda_{\max}(W_\psi) = \left\| \begin{bmatrix} e_1^{\mathrm{T}}V^{\mathrm{T}}\Lambda V e_1 \\ \vdots \\ e_p^{\mathrm{T}}V^{\mathrm{T}}\Lambda V e_p \end{bmatrix} \right\|_2 \leqslant \sum_{k=1}^{p} e_k^{\mathrm{T}}V^{\mathrm{T}}\Lambda V e_k = \mathrm{trace}(V^{\mathrm{T}}\Lambda V) \leqslant \sum_{k=1}^{p}\lambda_k = \eta_p.$$

In summary, we have

$$\mathrm{P}\{\|Z\|_2 \geqslant \alpha\} \leqslant (p+1) \inf_{\theta>0} \exp([4C_{\psi,d+1}]^{-1}\theta^2\psi^2\eta_p - \theta\alpha) = (p+1)\exp\bigg(-\frac{C_{\psi,d+1}\alpha^2}{\psi^2\eta_p}\bigg).$$

Substituting $\alpha = \widetilde{\eta}_p^{1/2}$, we have the claim (5.9). □

Lemma 5.2. *Suppose that the conditions of Theorem* 4.3 *hold. If* $n < N_{\mathrm{qb}}\{\Lambda\}$, *then*

$$\begin{aligned} V^{(n+1)} &= V^{(n)} + \beta Y^{(n+1)}(Z^{(n+1)})^{\mathrm{T}} \\ &\quad - \beta\bigg[1 + \frac{\beta}{2}(Y^{(n+1)})^{\mathrm{T}}Y^{(n+1)}\bigg]V^{(n)}Z^{(n+1)}(Z^{(n+1)})^{\mathrm{T}} + R^{(n)}(Z^{(n+1)})^{\mathrm{T}}, \end{aligned} \tag{5.10}$$

where $R^{(n)} \in \mathbb{R}^d$ *is a random vector with* $\|R^{(n)}\|_2 \leqslant C_V\nu^{1/2}\widetilde{\eta}_p^{3/2}\beta^2$ *and* C_V *is as in* (5.6a).

Proof. To avoid the cluttered superscripts, in this proof, we drop "$\cdot^{(n)}$" and use "$\cdot^{+}$" to replace "$\cdot^{(n+1)}$" on V, and drop "$\cdot^{(n+1)}$" on Y and Z.

On the set $\{N_{\mathrm{qb}}\{\Lambda\} > n\}$, by (4.8) and ($\beta$-2), we have

$$\alpha = \beta(2+\beta Y^{\mathrm{T}}Y)Z^{\mathrm{T}}Z \leqslant \beta(2+\nu\widetilde{\eta}_p\beta)\widetilde{\eta}_p \leqslant (2+\sqrt{2}-1)(\sqrt{2}-1)/\nu < 1.$$

By Taylor's expansion, there exists $\alpha > \xi > 0$ such that

$$(1+\alpha)^{-1/2} = 1 - \frac{1}{2}\alpha + \frac{3}{8}\frac{1}{(1+\xi)^{5/2}}\alpha^2 = 1 - \beta Z^{\mathrm{T}}Z - \frac{\beta^2}{2}Y^{\mathrm{T}}YZ^{\mathrm{T}}Z + \beta^2(Z^{\mathrm{T}}Z)^2\zeta,$$

where $\zeta = \frac{3}{8}\frac{1}{(1+\xi)^{5/2}}(2+\beta Y^{\mathrm{T}}Y)^2 \leqslant \frac{3}{8}(2+\nu\beta\widetilde{\eta}_p)^2$. Thus,

$$\begin{aligned} V^{+} &= (V+\beta YZ^{\mathrm{T}})\bigg(I - \bigg[\beta Z^{\mathrm{T}}Z + \frac{\beta^2}{2}Y^{\mathrm{T}}YZ^{\mathrm{T}}Z - \beta^2(Z^{\mathrm{T}}Z)^2\zeta\bigg]\frac{ZZ^{\mathrm{T}}}{Z^{\mathrm{T}}Z}\bigg) \\ &= V + \beta YZ^{\mathrm{T}} - \beta VZZ^{\mathrm{T}} - \frac{\beta^2}{2}(Y^{\mathrm{T}}Y)VZZ^{\mathrm{T}} + RZ^{\mathrm{T}}, \end{aligned}$$

where $R = -\frac{\beta^2}{2}(Z^{\mathrm{T}}Z)(2+\beta Y^{\mathrm{T}}Y)Y + \zeta\beta^2(Z^{\mathrm{T}}Z)VZ + \zeta\beta^3(Z^{\mathrm{T}}Z)^2Y$ for which

$$\begin{aligned} \|R\|_2 &\leqslant \frac{\beta^2}{2}\widetilde{\eta}_p(2+\beta\nu\widetilde{\eta}_p)(\nu\widetilde{\eta}_p)^{1/2} + \zeta\beta^2\widetilde{\eta}_p^{3/2} + \zeta\beta^3\widetilde{\eta}_p^2(\nu\widetilde{\eta}_p)^{1/2} \\ &= \bigg[\frac{1}{2}(2+\beta\nu\widetilde{\eta}_p) + \frac{3}{8}(2+\beta\nu\widetilde{\eta}_p)^2 + \frac{3}{8}(2+\beta\nu\widetilde{\eta}_p)^2(\beta\widetilde{\eta}_p)\bigg]\nu^{1/2}\widetilde{\eta}_p^{3/2}\beta^2 \\ &= C_V\nu^{1/2}\widetilde{\eta}_p^{3/2}\beta^2, \end{aligned}$$

as expected. □

Lemma 5.3. *Suppose that the conditions of Theorem* 4.3 *hold. Let* $\tau = \|T^{(n)}\|_2$, *and* C_T *be as in* (5.6c). *If* $n < \min\{N_{\mathrm{qb}}\{\Lambda\}, N_{\mathrm{out}}\{\mathbb{S}(\kappa)\}\}$, *then we have the following*:

(1) $T^{(n)}$ *and* $T^{(n+1)}$ *are well defined.*

(2) *Define* $E_T^{(n)}(V^{(n)}) := \mathrm{E}\{T^{(n+1)} - T^{(n)} \mid \mathbb{F}_n\} - \beta(\underline{\Lambda}T^{(n)} - T^{(n)}\bar{\Lambda})$. *Then*

(a) $\sup_{V\in\mathbb{S}(\kappa)}\|E_T^{(n)}(V)\|_2 \leqslant C_T\nu^{1/2}(\widetilde{\eta}_p\beta)^2(1+\tau^2)^{3/2}$;

(b) $\|T^{(n+1)} - T^{(n)}\|_2 \leqslant \nu^{1/2}(\widetilde{\eta}_p\beta)(1+\tau^2) + C_T\nu^{1/2}(\widetilde{\eta}_p\beta)^2(1+\tau^2)^{3/2}$.

(3) *Define* $R_\circ := \mathrm{var}_\circ(T^{(n+1)} - T^{(n)} \mid \mathbb{F}_n) - \beta^2 H_\circ$. *Then*

(a) $H_\circ = \mathrm{var}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}}) \leqslant 16\psi^4 H$, *where* $H = [\eta_{ij}]_{(d-p)\times p}$ *with* $\eta_{ij} = \lambda_{p+i}\lambda_j$ *for* $i = 1,\ldots,d-p$, $j = 1,\ldots,p$;

(b) $\|R_\circ\|_2 \leqslant (\nu\widetilde{\eta}_p\beta)^2\tau(1 + \frac{11}{2}\tau + \tau^2 + \frac{1}{4}\tau^3) + 4C_T\nu(\widetilde{\eta}_p\beta)^3(1+\tau^2)^{5/2} + 2C_T^2\nu(\widetilde{\eta}_p\beta)^4(1+\tau^2)^3$.

Proof. For readability, we drop "$\cdot^{(n)}$", and use "$\cdot^{+}$" to replace "$\cdot^{(n+1)}$" for V and R, drop "$\cdot^{(n+1)}$" on Y and Z, and drop the conditional sign " $\mid \mathbb{F}_n$" in the computation of $\mathrm{E}\{\cdot\}$, $\mathrm{var}(\cdot)$ and $\mathrm{cov}(\cdot)$ with the understanding that they are conditional with respect to $\mathbb{F}_n$. Finally, for any expression or variable F, we define $\Delta F := F^+ - F$.

Consider (1). Since $n < N_{\text{out}}\{\mathbb{S}(\kappa)\}$, we have $V \in \mathbb{S}(\kappa)$ and $\tau = \|T\|_2 \leqslant (\kappa^2-1)^{1/2}$. Thus, $\|\bar{V}^{-1}\|_2 \leqslant \kappa$ and $T = \underline{V}\bar{V}^{-1}$ is well defined. Recall (5.10) and the partitioning

$$Y = \begin{array}{c} \\ {\scriptstyle p} \\ {\scriptstyle d-p} \end{array}\!\!\begin{array}{c} {\scriptstyle 1} \\ \begin{bmatrix} \bar{Y} \\ \underline{Y} \end{bmatrix} \end{array}, \quad R = \begin{array}{c} \\ {\scriptstyle p} \\ {\scriptstyle d-p} \end{array}\!\!\begin{array}{c} {\scriptstyle 1} \\ \begin{bmatrix} \bar{R} \\ \underline{R} \end{bmatrix} \end{array}.$$

We have $\Delta\bar{V} = \beta(\bar{Y}Z^{\mathrm{T}} - (1+\frac{\beta}{2}Y^{\mathrm{T}}Y)\bar{V}ZZ^{\mathrm{T}}) + \bar{R}Z^{\mathrm{T}}$ and

$$\bar{R} = -\frac{\beta^2}{2}(Z^{\mathrm{T}}Z)(2+\beta Y^{\mathrm{T}}Y)\bar{Y} + \zeta\beta^2(Z^{\mathrm{T}}Z)\bar{V}Z + \zeta\beta^3(Z^{\mathrm{T}}Z)^2\bar{Y}.$$

Noticing $\|\bar{Y}\|_2 \leqslant \widetilde{\eta}_p^{1/2}$, we find

$$\|\Delta\bar{V}\|_2 \leqslant \beta\widetilde{\eta}_p + \beta\left(1+\frac{\beta}{2}\nu\widetilde{\eta}_p\right)\widetilde{\eta}_p + C_V\widetilde{\eta}_p^2\beta^2 \leqslant \left[2+\frac{\beta}{2}\nu\widetilde{\eta}_p + C_V\widetilde{\eta}_p\beta\right]\widetilde{\eta}_p\beta = C_\Delta\widetilde{\eta}_p\beta,$$

where C_Δ is as in (5.6b). Thus, $\|\Delta\bar{V}\bar{V}^{-1}\|_2 \leqslant \|\Delta\bar{V}\|_2\|\bar{V}^{-1}\|_2 \leqslant C_\Delta\widetilde{\eta}_p\beta\kappa \leqslant 1/2$ by (β-3). As a result, $\bar{V}^+$ is nonsingular, and

$$\|(\bar{V}^+)^{-1}\|_2 \leqslant \frac{\|\bar{V}^{-1}\|_2}{1-\|\bar{V}^{-1}\Delta\bar{V}\|_2} \leqslant 2\|\bar{V}^{-1}\|_2.$$

In particular, $T^+ = \underline{V}^+(\bar{V}^+)^{-1}$ is well defined. This proves (1).

For (2), using the Sherman-Morrison-Woodbury formula [11, p. 95], we obtain

$$\begin{aligned}
\Delta T &= (\underline{V}+\Delta\underline{V})(\bar{V}+\Delta\bar{V})^{-1} - \underline{V}\bar{V}^{-1} \\
&= (\underline{V}+\Delta\underline{V})(\bar{V}^{-1} - \bar{V}^{-1}\Delta\bar{V}(\bar{V}+\Delta\bar{V})^{-1}) - \underline{V}\bar{V}^{-1} \\
&= \Delta\underline{V}\bar{V}^{-1} - \underline{V}\bar{V}^{-1}\Delta\bar{V}(\bar{V}+\Delta\bar{V})^{-1} - \Delta\underline{V}\bar{V}^{-1}\Delta\bar{V}(\bar{V}+\Delta\bar{V})^{-1} \\
&= \Delta\underline{V}\bar{V}^{-1} - \underline{V}\bar{V}^{-1}\Delta\bar{V}(\bar{V}^{-1} - \bar{V}^{-1}\Delta\bar{V}(\bar{V}+\Delta\bar{V})^{-1}) - \Delta\underline{V}\bar{V}^{-1}\Delta\bar{V}(\bar{V}+\Delta\bar{V})^{-1} \\
&= \Delta\underline{V}\bar{V}^{-1} - T\Delta\bar{V}\bar{V}^{-1} + T\Delta\bar{V}\bar{V}^{-1}\Delta\bar{V}(\bar{V}^+)^{-1} - \Delta\underline{V}\bar{V}^{-1}\Delta\bar{V}(\bar{V}^+)^{-1} \\
&= [\Delta\underline{V} - T\Delta\bar{V}][I - (\bar{V}^+)^{-1}\Delta\bar{V}]\bar{V}^{-1}.
\end{aligned}$$

Write $T_L = [-T\ I]$ and $T_R = [\begin{smallmatrix} I \\ T \end{smallmatrix}]$. Then $T_LV = 0$ and $V = T_R\bar{V}$. Thus,

$$\Delta T = T_L\Delta V[I - (\bar{V}^+)^{-1}\Delta\bar{V}]V^{\mathrm{T}}T_R.$$

Since ΔV is rank-1, ΔT is also rank-1. By Lemma 5.2,

$$\begin{aligned}
\Delta T &= T_L\left[\beta YZ^{\mathrm{T}} - \beta\left(1+\frac{\beta}{2}Y^{\mathrm{T}}Y\right)VZZ^{\mathrm{T}} + RZ^{\mathrm{T}}\right][I - (\bar{V}^+)^{-1}\Delta\bar{V}]V^{\mathrm{T}}T_R \\
&= T_L[\beta YY^{\mathrm{T}}V + RZ^{\mathrm{T}}][I - (\bar{V}^+)^{-1}\Delta\bar{V}]V^{\mathrm{T}}T_R \\
&= T_L(\beta YY^{\mathrm{T}}VV^{\mathrm{T}} + R_T)T_R \\
&= T_L(\beta YY^{\mathrm{T}} + R_T)T_R,
\end{aligned}$$

where $R_T = RZ^{\mathrm{T}}V^{\mathrm{T}} - (\beta Y + R)Z^{\mathrm{T}}(\bar{V}^+)^{-1}\Delta\bar{V}V^{\mathrm{T}}$. Note that

$$T_LYY^{\mathrm{T}}T_R = \underline{Y}\bar{Y}^{\mathrm{T}} - T\bar{Y}\underline{Y}^{\mathrm{T}}T - T\bar{Y}\bar{Y}^{\mathrm{T}} + \underline{Y}\underline{Y}^{\mathrm{T}}T \tag{5.11}$$

and

$$\mathrm{E}\{\underline{Y}\bar{Y}^{\mathrm{T}}\} = 0, \quad \mathrm{E}\{T\bar{Y}\bar{Y}^{\mathrm{T}}\} = T\mathrm{E}\{\bar{Y}\bar{Y}^{\mathrm{T}}\} = T\bar{\Lambda}, \tag{5.12a}$$

$$\mathrm{E}\{T\bar{Y}\underline{Y}^{\mathrm{T}}T\} = T\mathrm{E}\{\bar{Y}\underline{Y}^{\mathrm{T}}\}T = 0, \quad \mathrm{E}\{\underline{Y}\underline{Y}^{\mathrm{T}}T\} = \mathrm{E}\{\underline{Y}\underline{Y}^{\mathrm{T}}\}T = \underline{\Lambda}T. \tag{5.12b}$$

Thus, $\mathrm{E}\{\Delta T\} = \beta(\underline{\Lambda} T - T\bar{\Lambda}) + E_T(V)$, where $E_T(V) = \mathrm{E}\{T_L R_T T_R\}$.

Since $V \in \mathbb{S}(\kappa)$, $\|T\|_2 \leqslant (\kappa^2 - 1)^{1/2}$ by (5.4). Thus,

$$\begin{aligned}\|R_T\|_2 &\leqslant \|R\|_2 \widetilde{\eta}_p^{1/2} + [(\nu\widetilde{\eta}_p)^{1/2}\beta + \|R\|_2]\widetilde{\eta}_p^{1/2} 2(1+\|T\|_2^2)^{1/2} C_\Delta \widetilde{\eta}_p \beta \\ &\leqslant C_V \nu^{1/2} \widetilde{\eta}_p^2 \beta^2 + (1+\|T\|_2^2)^{1/2}[1 + C_V\widetilde{\eta}_p\beta] 2 C_\Delta \nu^{1/2} \widetilde{\eta}_p^2 \beta^2 \\ &\leqslant C_T \nu^{1/2} (\widetilde{\eta}_p\beta)^2 (1+\|T\|_2^2)^{1/2},\end{aligned}$$

where $C_T = C_V + 2C_\Delta(1 + C_V\widetilde{\eta}_p\beta)$. Therefore, $\|E_T(V)\|_2 \leqslant \mathrm{E}\{\|T_L R_T T_R\|_2\} \leqslant (1 + \|T\|_2^2)\,\mathrm{E}\{\|R_T\|_2\}$. (2)(a) holds. For (2)(b), we have

$$\begin{aligned}\|\Delta T\|_2 &\leqslant (1+\|T\|_2^2)(\beta\|YY^{\mathrm{T}}VV^{\mathrm{T}}\|_2 + \|R_T\|_2) \\ &\leqslant \beta(\nu\widetilde{\eta}_p)^{1/2}\widetilde{\eta}_p^{1/2}(1+\|T\|_2^2) + C_T\nu^{1/2}(\widetilde{\eta}_p\beta)^2(1+\|T\|_2^2)^{3/2} \\ &\leqslant \nu^{1/2}\widetilde{\eta}_p\beta(1+\|T\|_2^2) + C_T\nu^{1/2}(\widetilde{\eta}_p\beta)^2(1+\|T\|_2^2)^{3/2}.\end{aligned}$$

The proof of (3) is similar to that of (2) but involves more complicated calculations, and it is deferred to Appendix A.1. □

5.3 Quasi-power iterative process

Let $D^{(n+1)} = T^{(n+1)} - \mathrm{E}\{T^{(n+1)} \mid \mathbb{F}_n\}$. We have $T^{(n)} - \mathrm{E}\{T^{(n)} \mid \mathbb{F}_n\} = 0$, $\mathrm{E}\{D^{(n+1)} \mid \mathbb{F}_n\} = 0$ and $\mathrm{E}\{D^{(n+1)} \circ D^{(n+1)} \mid \mathbb{F}_n\} = \mathrm{var}_\circ(T^{(n+1)} - T^{(n)} \mid \mathbb{F}_n)$. By Lemma 5.3(2), we have

$$\begin{aligned}T^{(n+1)} &= D^{(n+1)} + T^{(n)} + \mathrm{E}\{T^{(n+1)} - T^{(n)} \mid \mathbb{F}_n\} \\ &= D^{(n+1)} + T^{(n)} + \beta(\underline{\Lambda} T^{(n)} - T^{(n)}\bar{\Lambda}) + E_T^{(n)}(V^{(n)}) \\ &= \mathcal{L}T^{(n)} + D^{(n+1)} + E_T^{(n)}(V^{(n)}),\end{aligned}$$

where $\mathcal{L}\colon T \mapsto T + \beta\underline{\Lambda} T - \beta T\bar{\Lambda}$ is a bounded linear operator. It can be verified that $\mathcal{L}T = L \circ T$, the Hadamard product of L and T, where $L = [\lambda_{ij}]_{(d-p)\times p}$ with $\lambda_{ij} = 1 + \beta\lambda_{p+i} - \beta\lambda_j$. Moreover, it can be shown that[2] $\|\mathcal{L}\|_{\mathrm{ui}} = \rho(\mathcal{L}) = 1 - \beta\gamma$, where $\|\mathcal{L}\|_{\mathrm{ui}} = \sup_{\|T\|_{\mathrm{ui}}=1}\|\mathcal{L}T\|_{\mathrm{ui}}$ is an operator norm induced by the matrix norm $\|\cdot\|_{\mathrm{ui}}$. Recursively,

$$T^{(n)} = \mathcal{L}^n T^{(0)} + \sum_{s=1}^{n} \mathcal{L}^{n-s} D^{(s)} + \sum_{s=1}^{n} \mathcal{L}^{n-s} E_T^{(s-1)}(V^{(s-1)}) =: J_1 + J_2 + J_3. \tag{5.13}$$

Define events $\mathbb{M}_n(\chi)$, $\mathbb{T}_n(\chi)$ and $\mathbb{Q}_n$ as

$$\mathbb{M}_n(\chi) = \left\{\|T^{(n)} - \mathcal{L}^n T^{(0)}\|_2 \leqslant \frac{1}{2}(\kappa^2\beta^{2\chi-1} - 1)^{1/2}\beta^{\chi-3\varepsilon}\right\}, \tag{5.14}$$

$$\mathbb{T}_n(\chi) = \{\|T^{(n)}\|_2 \leqslant (\kappa^2\beta^{2\chi-1} - 1)^{1/2}\beta^{\chi-3\varepsilon}\}, \quad \mathbb{Q}_n = \{n < N_{\mathrm{qb}}\{\Lambda\}\}. \tag{5.15}$$

Lemma 5.4. *Suppose that the conditions of Theorem 4.3 hold and that* $\chi \in (5\varepsilon - 1/2, 0]$ *and* $\kappa > \sqrt{2}$. *If* $V^{(0)} \in \mathbb{S}(\kappa\beta^\chi)$ *and* $n < \min\{N_{\mathrm{qb}}\{\Lambda\}, N_{\mathrm{out}}\{\mathbb{S}(\kappa\beta^\chi)\}\}$, *then*

$$\mathrm{P}\{\mathbb{M}_n(\chi + 1/2)\} \geqslant 1 - 2d\exp(-C_\kappa\gamma\kappa^{-2}\nu^{-1}\eta_p^{-2}\beta^{-2\varepsilon}), \tag{5.16}$$

where C_κ *is as in* (5.6d).

[2] Since $\lambda(\mathcal{L}) = \{\lambda_{ij} : i = 1, \dots, d-p,\ j = 1, \dots, p\}$, we have the spectral radius $\rho(\mathcal{L}) = 1 - \beta(\lambda_p - \lambda_{p+1})$. Thus for any T,

$$\|\mathcal{L}T\|_{\mathrm{ui}} = \|T(I - \beta\bar{\Lambda}) + \beta\underline{\Lambda} T\|_{\mathrm{ui}} \leqslant \|I - \beta\bar{\Lambda}\|_2\|T\|_{\mathrm{ui}} + \|\beta\underline{\Lambda}\|_2\|T\|_{\mathrm{ui}} = (1 - \beta\lambda_p + \beta\lambda_{p+1})\|T\|_{\mathrm{ui}} = \rho(\mathcal{L})\|T\|_{\mathrm{ui}},$$

which means $\|\mathcal{L}\|_{\mathrm{ui}} \leqslant \rho(\mathcal{L})$. This ensures $\|\mathcal{L}\|_{\mathrm{ui}} = \rho(\mathcal{L})$.

Proof. Since $\kappa > \sqrt{2}$, we have $\kappa^2\beta^{2\chi} > 2$ and $\kappa\beta^\chi < [2(\kappa^2\beta^{2\chi}-1)]^{1/2}$. Thus, by ($\beta$-4),

$$4C_T\kappa^3\widetilde{\eta}_p^2\gamma^{-1}\beta^{1+3\chi}(\kappa^2\beta^{2\chi}-1)^{-1/2}\beta^{-1/2-\chi} \leqslant 4\sqrt{2}C_T\kappa^2\widetilde{\eta}_p^2\gamma^{-1}\beta^{1/2+\chi} \leqslant 1.$$

For any $n < \min\{N_{\rm qb}\{\Lambda\}, N_{\rm out}\{\mathbb{S}(\kappa\beta^\chi)\}\}$, $V^{(n)} \in \mathbb{S}(\kappa\beta^\chi)$ and thus $\|T^{(n)}\|_2 \leqslant \sqrt{\kappa^2\beta^{2\chi}-1}$ by (5.4). Therefore, by Lemma 5.3(2)(b), we have

$$\begin{aligned}\|D^{(n+1)}\|_2 &= \|T^{(n+1)} - T^{(n)} - \mathrm{E}\{T^{(n+1)} - T^{(n)} \mid \mathbb{F}_n\}\|_2 \\ &\leqslant \|T^{(n+1)} - T^{(n)}\|_2 + \mathrm{E}\{\|T^{(n+1)} - T^{(n)}\|_2 \mid \mathbb{F}_n\} \\ &\leqslant 2\nu^{1/2}\widetilde{\eta}_p\beta(1+\|T^{(n)}\|_2^2)[1 + C_T\widetilde{\eta}_p\beta(1+\|T^{(n)}\|_2^2)^{1/2}] \\ &\leqslant 2\kappa^2\nu^{1/2}\widetilde{\eta}_p\beta^{1+2\chi}[1 + C_T\kappa\widetilde{\eta}_p\beta^{1+\chi}]. \end{aligned} \tag{5.17}$$

For any $n < \min\{N_{\rm qb}\{\Lambda\}, N_{\rm out}\{\mathbb{S}(\kappa\beta^\chi)\}\}$,

$$\begin{aligned}\|J_3\|_2 &\leqslant \sum_{s=1}^{n}\|\mathcal{L}\|_2^{n-s}\|E_T^{(s-1)}(V^{(s-1)})\|_2 \\ &\leqslant C_T\nu^{1/2}\kappa^3\widetilde{\eta}_p^2\beta^{2+3\chi}\sum_{s=1}^{n}(1-\beta\gamma)^{n-s} \\ &\leqslant \frac{C_T\nu^{1/2}\kappa^3\widetilde{\eta}_p^2\beta^{2+3\chi}}{\beta\gamma} = C_T\nu^{1/2}\kappa^3\widetilde{\eta}_p^2\gamma^{-1}\beta^{1+3\chi} \leqslant \frac{1}{4}\nu^{1/2}(\kappa^2\beta^{2\chi}-1)^{1/2}\beta^{1/2+\chi}.\end{aligned}$$

Similarly,

$$\begin{aligned}\|J_2\|_2 &\leqslant \sum_{s=1}^{n}\|\mathcal{L}\|_2^{n-s}\|D^{(s)}\|_2 \\ &\leqslant \frac{2\kappa^2\nu^{1/2}\widetilde{\eta}_p\beta^{2\chi}(1 + C_T\kappa\widetilde{\eta}_p\beta^{1+\chi})}{\gamma} \\ &\leqslant \frac{2\kappa^2\nu^{1/2}\widetilde{\eta}_p\beta^{2\chi}}{\gamma} + \frac{1}{2}\nu^{1/2}(\kappa^2\beta^{2\chi}-1)^{1/2}\beta^{1/2+\chi}.\end{aligned}$$

Also, $\|J_1\|_2 \leqslant \|\mathcal{L}\|_2^n\|T^{(0)}\|_2 \leqslant \|T^{(0)}\|_2 \leqslant \nu^{1/2}(\kappa^2\beta^{2\chi}-1)^{1/2}$. For fixed $n > 0$ and $\beta > 0$,

$$\left\{M_0^{(n)} := \mathcal{L}^nT^{(0)}, M_t^{(n)} := \mathcal{L}^nT^{(0)} + \sum_{s=1}^{\min\{t, N_{\rm out}\{\mathbb{S}(\kappa)\}-1\}}\mathcal{L}^{n-s}D^{(s)} : 1 \leqslant t \leqslant n\right\}$$

forms a martingale with respect to $\mathbb{F}_t$, because $\mathrm{E}\{\|M_t^{(n)}\|_2\} \leqslant \|J_1\|_2 + \|J_2\|_2 < +\infty$, and

$$\mathrm{E}\{M_{t+1}^{(n)} - M_t^{(n)} \mid \mathbb{F}_t\} = \mathrm{E}\{\mathcal{L}^{n-t-1}D^{(t+1)} \mid \mathbb{F}_t\} = \mathcal{L}^{n-t-1}\mathrm{E}\{D^{(t+1)} \mid \mathbb{F}_t\} = 0.$$

Use the matrix version of Azuma's inequality [29, Subsection 7.2] to obtain, for any $\alpha > 0$,

$$\mathrm{P}\{\|M_n^{(n)} - M_0^{(n)}\|_2 \geqslant \alpha\} \leqslant 2d\exp\left(-\frac{\alpha^2}{2\sigma^2}\right),$$

where

$$\begin{aligned}\sigma^2 &= \sum_{s=1}^{\min\{n, N_{\rm out}\{\mathbb{S}(\kappa)\}-1\}}\|\mathcal{L}^{n-s}D^{(s)}\|_2^2 \\ &\leqslant [2\kappa^2\nu^{1/2}\widetilde{\eta}_p\beta^{1+2\chi}(1 + C_T\kappa\widetilde{\eta}_p\beta^{1+\chi})]^2\sum_{s=1}^{\min\{n, N_{\rm out}\{\mathbb{S}(\kappa)\}-1\}}(1-\beta\gamma)^{2(n-s)} \\ &\leqslant \frac{4\kappa^4\nu\widetilde{\eta}_p^2\beta^{2+4\chi}(1 + C_T\kappa\widetilde{\eta}_p\beta^{1+\chi})^2}{\beta\gamma[2-\beta\gamma]}\end{aligned}$$

$$
\begin{aligned}
&\leqslant \frac{4\kappa^4\nu\widetilde{\eta}_p^2\gamma^{-1}\beta^{1+4\chi}(1+\frac{C_T}{2C_\Delta})^2}{3-\sqrt{2}} \left(\text{by } (\beta\text{-3}) \text{ and } \widetilde{\eta}_p\beta^{1/2}\leqslant \frac{1}{2\kappa C_\Delta}\right)\\
&= C_\sigma\kappa^4\nu\gamma^{-1}\widetilde{\eta}_p^2\beta^{1+4\chi}
\end{aligned}
$$

and $C_\sigma = \frac{(C_T+2C_\Delta)^2}{(3-\sqrt{2})C_\Delta^2}$. Thus, noticing $J_2 = M_n^{(n)} - M_0^{(n)}$ for $n \leqslant N_{\text{out}}\{\mathbb{S}(\kappa)\} - 1$, we have

$$
\mathrm{P}\{\|J_2\|_2 \geqslant \alpha\} \leqslant 2d\exp\left(-\frac{\alpha^2}{2C_\sigma\kappa^4\nu\gamma^{-1}\widetilde{\eta}_p^2\beta^{1+4\chi}}\right).
$$

Choosing $\alpha = \frac{1}{4}(\kappa^2\beta^{2\chi}-1)^{1/2}\beta^{\chi+1/2-3\varepsilon}$ and noticing $T^{(n)} - \mathcal{L}^nT^{(0)} = J_2 + J_3$ and $\|J_3\|_2 \leqslant \frac{1}{4}(\kappa^2\beta^{2\chi} - 1)^{1/2}\beta^{\chi+1/2-3\varepsilon}$, we have

$$
\begin{aligned}
\mathrm{P}\{\mathbb{M}_n(\chi+1/2)^{\mathrm{c}}\} &= \mathrm{P}\left\{\|T^{(n)} - \mathcal{L}^nT^{(0)}\|_2 \geqslant \frac{1}{2}(\kappa^2\beta^{2\chi}-1)^{1/2}\beta^{\chi+1/2-3\varepsilon}\right\}\\
&\leqslant \mathrm{P}\left\{\|J_2\|_2 \geqslant \frac{1}{4}(\kappa^2\beta^{2\chi}-1)^{1/2}\beta^{\chi+1/2-3\varepsilon}\right\}\\
&\leqslant 2d\exp\left(-\frac{\kappa^2\beta^{2\chi}-1}{32C_\sigma\kappa^4\nu\gamma^{-1}\widetilde{\eta}_p^2\beta^{2\chi}}\beta^{-6\varepsilon}\right)\\
&\leqslant 2d\exp\left(-\frac{\kappa^2\beta^{2\chi}}{64C_\sigma\kappa^4\nu\gamma^{-1}\widetilde{\eta}_p^2\beta^{2\chi}}\beta^{-6\varepsilon}\right)\\
&= 2d\exp(-C_\kappa\gamma\kappa^{-2}\nu^{-1}\eta_p^{-2}\beta^{-2\varepsilon}),
\end{aligned}
$$

where $C_\kappa = \frac{1}{64C_\sigma}$ which is the same as in (5.6d). □

Lemma 5.5. *Suppose that the conditions of Theorem* 4.3 *hold. If*

$$
N_{2^{-m}(1-6\varepsilon)} < \min\{N_{\text{qb}}\{\Lambda\}, N_{\text{out}}\{\mathbb{S}(\kappa\beta^\chi)\}\}
$$

and $V^{(0)} \in \mathbb{S}(\beta^{(1-2^{1-m})(3\varepsilon-1/2)}\kappa_m/2)$ *with* $m \geqslant 2$*, then for* $\kappa_m > \sqrt{2}$*,*

$$
\mathrm{P}\{\mathbb{H}_m\} \geqslant 1 - 2dN_{2^{-m}(1-6\varepsilon)}\exp(-C_\kappa\gamma\kappa_m^{-2}\nu^{-1}\eta_p^{-2}\beta^{-2\varepsilon}),
$$

where $\mathbb{H}_m = \{N_{\text{in}}\{\mathbb{S}(\sqrt{3/2}\beta^{(1-2^{2-m})(3\varepsilon-1/2)}\kappa_m)\} \leqslant N_{2^{-m}(1-6\varepsilon)}\}$.

Proof. By the definition of the event $\mathbb{T}_n$,

$$
\mathbb{T}_n(2^{-m}[1-6\varepsilon]+3\varepsilon) = \{\|T^{(n)}\|_2 \leqslant (\kappa_m^2 - \beta^{(1-2^{1-m})(1-6\varepsilon)})^{1/2}\beta^{(1-2^{2-m})(3\varepsilon-1/2)}\}.
$$

For $n \geqslant N_{2^{-m}(1-6\varepsilon)}$ and $V^{(0)} \in \mathbb{S}(\beta^{(1-2^{1-m})(3\varepsilon-1/2)}\kappa_m/2)$, we know

$$
\mathbb{M}_n(2^{-m}(1-6\varepsilon)+3\varepsilon) \subset \mathbb{T}_n(2^{-m}(1-6\varepsilon)+3\varepsilon),
$$

because

$$
\begin{aligned}
\|T^{(n)}\|_2 &\leqslant \|T^{(n)} - \mathcal{L}^nT^{(0)}\|_2 + \|\mathcal{L}\|_2^n\|T^{(0)}\|_2\\
&\leqslant \frac{1}{2}(\kappa_m^2 - \beta^{(1-2^{1-m})(1-6\varepsilon)})^{1/2}\beta^{(1-2^{2-m})(3\varepsilon-1/2)}\\
&\quad + \beta^{2^{-m}(1-6\varepsilon)}\left(\frac{\kappa_m^2}{4} - \beta^{(1-2^{1-m})(1-6\varepsilon)}\right)^{1/2}\beta^{(1-2^{1-m})(3\varepsilon-1/2)}\\
&\leqslant (\kappa_m^2 - \beta^{(1-2^{1-m})(1-6\varepsilon)})^{1/2}\beta^{(1-2^{1-m})(3\varepsilon-1/2)}.
\end{aligned}
$$

Therefore, noticing

$$
(\kappa_m^2 - \beta^{(1-2^{1-m})(1-6\varepsilon)})^{1/2}\beta^{(1-2^{2-m})(3\varepsilon-1/2)} = (\beta^{(1-2^{2-m})(6\varepsilon-1)}\kappa_m^2 - \beta^{2^{1-m}(1-6\varepsilon)})^{1/2}
$$

$$\leqslant \left(\frac{3}{2}\beta^{(1-2^{2-m})(6\varepsilon-1)}\kappa_m^2 - 1\right)^{1/2},$$

we obtain

$$\mathbb{M}_{N_{2^{-m}(1-6\varepsilon)}}(2^{-m}(1-6\varepsilon)+3\varepsilon) \subset \{\widehat{N} \leqslant N_{2^{-m}(1-6\varepsilon)}\} = \mathbb{H}_m,$$

where $\widehat{N} = N_{\rm in}\{\mathbb{S}(\sqrt{3/2}\beta^{(1-2^{2-m})(3\varepsilon-1/2)}\kappa_m)\}$. Since

$$\begin{aligned}&\bigcap_{n\leqslant \min\{N_{2^{-m}(1-6\varepsilon)},\widehat{N}-1\}} \mathbb{M}_n(2^{-m}(1-6\varepsilon)+3\varepsilon) \cap \mathbb{H}_m^{\rm c}\\ &\subset \bigcap_{n\leqslant N_{2^{-m}(1-6\varepsilon)}} \mathbb{M}_n(2^{-m}(1-6\varepsilon)+3\varepsilon) \subset \mathbb{M}_{N_{2^{-m}(1-6\varepsilon)}}(2^{-m}(1-6\varepsilon)+3\varepsilon),\end{aligned}$$

we have

$$\bigcap_{n\leqslant \min\{N_{2^{-m}(1-6\varepsilon)},\widehat{N}-1\}} \mathbb{M}_n(2^{-m}(1-6\varepsilon)+3\varepsilon) \subset \mathbb{H}_m.$$

By Lemma 5.4 with $\chi = 2^{-m}(1-6\varepsilon)+3\varepsilon-\frac{1}{2} = 2^{-m}(1-2^{m-1})(1-6\varepsilon)$, we obtain

$$\begin{aligned}\mathrm{P}\{\mathbb{H}_m^{\rm c}\} &\leqslant \mathrm{P}\Bigg\{\bigcup_{n\leqslant \min\{N_{2^{-m}(1-6\varepsilon)},\widehat{N}-1\}} \mathbb{M}_n(2^{-m}(1-6\varepsilon)+3\varepsilon)^{\rm c}\Bigg\}\\ &\leqslant \min\{N_{2^{-m}(1-6\varepsilon)},\widehat{N}-1\} \times 2d\exp(-C_\kappa\gamma\kappa_m^{-2}\nu^{-1}\eta_p^{-2}\beta^{-2\varepsilon})\\ &\leqslant 2dN_{2^{-m}(1-6\varepsilon)}\exp(-C_\kappa\gamma\kappa_m^{-2}\nu^{-1}\eta_p^{-2}\beta^{-2\varepsilon}),\end{aligned}$$

as expected. □

Lemma 5.6. *Suppose that the conditions of Theorem* 4.3 *hold. If* $V^{(0)} \in \mathbb{S}(\kappa/2)$ *with* $\kappa > 2\sqrt{2}$ *and* $K > N_{1-6\varepsilon}$, *then there exists a high-probability event* $\mathbb{H}_1 \cap \mathbb{Q}_K = \bigcap_{n\in[N_{1/2-3\varepsilon},K]} \mathbb{T}_n(1/2) \cap \mathbb{Q}_K$ *satisfying*

$$\mathrm{P}\{\mathbb{H}_1\cap\mathbb{Q}_K\} \geqslant 1 - 2dK\exp(-C_\kappa\gamma\kappa^{-2}\nu^{-1}\eta_p^{-2}\beta^{-2\varepsilon}) - K(\mathrm{e}d+p+1)\exp(-C_\psi\min\{\psi^{-1},\psi^{-2}\}\beta^{-2\varepsilon}),$$

such that for any $n \in [N_{1-6\varepsilon}, K]$,

$$\mathrm{E}\{T^{(n)}\circ T^{(n)};\mathbb{H}_1\cap\mathbb{Q}_K\} \leqslant \mathcal{L}^{2n}T^{(0)}\circ T^{(0)} + 2\beta^2[I-\mathcal{L}^2]^{-1}[I-\mathcal{L}^{2n}]H_\circ + R_E,$$

where $\|R_E\|_2 \leqslant C_\circ\kappa^4\gamma^{-1}\nu^2\widetilde{\eta}_p^2\beta^{3/2-3\varepsilon}$, $H_\circ = \mathrm{var}_\circ(\underline{Y}\bar{Y}^{\rm T}) \leqslant 16\psi^4 H$ *is as in Lemma* 5.3(3)(a), *and* $C_\circ$ *is as in* (5.6f).

Proof. First we estimate the probability of the event $\mathbb{H}_1$. We know $\mathbb{T}_n(1/2) \subset \{\|T^{(n)}\|_2 \leqslant (\kappa^2-1)^{1/2}\}$. If $K \geqslant N_{\rm out}\{\mathbb{S}(\kappa)\}$, then there exists some $n \leqslant K$, such that $V^{(n)} \notin \mathbb{S}(\kappa)$, i.e., $\|T^{(n)}\|_2 > (\kappa^2-1)^{1/2}$ by (5.4). Thus,

$$\{K \geqslant N_{\rm out}\{\mathbb{S}(\kappa)\}\} \subset \bigcup_{n\leqslant K}\{\|T^{(n)}\|_2 > (\kappa^2-1)^{1/2}\} \subset \bigcup_{n\leqslant K}\mathbb{T}_n(1/2)^{\rm c}.$$

On the other hand, for $n \geqslant N_{1/2-3\varepsilon}$ and $V^{(0)} \in \mathbb{S}(\kappa/2)$, $\mathbb{M}_n(1/2) \subset \mathbb{T}_n(1/2)$ because

$$\begin{aligned}\|T^{(n)}\|_2 &\leqslant \|T^{(n)} - \mathcal{L}^nT^{(0)}\|_2 + \|\mathcal{L}\|_2^n\|T^{(0)}\|_2\\ &\leqslant \frac{1}{2}(\kappa^2-1)^{1/2}\beta^{1/2-3\varepsilon} + \beta^{1/2-3\varepsilon}\left(\frac{\kappa^2}{4}-1\right)^{1/2}\\ &\leqslant (\kappa^2-1)^{1/2}\beta^{1/2-3\varepsilon}.\end{aligned} \tag{5.18}$$

Therefore,

$$\bigcap_{n\in[N_{1/2-3\varepsilon},K]}\mathbb{M}_n(1/2) \subset \bigcap_{n\in[N_{1/2-3\varepsilon},K]}\mathbb{T}_n(1/2) \subset \{K \leqslant N_{\rm out}\{\mathbb{S}(\kappa)\}-1\},$$

so

$$\bigcap_{n\leqslant\min\{K,N_{\rm out}\{\mathbb{S}(\kappa)\}-1\}}\mathbb{M}_n(1/2)\subset\bigcap_{n\in[N_{1/2-3\varepsilon},\min\{K,N_{\rm out}\{\mathbb{S}(\kappa)\}-1\}]}\mathbb{M}_n(1/2)$$
$$=\bigcap_{n\in[N_{1/2-3\varepsilon},K]}\mathbb{M}_n(1/2)$$
$$\subset\bigcap_{n\in[N_{1/2-3\varepsilon},K]}\mathbb{T}_n(1/2)=:\mathbb{H}_1.$$

By Lemma 5.4 with $\chi=0$, we have

$$\begin{aligned}&{\rm P}\bigg\{\bigcup_{n\leqslant\min\{K,N_{\rm out}\{\mathbb{S}(\kappa)\}-1\}}\mathbb{M}_n(1/2)^{\rm c}\cap\mathbb{Q}_K\bigg\}\\&\leqslant\min\{K,N_{\rm out}\{\mathbb{S}(\kappa)\}-1\}\cdot 2d\exp(-C_\kappa\gamma\kappa^{-2}\nu^{-1}\eta_p^{-2}\beta^{-2\varepsilon})\\&=2dK\exp(-C_\kappa\gamma\kappa^{-2}\nu^{-1}\eta_p^{-2}\beta^{-2\varepsilon}).\end{aligned}$$

Thus, by Lemma 5.1,

$$\begin{aligned}{\rm P}\{(\mathbb{H}_1\cap\mathbb{Q}_K)^{\rm c}\}&={\rm P}\{\mathbb{H}_1^{\rm c}\cup\mathbb{Q}_K^{\rm c}\}={\rm P}\{\mathbb{H}_1^{\rm c}\cap\mathbb{Q}_K\}+{\rm P}\{\mathbb{Q}_K^{\rm c}\}\\&\leqslant{\rm P}\bigg\{\bigcup_{n\leqslant\min\{K,N_{\rm out}\{\mathbb{S}(\kappa)\}-1\}}\mathbb{M}_n(1/2)^{\rm c}\cap\mathbb{Q}_K\bigg\}+{\rm P}\{\mathbb{Q}_K^{\rm c}\}\\&\leqslant 2dK\exp(-C_\kappa\gamma\kappa^{-2}\nu^{-1}\eta_p^{-2}\beta^{-2\varepsilon})+K({\rm e}d+p+1)\exp(-C_\psi\min\{\psi^{-1},\psi^{-2}\}\beta^{-2\varepsilon}).\end{aligned}$$

Next, we estimate the expectation. Since

$$\mathbb{H}_1=\bigcap_{n\in[N_{1/2-3\varepsilon},K]}\mathbb{T}_n(1/2)\subset\bigcap_{n\in[N_{1/2-3\varepsilon},K]}\{\mathbf{1}_{\mathbb{T}_{n-1}}D^{(n)}=D^{(n)}\},$$

we have that for $n\in[N_{1/2-3\varepsilon},K]$,

$$\begin{aligned}T^{(n)}\mathbf{1}_{\mathbb{H}_1\cap\mathbb{Q}_K}&=\mathbf{1}_{\mathbb{Q}_K}\bigg(\mathcal{L}^nT^{(0)}+\sum_{s=1}^{N_{1/2-3\varepsilon}-1}\mathcal{L}^{n-s}D^{(s)}+\sum_{s=N_{1/2-3\varepsilon}}^{n}\mathcal{L}^{n-s}D^{(s)}\mathbf{1}_{\mathbb{T}_{s-1}}\sum_{s=1}^{n}\mathcal{L}^{n-s}E_T^{(s-1)}(V^{(s-1)})\bigg)\\&=:\widetilde{J}_1+\widetilde{J}_{21}+\widetilde{J}_{22}+\widetilde{J}_3.\end{aligned}$$

In what follows, we simply write $E_T^{(n)}=E_T^{(n)}(V^{(n)})$ for convenience. Then

$$\begin{aligned}{\rm E}\{T^{(n)}\circ T^{(n)};\mathbb{H}_1\cap\mathbb{Q}_K\}&={\rm E}\{T^{(n)}\circ T^{(n)}\mathbf{1}_{\mathbb{H}_1\cap\mathbb{Q}_K}\}\\&={\rm E}\{\widetilde{J}_1\circ\widetilde{J}_1\}+2{\rm E}\{\widetilde{J}_1\circ\widetilde{J}_{21}\}+2{\rm E}\{\widetilde{J}_1\circ\widetilde{J}_{22}\}+2{\rm E}\{\widetilde{J}_1\circ\widetilde{J}_3\}\\&\quad+{\rm E}\{[\widetilde{J}_{21}+\widetilde{J}_{22}]\circ[\widetilde{J}_{21}+\widetilde{J}_{22}]\}+2{\rm E}\{[\widetilde{J}_{21}+\widetilde{J}_{22}]\circ\widetilde{J}_3\}+{\rm E}\{\widetilde{J}_3\circ\widetilde{J}_3\}\\&\leqslant{\rm E}\{\widetilde{J}_1\circ\widetilde{J}_1\}+2{\rm E}\{\widetilde{J}_1\circ\widetilde{J}_{21}\}+2{\rm E}\{\widetilde{J}_1\circ\widetilde{J}_{22}\}+2{\rm E}\{\widetilde{J}_1\circ\widetilde{J}_3\}\\&\quad+2{\rm E}\{\widetilde{J}_{21}\circ\widetilde{J}_{21}\}+4{\rm E}\{\widetilde{J}_{21}\circ\widetilde{J}_{22}\}+2{\rm E}\{\widetilde{J}_{22}\circ\widetilde{J}_{22}\}+2{\rm E}\{\widetilde{J}_3\circ\widetilde{J}_3\}.\end{aligned}$$

Each summand above for $n\in[N_{1-6\varepsilon},K]$ can be estimated with careful calculation (see Appendix A.2), which reads

(1) ${\rm E}\{\widetilde{J}_1\circ\widetilde{J}_1\}=\mathcal{L}^{2n}T^{(0)}\circ T^{(0)}$;
(2) ${\rm E}\{\widetilde{J}_1\circ\widetilde{J}_{21}\}=0$;
(3) ${\rm E}\{\widetilde{J}_1\circ\widetilde{J}_{22}\}=0$.
(4) $\|{\rm E}\{\widetilde{J}_1\circ\widetilde{J}_3\}\|_2\leqslant\frac{1}{2}C_T\nu^{1/2}\widetilde{\eta}_p^2\gamma^{-1}\kappa^4\beta^{2-6\varepsilon}$;
(5) ${\rm E}\{\widetilde{J}_{21}\circ\widetilde{J}_{22}\}=0$;

(6) $\mathrm{E}\{\widetilde{J}_{21} \circ \widetilde{J}_{21}\} = \beta^2 \sum_{s=1}^{N_{1/2-3\varepsilon}-1} \mathcal{L}^{2(n-s)} H_\circ + E_{21}$, where

$$\|E_{21}\|_2 \leqslant \left(\frac{29+8\sqrt{2}}{64} + 2C_T\kappa(\widetilde{\eta}_p\beta) + C_T^2\kappa^2(\widetilde{\eta}_p\beta)^2\right)\gamma^{-1}\kappa^4\nu^2\widetilde{\eta}_p^2\beta^{2-6\varepsilon};$$

(7) $\mathrm{E}\{\widetilde{J}_{22} \circ \widetilde{J}_{22}\} = \beta^2 \sum_{s=N_{1/2-3\varepsilon}}^{n} \mathcal{L}^{2(n-s)} H_\circ + E_{22}$, where

$$\|E_{22}\|_2 \leqslant \frac{1}{3-\sqrt{2}}\left(\frac{29+8\sqrt{2}}{32} + 4C_T\kappa\widetilde{\eta}_p\beta^{1/2+3\varepsilon} + 2C_T^2\kappa^2\widetilde{\eta}_p^2\beta^{3/2+3\varepsilon}\right)\gamma^{-1}\kappa^4\nu^2\widetilde{\eta}_p^2\beta^{3/2-3\varepsilon};$$

(8) $\|\mathrm{E}\{\widetilde{J}_3 \circ \widetilde{J}_3\}\|_2 \leqslant \frac{1}{3-\sqrt{2}} C_T^2\nu\widetilde{\eta}_p^4\gamma^{-1}\kappa^6\beta^3$.

Collecting all the estimates together, we obtain

$$\begin{aligned}\mathrm{E}\{T^{(n)} \circ T^{(n)}; \mathbb{H}_1 \cap \mathbb{Q}_K\} &\leqslant \mathcal{L}^{2n} T^{(0)} \circ T^{(0)} + 2\beta^2 \sum_{s=1}^{n} \mathcal{L}^{2(n-s)} H_\circ + R_E \\ &\leqslant \mathcal{L}^{2n} T^{(0)} \circ T^{(0)} + 2\beta^2 [I-\mathcal{L}^2]^{-1}[I-\mathcal{L}^{2n}] H_\circ + R_E,\end{aligned}$$

where by (β-3), $2C_\Delta\kappa\widetilde{\eta}_p\beta^{1/2} \leqslant 1$, and

$$\begin{aligned}\|R_E\|_2 \leqslant{}& 2\Bigg[\frac{C_T}{2}\beta^{1/2-3\varepsilon} + \left(\frac{29+8\sqrt{2}}{64} + 2C_T\kappa\widetilde{\eta}_p\beta + C_T^2\kappa^2(\widetilde{\eta}_p\beta)^2\right)\beta^{1/2-3\varepsilon} + \frac{C_T^2}{3-\sqrt{2}}\widetilde{\eta}_p^2\kappa^2\beta^{3/2+3\varepsilon} \\ &+ \frac{2}{3-\sqrt{2}}\left(\frac{29+8\sqrt{2}}{64} + 2C_T\kappa\widetilde{\eta}_p\beta^{1/2+3\varepsilon} + C_T^2\kappa^2\widetilde{\eta}_p^2\beta^{3/2+3\varepsilon}\right)\Bigg]\kappa^4\gamma^{-1}\nu^2\widetilde{\eta}_p^2\beta^{3/2-3\varepsilon} \\ \leqslant{}& 2\Bigg[\frac{C_T}{2}\beta^{1/2-3\varepsilon} + \left(\frac{29+8\sqrt{2}}{64} + \frac{C_T}{C_\Delta}\beta^{1/2} + \frac{C_T^2}{4C_\Delta^2}\beta\right)\beta^{1/2-3\varepsilon} + \frac{C_T^2}{4(3-\sqrt{2})C_\Delta^2}\beta^{1/2+3\varepsilon} \\ &+ \frac{2}{3-\sqrt{2}}\left(\frac{29+8\sqrt{2}}{64} + \frac{C_T}{C_\Delta}\beta^{3\varepsilon} + \frac{C_T^2}{4C_\Delta^2}\beta^{1/2+3\varepsilon}\right)\Bigg]\kappa^4\gamma^{-1}\nu^2\widetilde{\eta}_p^2\beta^{3/2-3\varepsilon} \\ ={}& C_\circ\kappa^4\gamma^{-1}\nu^2\widetilde{\eta}_p^2\beta^{3/2-3\varepsilon},\end{aligned}$$

where $C_\circ$ is as given in (5.6f). □

5.4 Proof of Theorem 4.3

Write $\widetilde{N}_s = \frac{s\ln\beta}{\ln(1-\beta\gamma)}$. Then $(1-\beta\gamma)^{\widetilde{N}_s} = \beta^s$ and $N_s = \lceil\widetilde{N}_s\rceil$, where N_s is defined in (4.5). It can be verified that $\widetilde{N}_{s_1} + \widetilde{N}_{s_2} = \widetilde{N}_{s_1+s_2}$ for any s_1 and s_2.

Write $\kappa_m = 6^{(1-m)/2}\kappa$ for $m = 1, \ldots, M \equiv M(\epsilon)$. Since $d\beta^{1-7\varepsilon} \leqslant (\sqrt{2}-1)\lambda_1^{-1}\omega$, we know

$$\phi d^{1/2} \leqslant \phi\omega^{1/2}\beta^{7\varepsilon/2-1/2} \leqslant \beta^{(1-2^{1-M})(3\varepsilon-1/2)}\kappa_M/2.$$

The key to our proof is to divide the whole process into M segments of iterations. Thanks to the strong Markov property of the process, we can use the final value of the current segment as the initial guess of the very next one. By Lemma 5.5, after the first segment of

$$n_1 := \min\{N_{\mathrm{in}}\{\mathbb{S}(\sqrt{3/2}\beta^{(1-2^{2-M})(3\varepsilon-1/2)}\kappa_1)\}, N_{2^{-M}(1-6\varepsilon)}\}$$

iterations, $V^{(n_1)}$ lies in $\mathbb{S}(\sqrt{3/2}\beta^{(1-2^{2-M})(3\varepsilon-1/2)}\kappa_1) = \mathbb{S}(\beta^{(1-2^{2-M})(3\varepsilon-1/2)}\kappa_2/2)$ with high probability, which will be a good initial guess for the second segment. In general, the i-th segment of iterations starts with $V^{(n_{i-1})}$ and ends with $V^{(n_i)}$, where

$$n_i = \min\left\{N_{\mathrm{in}}\{\mathbb{S}(\beta^{(1-2^{i+1-M})(3\varepsilon-1/2)}\kappa_{i+1}/2)\}, \left\lceil \sum_{m=M+1-i}^{M} \widetilde{N}_{2^{-m}(1-6\varepsilon)} \right\rceil\right\}.$$

At the end of the $(M-1)$-st segment of iterations, $V^{(n_{M-1})}$ is produced and it is going to be used as an initial guess for the last step, at which we can apply Lemma 5.6. Now $n_{M-1} = \min\{N_{\rm in}\{\mathbb{S}(\kappa_M/2)\}, \widehat{K}\}$, where $\widehat{K} = \lceil \sum_{m=2}^{M} \widetilde{N}_{2^{-m}(1-6\varepsilon)} \rceil = \lceil \widetilde{N}_{(1-2^{1-M})(1/2-3\varepsilon)} \rceil$. By $2^{2-M} \geqslant \frac{\varepsilon/2}{1/2-3\varepsilon} \geqslant 2^{1-M}$, we have

$$N_{1/2-7\varepsilon/2} = \lceil \widetilde{N}_{1/2-7\varepsilon/2} \rceil \leqslant \widehat{K} \leqslant \lceil \widetilde{N}_{1/2-13\varepsilon/4} \rceil \leqslant N_{1/2-13\varepsilon/4}.$$

Let $\widehat{N} = N_{\rm in}\{\mathbb{S}(\sqrt{3/2}\beta^{(1-2^{2-m})(3\varepsilon-1/2)}\kappa_{M+1-m})\}$, and

$$\begin{aligned}
\widetilde{\mathbb{H}}_m &= \{\widehat{N} \leqslant \widetilde{N}_{2^{-m}(1-6\varepsilon)} + n_{M-m}\} \quad \text{for } 2 \leqslant m \leqslant M, \\
\widetilde{\mathbb{H}}_1 &= \bigcap_{n \in [N_{1/2-3\varepsilon}, K - N_{\rm in}\{\mathbb{S}(\kappa_M/2)\}]} \mathbb{T}_{n+N_{\rm in}\{\mathbb{S}(\kappa_M/2)\}}(1/2), \\
\mathbb{H} &= \bigcap_{m=1}^{M} \widetilde{\mathbb{H}}_m \cap \mathbb{Q}_K,
\end{aligned}$$

where $n_0 = 0$. We have

$$\begin{aligned}
\mathrm{P}\{\mathbb{H}^{\rm c}\} &= \mathrm{P}\bigg\{\bigcup_{m=1}^{M} \widetilde{\mathbb{H}}_m^{\rm c} \cup \mathbb{Q}_K^{\rm c}\bigg\} \leqslant \sum_{m=1}^{M} \mathrm{P}\{\widetilde{\mathbb{H}}_m^{\rm c} \cup \mathbb{Q}_K^{\rm c}\} \\
&\leqslant \sum_{m=2}^{M} 2dN_{2^{-m}(1-6\varepsilon)} \exp(-C_\kappa \gamma \kappa_{M+1-m}^{-2} \nu^{-1} \eta_p^{-2} \beta^{-2\varepsilon}) \\
&\quad + 2d\bigg(K - \sum_{m=2}^{M} N_{2^{-m}(1-6\varepsilon)}\bigg) \exp(-C_\kappa \gamma \kappa_M^{-2} \nu^{-1} \eta_p^{-2} \beta^{-2\varepsilon}) \\
&\quad + K(\mathrm{e}d + p + 1) \exp(-C_\psi \min\{\psi^{-1}, \psi^{-2}\} \beta^{-2\varepsilon}) \\
&\leqslant 2dK \exp(-C_\kappa \gamma \kappa^{-2} \nu^{-1} \eta_p^{-2} \beta^{-2\varepsilon}) + K(\mathrm{e}d + p + 1) \exp(-C_\psi \min\{\psi^{-1}, \psi^{-2}\} \beta^{-2\varepsilon}) \\
&\leqslant 2dK \exp(-C_\kappa 4\sqrt{2} C_T \nu^{-1} \beta^{\varepsilon} \beta^{-2\varepsilon}) + K(\mathrm{e}d + p + 1) \exp(-C_\psi \min\{\psi^{-1}, \psi^{-2}\} \beta^{-2\varepsilon}) \ (\text{by } (\beta\text{-}4)) \\
&\leqslant 2dK \exp(-4\sqrt{2} C_T C_\kappa \nu^{-1} \beta^{-\varepsilon}) + K(\mathrm{e}d + p + 1) \exp(-C_\psi \min\{\psi^{-1}, \psi^{-2}\} \beta^{-\varepsilon}) \\
&\leqslant K[(2+\mathrm{e})d + p + 1] \exp(-\max\{C_\nu \nu^{-1}, C_\psi \min\{\psi^{-1}, \psi^{-2}\}\} \beta^{-\varepsilon}),
\end{aligned}$$

where $C_\nu = 4\sqrt{2} C_T C_\kappa$ is as given in (5.6e).

Set $\mathbb{H}'_{n'} := \{N_{\rm in}\{\mathbb{S}(\kappa/2)\} = n'\}$. If $n' > \widehat{K}$, then $\mathbb{H} \cap \mathbb{H}'_{n'} = \emptyset$. Otherwise if $n' \leqslant \widehat{K}$, then by Lemma 5.5, $V^{(n')} \in \mathbb{S}(\kappa_M/2)$ and then $\|T^{(n')}\|_{\rm F}^2 \leqslant p((\frac{\kappa_M}{2})^2 - 1)$. Thus,

$$\phi^2 d(1-\beta\gamma)^{2(n'-1)} \geqslant \phi^2 d(1-\beta\gamma)^{2(\widehat{K}-1)} > \left(\frac{\kappa_M}{2}\right)^2 \geqslant \frac{1}{p}\|T^{(n')}\|_{\rm F}^2.$$

Hence, for any $n \in [N_{1-6\varepsilon} + N_{\rm in}\{\mathbb{S}(\kappa/2)\}, K] \subset [N_{1-6\varepsilon} + n', K + n']$, by Lemma 5.6, we have

$$\mathrm{E}\{T^{(n)} \circ T^{(n)} \mathbf{1}_{\mathbb{H}} \mid \mathbb{H}'_{n'} \cap \mathbb{F}_{n'}\} \leqslant \mathcal{L}^{2(n-n')} T^{(n')} \circ T^{(n')} + 2\beta^2 [I - \mathcal{L}^2]^{-1} [I - \mathcal{L}^{2(n-n')}] H_\circ + R_E.$$

Recall that $\mathbb{F}_{n'}$ is the σ-algebra filtration, i.e., the information known by step n'. Introduce $\mathrm{sum}(A)$ for the sum of all the entries of a matrix A. In particular, $\mathrm{sum}(A \circ A) = \|A\|_{\rm F}^2$. We have

$$\begin{aligned}
&\mathrm{E}\{\|T^{(n)}\|_{\rm F}^2 \mathbf{1}_{\mathbb{H}} \mid \mathbb{H}'_{n'}\} \\
&\quad = \mathrm{E}\{\mathrm{E}\{\|T^{(n)}\|_{\rm F}^2 \mathbf{1}_{\mathbb{H}} \mid \mathbb{H}'_{n'} \cap \mathbb{F}_{n'}\}\} \\
&\quad \leqslant \mathrm{E}\{(1-\beta\gamma)^{2(n-n')} \|T^{(n')}\|_{\rm F}^2 + 2\beta^2 \,\mathrm{sum}([I - \mathcal{L}^2]^{-1} H_\circ) + \mathrm{sum}(R_E)\} \\
&\quad \leqslant (1-\beta\gamma)^{2(n-1)} p\phi^2 d + 2\beta^2 \,\mathrm{sum}([I - \mathcal{L}^2]^{-1} H_\circ) + \sqrt{p(d-p)} \|R_E\|_{\rm F} \\
&\quad \leqslant (1-\beta\gamma)^{2(n-1)} p\phi^2 d + 2\beta^2 \frac{1}{\beta(2-\lambda_1\beta)} \,\mathrm{sum}(G \circ H_\circ) + \sqrt{p(d-p)} C_\circ \sqrt{p} \kappa^4 (\nu \widetilde{\eta}_p)^2 \gamma^{-1} \beta^{3/2-3\varepsilon},
\end{aligned}$$

where $G=[\gamma_{ij}]_{(d-p)\times p}$ with $\gamma_{ij}=\frac{1}{\lambda_j-\lambda_{p+i}}$. Putting all the above together, we obtain

$$\begin{aligned}\mathrm{E}\{\|T^{(n)}\|_{\mathrm{F}}^2;\mathbb{H}\} &= \mathrm{E}\{\mathrm{E}\{\|T^{(n)}\|_{\mathrm{F}}^2\mathbf{1}_{\mathbb{H}}\mid\mathbb{H}'_{n'}\}\} \\ &\leqslant (1-\beta\gamma)^{2(n-1)}p\phi^2d+\frac{2\beta}{2-\lambda_1\beta}\operatorname{sum}(G\circ H_\circ)+C_\circ\kappa^4\nu^2\widetilde{\eta}_p^2p\sqrt{d-p}\gamma^{-1}\beta^{3/2-3\varepsilon}.\end{aligned}$$

Note that on $\mathbb{H}$, $N_{\mathrm{in}}\{\mathbb{S}(\kappa/2)\}\leqslant\widehat{K}$. So the expectation is valid for any $n\in[N_{1-2\varepsilon}+\widehat{K},K]$. Finally, we estimate $\operatorname{sum}(G\circ H_\circ)$. By Lemma 5.3, $H_\circ\leqslant 16\psi^4H$, and hence,

$$\operatorname{sum}(G\circ H_\circ)\leqslant\sum_{j=1}^{p}\sum_{i=1}^{d-p}\frac{16\psi^4\lambda_{p+i}\lambda_j}{\lambda_j-\lambda_{p+i}}=16\psi^4\varphi(p,d;\Lambda).$$

This completes the proof.

6 Proofs of Theorems 4.5 and 4.6

To prove Theorem 4.5, we first prove that it is a high-probability event that $V^{(0)}$ satisfies the initial condition there, which is the result of Lemma 6.2 below. Then together with Theorem 4.3, we have the conclusion. During estimating the probability, we need a property on the Gaussian hypergeometric function of a matrix argument, as in Lemma 6.1.

The gamma function and the multivariate gamma function are

$$\Gamma(x):=\int_0^\infty t^{x-1}\exp(-t)dt,\quad \Gamma_m(x):=\pi^{m(m-1)/4}\prod_{i=1}^m\Gamma\left(x-\frac{i-1}{2}\right),$$

respectively. Denote by ${}_2F_1$ the Gaussian hypergeometric function of matrix argument (see [23, Definition 7.3.1]), and also by ${}_1F_0$ and ${}_1F_1$ the generalized hypergeometric functions that will be used later.

Lemma 6.1. *For any scalar a,b,c and a symmetric matrix $T\in\mathbb{R}^{m\times m}$,*

$$\begin{aligned}&{}_2F_1(a,b;c;T)\\ &\quad=\frac{\Gamma_m(c-a-b)\Gamma_m(c)}{\Gamma_m(c-a)\Gamma_m(c-b)}{}_2F_1\left(a,b;a+b-c+\frac{m+1}{2};I-T\right)\\ &\qquad+\frac{\Gamma_m(a+b-c)\Gamma_m(c)}{\Gamma_m(a)\Gamma_m(b)}\det(I-T)^{c-a-b}{}_2F_1\left(c-a,c-b;c-a-b+\frac{m+1}{2};I-T\right).\end{aligned}\tag{6.1}$$

Our proof of Lemma 6.1 is similar to that for the case $p=1$ by Kummer's solutions of the hypergeometric differential equation (see, e.g., [20, Subsection 3.8]), and we leave it to Appendix A.3.

Lemma 6.2. *Suppose $p<(d+1)/2$. If $V^{(0)}$ satisfies the condition that $\mathcal{R}(V^{(0)})$ is uniformly sampled from $\mathbb{G}_p(\mathbb{R}^d)$, then for sufficiently large d and $\delta\in[0,1]$, there exists a constant C_p, independent of δ and d, such that*

$$\mathrm{P}\{V^{(0)}\in\mathbb{S}(C_p\delta^{-1}d^{1/2})\}\geqslant 1-\delta^{p^2}.\tag{6.2}$$

Proof. Let $1\geqslant\sigma_1\geqslant\cdots\geqslant\sigma_p\geqslant 0$ be the singular values of $\bar{V}^{(0)}$, and then $\sigma_i=\cos\theta_i$, where θ_i's are the canonical angles between $\mathcal{R}(V^{(0)})$ and $\mathcal{R}(V_*)$ (recall (5.1)). By [2, Theorem 1], since $p<(d+1)/2$, the probability distribution function of σ_p is

$$\begin{aligned}\mathrm{P}\{V^{(0)}\in\mathbb{S}(1/x)\}&=\mathrm{P}\{\sigma_p\geqslant x\}=\mathrm{P}\{\theta_p\leqslant\arccos x\}\\ &=\frac{\Gamma(\frac{p+1}{2})\Gamma(\frac{d-p+1}{2})}{\Gamma(\frac{1}{2})\Gamma(\frac{d+1}{2})}(1-x^2)^{p(d-p)/2}{}_2F_1\left(\frac{d-p}{2},\frac{1}{2};\frac{d+1}{2};(1-x^2)I_p\right).\end{aligned}$$

Set

$$f_d:=\frac{\Gamma_p(\frac{d+1}{2})\Gamma_p(\frac{p}{2})}{\Gamma_p(\frac{p+1}{2})\Gamma_p(\frac{d}{2})},\quad g_d:=\frac{\Gamma_p(\frac{d+1}{2})\Gamma_p(-\frac{p}{2})}{\Gamma_p(\frac{d-p}{2})\Gamma_p(\frac{1}{2})}.$$

After some calculations that are deferred to Appendix A.4, we know

- in defining g_d, although $\Gamma_p(-\frac{p}{2})$ and $\Gamma_p(\frac{1}{2})$ may be ∞, by analytic continuation, $\Gamma_p(-\frac{p}{2})/\Gamma_p(\frac{1}{2})$ is well defined;
- $f_d^{-1}g_d = \frac{\Gamma(\frac{p+1}{2})\Gamma_p(\frac{d}{2})\Gamma_p(-\frac{p}{2})}{\Gamma(\frac{1}{2})\Gamma_p(\frac{d-p}{2})\Gamma_p(\frac{1}{2})}$;
- $\frac{\Gamma_p(\frac{d}{2})}{\Gamma_p(\frac{d-p}{2})} = (\frac{d}{2})^{p^2/2}[1+\mathrm{o}(1)]$ as $d\to\infty$.

By (6.1), we have

$$\begin{aligned}&{}_2F_1\left(\frac{d-p}{2},\frac{1}{2};\frac{d+1}{2};(1-x^2)I_p\right)\\&\quad= f_d\,{}_2F_1\left(\frac{d-p}{2},\frac{1}{2};\frac{1}{2};x^2I_p\right)+g_d\det(x^2I_p)^{p/2}{}_2F_1\left(\frac{p+1}{2},\frac{d}{2};\frac{2p+1}{2};x^2I_p\right).\end{aligned}$$

Also, [23, Definition 7.3.1 and Corollary 7.3.5] give

$${}_2F_1\left(\frac{d-p}{2},\frac{1}{2};\frac{1}{2};x^2I_p\right)={}_1F_0\left(\frac{d-p}{2};x^2I_p\right)=\det(I_p-x^2I_p)^{-(d-p)/2}=(1-x^2)^{-p(d-p)/2}.$$

Therefore,

$$\mathrm{P}\{V^{(0)}\in\mathbb{S}(1/x)\}=1+f_d^{-1}g_d\,(1-x^2)^{p(d-p)/2}x^{p^2}{}_2F_1\left(\frac{p+1}{2},\frac{d}{2};\frac{2p+1}{2};x^2I_p\right).$$

Substituting $x=(\delta^{-1}d^{1/2})^{-1}$ and by [23, (8) of Subsection 7.4], we obtain that as $d\to\infty$,

$$\begin{aligned}&\mathrm{P}\{V^{(0)}\notin\mathbb{S}(\delta^{-1}d^{1/2})\}\\&\quad=-f_d^{-1}g_d(1-\delta^2d^{-1})^{p(d-p)/2}(\delta^2d^{-1})^{p^2/2}{}_2F_1\left(\frac{p+1}{2},\frac{d}{2};\frac{2p+1}{2};\frac{\delta^2}{d}I_p\right)\\&\quad=\frac{\Gamma(\frac{p+1}{2})\Gamma_p(-\frac{p}{2})}{-\Gamma(\frac{1}{2})\Gamma_p(\frac{1}{2})}\frac{\Gamma_p(\frac{d}{2})}{\Gamma_p(\frac{d-p}{2})}\left(1-\frac{\delta^2}{d}\right)^{pd/2}\left(\frac{d}{\delta^2}-1\right)^{-p^2/2}\left[{}_1F_1\left(\frac{p+1}{2};\frac{2p+1}{2};\frac{\delta^2}{2}I_p\right)+\mathrm{o}(1)\right]\\&\quad=\frac{\Gamma(\frac{p+1}{2})\Gamma_p(-\frac{p}{2})}{-\Gamma(\frac{1}{2})\Gamma_p(\frac{1}{2})}\left(\frac{d}{2}\right)^{p^2/2}[1+\mathrm{o}(1)]\left[\exp\left(-\frac{p\delta^2}{2}\right)+\mathrm{o}(1)\right]\left[\frac{\delta^{p^2}}{d^{p^2/2}}+\mathrm{o}(1)\right]\\&\quad\quad\times\left[{}_1F_1\left(\frac{p+1}{2};\frac{2p+1}{2};\frac{\delta^2}{2}I_p\right)+\mathrm{o}(1)\right]\\&\quad=\frac{\Gamma(\frac{p+1}{2})\Gamma_p(-\frac{p}{2})}{-\Gamma(\frac{1}{2})\Gamma_p(\frac{1}{2})}\exp\left(-\frac{p\delta^2}{2}\right){}_1F_1\left(\frac{p+1}{2};\frac{2p+1}{2};\frac{\delta^2}{2}I_p\right)\delta^{p^2}[1+\mathrm{o}(1)]\\&\quad\leqslant\frac{\Gamma(\frac{p+1}{2})\Gamma_p(-\frac{p}{2})}{-\Gamma(\frac{1}{2})\Gamma_p(\frac{1}{2})}{}_1F_1\left(\frac{p+1}{2};\frac{2p+1}{2};\frac{1}{2}I_p\right)\delta^{p^2}2=:C_p^{p^2}\delta^{p^2},\end{aligned}\tag{6.3}$$

where the inequality is guaranteed by ${}_1F_1(\frac{p+1}{2};\frac{2p+1}{2};\frac{\delta^2}{2}I_p)\leqslant{}_1F_1(\frac{p+1}{2};\frac{2p+1}{2};\frac{1}{2}I_p)$, according to [23, Theorem 7.5.6]. Substituting δ/C_p for δ, we infer from (6.3) that $\mathrm{P}\{V^{(0)}\notin\mathbb{S}(C_p\delta^{-1}d^{1/2})\}\leqslant\delta^{p^2}$. The claim (6.2) is now a simple consequence. □

Now we are ready to prove Theorem 4.5.

Proof of Theorem 4.5. Define the event $\mathbb{H}_*'=\{V^{(0)}\in\mathbb{S}(C_p\delta^{-1}d^{1/2})\}$. Since $\mathcal{R}(V^{(0)})$ is uniformly sampled from $\mathbb{G}_p(\mathbb{R}^d)$, Lemma 6.2 says $\mathrm{P}\{\mathbb{H}_*'\}\geqslant 1-\delta^{p^2}$. In the following, we will apply Theorem 4.3 with $\phi=C_p\delta^{-1}$ and $\omega=(\sqrt{2}+1)\lambda_1\delta^2$. Since Theorem 4.3 is valid on $\mathbb{H}_*'$, and

$$K[(2+\mathrm{e})d+p+1]\exp(-C_{\nu\psi}\beta^{-\varepsilon})\leqslant\delta^{p^2},$$

there exists an event $\mathbb{H}$ with

$$\mathrm{P}\{\mathbb{H}\mid\mathbb{H}_*'\}\geqslant 1-K[(2+\mathrm{e})d+p+1]\exp(-C_{\nu\psi}\beta^{-\varepsilon})\geqslant 1-\delta^{p^2},$$

such that for any $n \in [N_{3/2-37\varepsilon/4}(\beta), K]$,

$$\begin{aligned}
\mathrm{E}\{\|T^{(n)}\|_{\mathrm{F}}^2; \mathbb{H} \cap \mathbb{H}'_*\} &= \mathrm{P}\{\mathbb{H}'_*\}\mathrm{E}\{\|T^{(n)}\|_{\mathrm{F}}^2 \mathbf{1}_{\mathbb{H}} \mid \mathbb{H}'_*\} \\
&\leqslant \mathrm{E}\{\|T^{(n)}\|_{\mathrm{F}}^2 \mathbf{1}_{\mathbb{H}} \mid \mathbb{H}'_*\} \\
&\leqslant (1-\beta\gamma)^{2(n-1)} p C_p^2 \delta^{-2} d + \frac{32\psi^4\beta}{2-\lambda_1\beta}\varphi(p,d;\Lambda) + C_\circ \kappa^4 \nu^2 \eta_p^2 \gamma^{-1} p\sqrt{d-p}\beta^{3/2-5\varepsilon}.
\end{aligned}$$

Let $\mathbb{H}_* = \mathbb{H} \cap \mathbb{H}'_*$ for which $\mathrm{P}\{\mathbb{H}_*\} = \mathrm{P}\{\mathbb{H} \mid \mathbb{H}'_*\}\,\mathrm{P}\{\mathbb{H}'_*\} \geqslant (1-\delta^{p^2})^2 \geqslant 1 - 2\delta^{p^2}$, as expected. □

Finally, we prove Theorem 4.6.

Proof of Theorem 4.6. First we examine the conditions of Theorem 4.5 to make sue that they are satisfied. It can be seen that $\beta_* \to 0$ as $N_* \to \infty$. Thus, β_* satisfies (4.6) for sufficiently large N_*. We have

$$\begin{aligned}
(1-\beta_*\gamma)^{N_*} &= \left(1 - \frac{3\ln N_*}{2N_*}\right)^{N_*} = \exp\left(-\frac{3}{2}\ln N_*\right)[1+\mathrm{o}(1)] = N_*^{-3/2}[1+\mathrm{o}(1)] \\
&= \left(\frac{3\ln N_*}{2\gamma\beta_*}\right)^{-3/2}[1+\mathrm{o}(1)] = \frac{\beta_*^{3/2}\gamma^{3/2}}{(3/2)^{3/2}(\ln N_*)^{3/2}}[1+\mathrm{o}(1)] \leqslant \beta_*^{3/2},
\end{aligned}$$

which implies $N_* \geqslant N_{3/2}(\beta) \geqslant N_{3/2-9\varepsilon}(\beta)$.

The conclusion of the theorem will be a straightforward consequence if

$$\widetilde{C}(d, N_*, \delta) := \frac{(1-\beta_*\gamma)^{2(N_*-1)} p C_p^2 \delta^{-2} d + \frac{32\psi^4\beta_*}{2-\lambda_1\beta_*}\varphi(p,d;\Lambda) + C_\circ\kappa^4\nu^2\eta_p^2\gamma^{-1}p\sqrt{d-p}\beta_*^{3/2-7\varepsilon}}{\frac{\varphi(p,d;\Lambda)}{\lambda_p-\lambda_{p+1}}\frac{\ln N_*}{N_*}}$$

is bounded, say by $C_*(d, N_*, \delta)$ to be defined. In fact,

$$\begin{aligned}
\widetilde{C}(d, N_*, \delta) &= \gamma\frac{N_*}{\ln N_*}\left[(1-\beta_*\gamma)^{2(N_*-1)} C_p^2 \delta^{-2}\frac{pd}{\varphi(p,d;\Lambda)} + \frac{32\psi^4\beta_*}{2-\lambda_1\beta_*} + \frac{C_\circ\kappa^4\nu^2\eta_p^2\gamma^{-1}p\sqrt{d-p}}{\varphi(p,d;\Lambda)}\beta_*^{3/2-7\varepsilon}\right] \\
&\leqslant \gamma\frac{N_*}{\ln N_*}\left[\frac{\beta_*^3}{(1-\beta_*\gamma)^2} C_p^2 \delta^{-2}\frac{pd}{\varphi(p,d;\Lambda)} + \frac{32\psi^4\beta_*}{2-\lambda_1\beta_*} + \frac{C_\circ\kappa^4\nu^2\eta_p^2\gamma^{-1}p\sqrt{d-p}}{\varphi(p,d;\Lambda)}\beta_*^{3/2-7\varepsilon}\right] \\
&\quad (\text{by } N_* \geqslant N_{3/2}, \text{ or equivalently, } (1-\beta_*\gamma)^{N_*} \leqslant \beta_*^{3/2}) \\
&\leqslant \gamma\frac{N_*}{\ln N_*}\beta_*\left[\frac{\beta_*^2}{(1-\beta_*\gamma)^2} C_p^2\delta^{-2}\frac{d}{p}\frac{1}{\frac{\lambda_1\lambda_d}{\lambda_1-\lambda_d}} + \frac{32\psi^4}{2-\lambda_1\beta_*} + \frac{C_\circ\kappa^4\nu^2\eta_p^2\gamma^{-1}}{\sqrt{p}\frac{\lambda_1\lambda_d}{\lambda_1-\lambda_d}}\beta_*^{1/2-7\varepsilon}\right] \\
&\quad \left(\text{by } \varphi(p,d;\Lambda) \geqslant \frac{p(d-p)\lambda_1\lambda_d}{\lambda_1-\lambda_d} \text{ and } d \geqslant 2p\right) \\
&\leqslant \frac{3}{2}\left[\frac{\beta_*^{1+3\varepsilon}}{(1-\beta_*\gamma)^2}\frac{C_p^2}{p}\frac{\lambda_1-\lambda_d}{\lambda_1\lambda_d} + \frac{32\psi^4}{2-\lambda_1\beta_*} + C_\circ\kappa^4\nu^2\eta_p^2\gamma^{-1}p^{-1/2}\frac{\lambda_1-\lambda_d}{\lambda_1\lambda_d}\beta_*^{1/2-7\varepsilon}\right] \\
&\quad (\text{by } d\beta_*^{1-3\varepsilon} \leqslant \delta^2) \\
&=: C_*(d, N_*, \delta).
\end{aligned}$$

Since $\beta_* \leqslant 1$ and $\beta_*\gamma \leqslant \lambda_1\beta_* \leqslant \sqrt{2}-1$, we have

$$C_*(d, N_*, \delta) \leqslant \frac{3}{2}\left[\frac{C_p^2}{2(3-2\sqrt{2})p}\frac{\lambda_1-\lambda_d}{\lambda_1\lambda_d} + \frac{32\psi^4}{3-\sqrt{2}} + \frac{C_\circ\kappa^4\nu^2\eta_p^2(\lambda_1-\lambda_d)}{p^{1/2}\gamma\lambda_1\lambda_d}\right],$$

and also $C_*(d, N_*, \delta) \to 24\psi^4$ as $d \to \infty, N_* \to \infty$, as was to be shown. □

7 Conclusion

We have presented a detailed convergence analysis for the multi-dimensional subspace online PCA iteration on sub-Gaussian samples, following the recent work [19] by Li et al. who considered only the one-dimensional case, i.e., the most significant principal component. Our results bear similar forms to theirs and when applied to the one-dimensional case yield estimates of essentially the same quality, as expected. As we embarked on the analysis presented in this paper, we found that a straightforward extension of the analysis in [19] was not possible because of the involvement of a cot-matrix of dimension higher than 1 in the multi-dimensional case but just a scalar in the one-dimensional case. Our results yield an explicit convergence rate, and it is *nearly optimal* because it nearly attains the minimax information lower bound for sub-Gaussian PCA under a constraint, as well as *nearly global* because the finite sample error bound holds with high probability if the initial value is uniformly sampled from the Grassmann manifold.

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Appendix A Supplementary proofs

Appendix A.1 Proof of Lemma 5.3(3)

We have

$$\operatorname{var}_\circ(\Delta T) = \operatorname{var}_\circ(T_L(\beta YY^{\mathrm{T}} + R_T)T_R) = \beta^2 \operatorname{var}_\circ(T_L YY^{\mathrm{T}} T_R) + 2\beta R_{\circ,1} + R_{\circ,2}, \tag{A.1}$$

where $R_{\circ,1} = \operatorname{cov}_\circ(T_L YY^{\mathrm{T}} T_R, T_L R_T T_R)$ and $R_{\circ,2} = \operatorname{var}_\circ(T_L R_T T_R)$. By (5.11),

$$\operatorname{var}_\circ(T_L YY^{\mathrm{T}} T_R) = \operatorname{var}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}}) + R_{\circ,0}, \tag{A.2}$$

where

$$\begin{aligned} R_{\circ,0} = {} & \operatorname{var}_\circ(T\bar{Y}\underline{Y}^{\mathrm{T}}T) + \operatorname{var}_\circ(T\bar{Y}\bar{Y}^{\mathrm{T}}) + \operatorname{var}_\circ(\underline{Y}\underline{Y}^{\mathrm{T}}T) \\ & - 2\operatorname{cov}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}}, T\bar{Y}\underline{Y}^{\mathrm{T}}T) - 2\operatorname{cov}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}}, T\bar{Y}\bar{Y}^{\mathrm{T}}) + 2\operatorname{cov}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}}, \underline{Y}\underline{Y}^{\mathrm{T}}T) \\ & + 2\operatorname{cov}_\circ(T\bar{Y}\underline{Y}^{\mathrm{T}}T, T\bar{Y}\bar{Y}^{\mathrm{T}}) - 2\operatorname{cov}_\circ(T\bar{Y}\underline{Y}^{\mathrm{T}}T, \underline{Y}\underline{Y}^{\mathrm{T}}T) \\ & - 2\operatorname{cov}_\circ(T\bar{Y}\bar{Y}^{\mathrm{T}}, \underline{Y}\underline{Y}^{\mathrm{T}}T). \end{aligned}$$

Examine (A.1) and (A.2) together to obtain $H_\circ = \operatorname{var}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}})$ and $R_\circ = \beta^2 R_{\circ,0} + 2\beta R_{\circ,1} + R_{\circ,2}$. We note

$$\begin{aligned} & Y_j = e_j^{\mathrm{T}} Y = e_j^{\mathrm{T}} \Lambda^{1/2}\Lambda^{-1/2} Y = \lambda_j^{1/2} e_j^{\mathrm{T}} \Lambda^{-1/2} Y, \\ & e_i^{\mathrm{T}} \operatorname{var}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}}) e_j = \operatorname{var}(e_i^{\mathrm{T}} \underline{Y}\bar{Y}^{\mathrm{T}} e_j) = \operatorname{var}(Y_{p+i} Y_j) = \mathrm{E}\{Y_{p+i}^2 Y_j^2\}. \end{aligned}$$

By [31, (5.11)],

$$\mathrm{E}\{Y_j^4\} = \lambda_j^2 \mathrm{E}\{(e_j^{\mathrm{T}}\Lambda^{-1/2}Y)^4\} \leqslant 16\lambda_j^2 \|e_j^{\mathrm{T}}\Lambda^{-1/2}Y\|_{\psi_2}^4 \leqslant 16\lambda_j^2 \|\Lambda^{-1/2}Y\|_{\psi_2}^4 = 16\lambda_j^2\psi^4.$$

Therefore, $e_i^{\mathrm{T}} \operatorname{var}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}}) e_j \leqslant [\mathrm{E}\{Y_{p+i}^4\}\mathrm{E}\{Y_j^4\}]^{1/2} \leqslant 16\lambda_{p+i}\lambda_j\psi^4$, i.e., $H_\circ = \operatorname{var}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}}) \leqslant 16\psi^4 H$. This proves (3)(a). To show (3)(b), first we bound the entrywise variance and covariance. For any matrices A_1 and A_2 of the same size, it holds that (see [14, p. 233])

$$\|A_1 \circ A_2\|_2 \leqslant \|A_1\|_2 \|A_2\|_2, \tag{A.3}$$

and thus

$$\|\operatorname{cov}_\circ(A_1, A_2)\|_2 = \|\mathrm{E}\{A_1 \circ A_2\} - \mathrm{E}\{A_1\} \circ \mathrm{E}\{A_2\}\|_2$$

$$\leqslant \mathrm{E}\{\|A_1\|_2\|A_2\|_2\} + \|\mathrm{E}\{A_1\}\|_2\|\mathrm{E}\{A_2\}\|_2, \tag{A.4a}$$

$$\|\mathrm{var}_\circ(A_1)\|_2 \leqslant \mathrm{E}\{\|A_1\|_2^2\} + \|\mathrm{E}\{A_1\}\|_2^2. \tag{A.4b}$$

Apply (A.4) to $R_{\circ,1}$ and $R_{\circ,2}$ to obtain

$$\|R_{\circ,1}\|_2 \leqslant 2C_T\nu\widetilde{\eta}_p^3\beta^2(1+\|T\|_2^2)^{5/2}, \quad \|R_{\circ,2}\|_2 \leqslant 2C_T^2\nu(\widetilde{\eta}_p\beta)^4(1+\|T\|_2^2)^3, \tag{A.5}$$

upon using

$$\|T_LYY^{\mathrm{T}}T_R\|_2 = \|T_LYY^{\mathrm{T}}VV^{\mathrm{T}}T_R\|_2 \leqslant \nu^{1/2}\widetilde{\eta}_p(1+\|T\|_2^2), \quad \|T_LR_TT_R\|_2 \leqslant C_T\nu^{1/2}(\widetilde{\eta}_p\beta)^2(1+\|T\|_2^2)^{3/2}.$$

For $R_{\circ,0}$, by (5.12), we have

$$\begin{aligned}
&\|\mathrm{cov}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}}, T\bar{Y}\underline{Y}^{\mathrm{T}}T)\|_2 \leqslant \mathrm{E}\{\|\underline{Y}\bar{Y}^{\mathrm{T}}\|_2^2\}\|T\|_2^2,\\
&\|\mathrm{cov}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}}, T\bar{Y}\bar{Y}^{\mathrm{T}})\|_2 \leqslant \mathrm{E}\{\|\underline{Y}\bar{Y}^{\mathrm{T}}\|_2\|\bar{Y}\bar{Y}^{\mathrm{T}}\|_2\}\|T\|_2,\\
&\|\mathrm{cov}_\circ(\underline{Y}\bar{Y}^{\mathrm{T}}, \underline{Y}\underline{Y}^{\mathrm{T}}T)\|_2 \leqslant \mathrm{E}\{\|\underline{Y}\bar{Y}^{\mathrm{T}}\|_2\|\underline{Y}\underline{Y}^{\mathrm{T}}\|_2\}\|T\|_2,\\
&\|\mathrm{cov}_\circ(T\bar{Y}\underline{Y}^{\mathrm{T}}T, T\bar{Y}\bar{Y}^{\mathrm{T}})\|_2 \leqslant \mathrm{E}\{\|\underline{Y}\bar{Y}^{\mathrm{T}}\|_2\|\bar{Y}\bar{Y}^{\mathrm{T}}\|_2\}\|T\|_2^3,\\
&\|\mathrm{cov}_\circ(T\bar{Y}\underline{Y}^{\mathrm{T}}T, \underline{Y}\underline{Y}^{\mathrm{T}}T)\|_2 \leqslant \mathrm{E}\{\|\underline{Y}\bar{Y}^{\mathrm{T}}\|_2\|\underline{Y}\underline{Y}^{\mathrm{T}}\|_2\}\|T\|_2^3,\\
&\|\mathrm{var}_\circ(T\bar{Y}\underline{Y}^{\mathrm{T}}T)\|_2 \leqslant \mathrm{E}\{\|\underline{Y}\bar{Y}^{\mathrm{T}}\|_2^2\}\|T\|_2^4,\\
&\|\mathrm{var}_\circ(T\bar{Y}\bar{Y}^{\mathrm{T}})\|_2 \leqslant \mathrm{E}\{\|\bar{Y}\bar{Y}^{\mathrm{T}}\|_2^2\}\|T\|_2^2 + \|T\bar{\Lambda}\|_2^2,\\
&\|\mathrm{var}_\circ(\underline{Y}\underline{Y}^{\mathrm{T}}T)\|_2 \leqslant \mathrm{E}\{\|\underline{Y}\underline{Y}^{\mathrm{T}}\|_2^2\}\|T\|_2^2 + \|\underline{\Lambda}T\|_2^2,\\
&\|\mathrm{cov}_\circ(T\bar{Y}\bar{Y}^{\mathrm{T}}, \underline{Y}\underline{Y}^{\mathrm{T}}T)\|_2 \leqslant \mathrm{E}\{\|\bar{Y}\bar{Y}^{\mathrm{T}}\|_2\|\underline{Y}\underline{Y}^{\mathrm{T}}\|_2\}\|T\|_2^2 + \|T\bar{\Lambda}\|_2\|\underline{\Lambda}T\|_2.
\end{aligned}$$

Since

$$\begin{aligned}
&\|\bar{Y}\bar{Y}^{\mathrm{T}}\|_2 + \|\underline{Y}\underline{Y}^{\mathrm{T}}\|_2 = \bar{Y}^{\mathrm{T}}\bar{Y} + \underline{Y}^{\mathrm{T}}\underline{Y} = Y^{\mathrm{T}}Y \leqslant \nu\widetilde{\eta}_p,\\
&\|\underline{Y}\bar{Y}^{\mathrm{T}}\|_2 = (\bar{Y}^{\mathrm{T}}\bar{Y})^{1/2}(\underline{Y}^{\mathrm{T}}\underline{Y})^{1/2} \leqslant \frac{\bar{Y}^{\mathrm{T}}\bar{Y} + \underline{Y}^{\mathrm{T}}\underline{Y}}{2} \leqslant \frac{\nu\widetilde{\eta}_p}{2},
\end{aligned}$$

we have

$$\begin{aligned}
\|R_{\circ,0}\|_2 &\leqslant \mathrm{E}\{2\|\underline{Y}\bar{Y}^{\mathrm{T}}\|_2^2 + (\|\bar{Y}\bar{Y}^{\mathrm{T}}\|_2 + \|\underline{Y}\underline{Y}^{\mathrm{T}}\|_2)^2\}\|T\|_2^2 + (\|T\bar{\Lambda}\|_2 + \|\underline{\Lambda}T\|_2)^2\\
&\quad + 2\mathrm{E}\{\|\underline{Y}\bar{Y}^{\mathrm{T}}\|_2(\|\bar{Y}\bar{Y}^{\mathrm{T}}\|_2 + \|\underline{Y}\underline{Y}^{\mathrm{T}}\|_2)\}(\|T\|_2 + \|T\|_2^3) + \mathrm{E}\{\|\underline{Y}\bar{Y}^{\mathrm{T}}\|_2^2\}\|T\|_2^4\\
&\leqslant (\nu\widetilde{\eta}_p)^2\|T\|_2 + \left[\frac{3}{2}(\nu\widetilde{\eta}_p)^2 + (\lambda_1+\lambda_{p+1})^2\right]\|T\|_2^2 + (\nu\widetilde{\eta}_p)^2\|T\|_2^3 + \frac{1}{4}(\nu\widetilde{\eta}_p)^2\|T\|_2^4\\
&\leqslant (\nu\widetilde{\eta}_p)^2\|T\|_2\left(1 + \frac{11}{2}\|T\|_2 + \|T\|_2^2 + \frac{1}{4}\|T\|_2^3\right).
\end{aligned} \tag{A.6}$$

Finally, collecting (A.5) and (A.6) yields the desired bound on $R_\circ = \beta^2R_{\circ,0} + 2\beta R_{\circ,1} + R_{\circ,2}$.

Appendix A.2 Estimation in the proof of Lemma 5.6

(1) $\mathrm{E}\{\widetilde{J}_1 \circ \widetilde{J}_1\} = \mathcal{L}^{2n}T^{(0)} \circ T^{(0)}$.

(2) $\mathrm{E}\{\widetilde{J}_1 \circ \widetilde{J}_{21}\} = \sum_{s=1}^{N_{1/2-3\varepsilon}-1}\mathcal{L}^{2n-s}T^{(0)} \circ \mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\} = 0$, because

$$\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\} = \mathrm{E}\{\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K} \mid \mathbb{F}_{s-1}\}\} = 0.$$

(3) $\mathrm{E}\{\widetilde{J}_1 \circ \widetilde{J}_{22}\} = \sum_{s=N_{1/2-3\varepsilon}}^{n}\mathcal{L}^{2n-s}T^{(0)} \circ \mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{T}_{s-1}}\mathbf{1}_{\mathbb{Q}_K}\} = 0$, because $\mathbb{T}_{s-1} \subset \mathbb{F}_{s-1}$, so

$$\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{T}_{s-1}}\mathbf{1}_{\mathbb{Q}_K}\} = \mathrm{P}\{\mathbb{T}_{s-1}\}\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K} \mid \mathbb{T}_{s-1}\} = \mathrm{P}\{\mathbb{T}_{s-1}\}\mathrm{E}\{\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K} \mid \mathbb{F}_{s-1}\} \mid \mathbb{T}_{s-1}\} = 0.$$

(4) $\mathrm{E}\{\widetilde{J}_1 \circ \widetilde{J}_3\} = \sum_{s=1}^{n}\mathcal{L}^{2n-s}T^{(0)} \circ \mathrm{E}\{E_T^{(s-1)}\mathbf{1}_{\mathbb{Q}_K}\}$. Recall (A.3). By Lemma 5.3(2)(a), we have

$$\|\mathrm{E}\{\widetilde{J}_1 \circ \widetilde{J}_3\|\}_2 \leqslant \sum_{s=1}^{n}\|\mathcal{L}\|_2^{2n-s}\|T^{(0)}\|_2\|\mathrm{E}\{E_T^{(s-1)}\mathbf{1}_{\mathbb{Q}_K}\}\|_2$$

$$
\begin{aligned}
&\leqslant \sum_{s=1}^{n}(1-\beta\gamma)^{2n-s}\left(\frac{\kappa^2}{4}-1\right)^{1/2}C_T\nu^{1/2}(\widetilde{\eta}_p\beta)^2\kappa^3\\
&\leqslant (1-\beta\gamma)^n\frac{(\kappa^2-1)^{1/2}C_T\nu^{1/2}\widetilde{\eta}_p^2\beta^2\kappa^3}{2\beta\gamma}\\
&\leqslant \frac{1}{2}\beta^{1-6\varepsilon}C_T\nu^{1/2}\widetilde{\eta}_p^2\gamma^{-1}\beta\kappa^4 \ (\text{by } n\geqslant N_{1-6\varepsilon}).
\end{aligned}
$$

(5) $\mathrm{E}\{\widetilde{J}_{21}\circ\widetilde{J}_{22}\}=\sum_{s=1}^{N_{1/2-3\varepsilon}-1}\sum_{s'=N_{1/2-3\varepsilon}}^{n}\mathcal{L}^{2n-s-s'}\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\circ D^{(s')}\mathbf{1}_{\mathbb{T}_{s'-1}}\mathbf{1}_{\mathbb{Q}_K}\}=0$, because $s<s'$ and

$$
\begin{aligned}
\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\circ D^{(s')}\mathbf{1}_{\mathbb{T}_{s'-1}}\mathbf{1}_{\mathbb{Q}_K}\}&=\mathrm{E}\{D^{(s)}\circ D^{(s')}\mathbf{1}_{\mathbb{T}_{s'-1}}\mathbf{1}_{\mathbb{Q}_K}\}\\
&=\mathrm{P}\{\mathbb{T}_{s'-1}\}\mathrm{E}\{D^{(s)}\circ D^{(s')}\mathbf{1}_{\mathbb{Q}_K}\mid\mathbb{T}_{s'-1}\}\\
&=\mathrm{P}\{\mathbb{T}_{s'-1}\}\mathrm{E}\{\mathrm{E}\{D^{(s)}\circ D^{(s')}\mathbf{1}_{\mathbb{Q}_K}\mid\mathbb{F}_{s'-1}\}\mid\mathbb{T}_{s'-1}\}\\
&=\mathrm{P}\{\mathbb{T}_{s'-1}\}\mathrm{E}\{\mathrm{E}\{D^{(s')}\mathbf{1}_{\mathbb{Q}_K}\mid\mathbb{F}_{s'-1}\}\circ D^{(s)}\mid\mathbb{T}_{s'-1}\}\\
&=0.
\end{aligned}
$$

(6) We have

$$
\begin{aligned}
\mathrm{E}\{\widetilde{J}_{21}\circ\widetilde{J}_{21}\}&=\sum_{s=1}^{N_{1/2-3\varepsilon}-1}\sum_{s'=1}^{N_{1/2-3\varepsilon}-1}\mathcal{L}^{2n-s-s'}\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\circ D^{(s')}\mathbf{1}_{\mathbb{Q}_K}\}\\
&=\sum_{s=1}^{N_{1/2-3\varepsilon}-1}\mathcal{L}^{2(n-s)}\mathrm{E}\{D^{(s)}\circ D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\},
\end{aligned}
$$

because for $s\neq s'$,

$$
\begin{aligned}
\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\circ D^{(s')}\mathbf{1}_{\mathbb{Q}_K}\}&=\mathrm{E}\{D^{(s)}\circ D^{(s')}\mathbf{1}_{\mathbb{Q}_K}\}\\
&=\mathrm{E}\{\mathrm{E}\{D^{(\max\{s,s'\})}\mathbf{1}_{\mathbb{Q}_K}\mid\mathbb{F}_{\max\{s,s'\}-1}\}\circ D^{(\min\{s,s'\})}\}\\
&=0.
\end{aligned}
$$

Use (3)(a) and (3)(b) of Lemma 5.3 to obtain

$$
\begin{aligned}
\mathrm{E}\{D^{(s)}\circ D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\}&=\mathrm{E}\{\mathrm{E}\{D^{(s)}\circ D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\mid\mathbb{F}_{s-1}\}\}\\
&=\mathrm{E}\{\mathrm{var}_\circ([T^{(n+1)}-T^{(n)}]\mathbf{1}_{\mathbb{Q}_K}\mid\mathbb{F}_{s-1})\}\\
&=\mathrm{E}\{\beta^2H_\circ+R_\circ\}=\beta^2H_\circ+\mathrm{E}\{R_\circ\}.
\end{aligned}
$$

Therefore, $\mathrm{E}\{\widetilde{J}_{21}\circ\widetilde{J}_{21}\}=\beta^2\sum_{s=1}^{N_{1/2-3\varepsilon}-1}\mathcal{L}^{2(n-s)}H_\circ+\sum_{s=1}^{N_{1/2-3\varepsilon}-1}\mathcal{L}^{2(n-s)}\mathrm{E}\{R_\circ\}$. We have that for $\kappa>2\sqrt{2}$,

$$
\begin{aligned}
\|R_\circ\|_2&\leqslant(\nu\widetilde{\eta}_p\beta)^2\tau_{s-1}\left(1+\frac{11}{2}\tau_{s-1}+\tau_{s-1}^2+\frac{1}{4}\tau_{s-1}^3\right)+4C_T\kappa^5\nu(\widetilde{\eta}_p\beta)^3+2C_T^2\kappa^6\nu(\widetilde{\eta}_p\beta)^4\\
&\leqslant(\nu\widetilde{\eta}_p\beta)^2\tau_{s-1}\left(\kappa^2+\frac{21}{4}\kappa+\frac{1}{4}\kappa^3\right)+4C_T\kappa^5\nu(\widetilde{\eta}_p\beta)^3+2C_T^2\kappa^6\nu(\widetilde{\eta}_p\beta)^4\\
&\leqslant\frac{29+8\sqrt{2}}{32}\kappa^3\nu^2(\widetilde{\eta}_p\beta)^2\tau_{s-1}+4C_T\kappa^5\nu(\widetilde{\eta}_p\beta)^3+2C_T^2\kappa^6\nu(\widetilde{\eta}_p\beta)^4,
\end{aligned}
$$

where $\tau_{s-1}=\|T^{(s-1)}\|_2\leqslant(\kappa^2-1)^{1/2}$. Write $E_{21}:=\sum_{s=1}^{N_{1/2-3\varepsilon}-1}\mathcal{L}^{2(n-s)}\mathrm{E}\{R_\circ\}$. Since $2N_{1/2-3\varepsilon}-1\leqslant N_{1-6\varepsilon}\leqslant 2N_{1/2-3\varepsilon}$ by definition, we obtain

$$
\|E_{21}\|_2\leqslant\sum_{s=1}^{N_{1/2-3\varepsilon}-1}\|\mathcal{L}\|_2^{2(n-s)}\mathrm{E}\{\|R_\circ\|_2\}
$$

$$
\begin{aligned}
&\leqslant \frac{(1-\beta\gamma)^{2(n+1-N_{1/2-3\varepsilon})}}{\beta\gamma[2-\beta\gamma]} \mathrm{E}\{\|R_\circ\|_2\} \\
&\leqslant \frac{1-\beta\gamma}{2-\beta\gamma}\frac{(1-\beta\gamma)^n}{\beta\gamma} \mathrm{E}\{\|R_\circ\|_2\} \\
&\leqslant \frac{1}{2}\beta^{1-6\varepsilon}\gamma^{-1}\beta\kappa^4\nu\widetilde{\eta}_p^2\left(\frac{29+8\sqrt{2}}{32}\nu + 4C_T\kappa(\widetilde{\eta}_p\beta) + 2C_T^2\kappa^2(\widetilde{\eta}_p\beta)^2\right) \\
&\leqslant \left(\frac{29+8\sqrt{2}}{64} + 2C_T\kappa(\widetilde{\eta}_p\beta) + C_T^2\kappa^2(\widetilde{\eta}_p\beta)^2\right)\gamma^{-1}\kappa^4\nu^2\widetilde{\eta}_p^2\beta^{2-6\varepsilon}.
\end{aligned}
$$

(7) We have

$$
\begin{aligned}
\mathrm{E}\{\widetilde{J}_{22}\circ\widetilde{J}_{22}\} &= \sum_{s=N_{1/2-3\varepsilon}}^{n} \mathcal{L}^{2(n-s)}\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\mathbf{1}_{\mathbb{T}_{s-1}} \circ D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\mathbf{1}_{\mathbb{T}_{s-1}}\} \\
&= \beta^2 \sum_{s=N_{1/2-3\varepsilon}}^{n} \mathcal{L}^{2(n-s)} H_\circ + \sum_{s=N_{1/2-3\varepsilon}}^{n} \mathcal{L}^{2(n-s)}\mathrm{E}\{R_\circ\mathbf{1}_{\mathbb{T}_{s-1}}\},
\end{aligned}
$$

because for $s\neq s'$,

$$
\begin{aligned}
&\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\mathbf{1}_{\mathbb{T}_{s-1}} \circ D^{(s')}\mathbf{1}_{\mathbb{Q}_K}\mathbf{1}_{\mathbb{T}_{s'-1}}\} \\
&\quad= \mathrm{E}\{D^{(s)}\circ D^{(s')}\mathbf{1}_{\mathbb{Q}_K}\mathbf{1}_{\mathbb{T}_{s-1}}\mathbf{1}_{\mathbb{T}_{s'-1}}\} \\
&\quad= \mathrm{E}\{D^{(s)}\circ D^{(s')}\mathbf{1}_{\mathbb{Q}_K} \mid \mathbb{T}_{s-1}\cap\mathbb{T}_{s'-1}\}\,\mathrm{P}\{\mathbb{T}_{s-1}\cap\mathbb{T}_{s'-1}\} \\
&\quad= \mathrm{E}\{\mathrm{E}\{D^{(\max\{s,s'\})}\mathbf{1}_{\mathbb{Q}_K} \mid \mathbb{F}_{\max\{s,s'\}-1}\}\circ D^{(\min\{s,s'\})} \mid \mathbb{T}_{s-1}\cap\mathbb{T}_{s'-1}\}\,\mathrm{P}\{\mathbb{T}_{s-1}\cap\mathbb{T}_{s'-1}\} \\
&\quad= 0
\end{aligned}
$$

and

$$
\begin{aligned}
\mathrm{E}\{D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\mathbf{1}_{\mathbb{T}_{s-1}} \circ D^{(s)}\mathbf{1}_{\mathbb{Q}_K}\mathbf{1}_{\mathbb{T}_{s-1}}\} &= \mathrm{E}\{D^{(s)}\circ D^{(s')}\mathbf{1}_{\mathbb{Q}_K}\mathbf{1}_{\mathbb{T}_{s-1}}\} \\
&= \mathrm{P}\{\mathbb{T}_{s-1}\}\mathrm{E}\{\mathrm{E}\{D^{(s)}\circ D^{(s)}\mathbf{1}_{\mathbb{Q}_K} \mid \mathbb{F}_{s-1}\} \mid \mathbb{T}_{s-1}\} \\
&\leqslant \beta^2 H_\circ + \mathrm{E}\{R_\circ\mathbf{1}_{\mathbb{T}_{s-1}}\}.
\end{aligned}
$$

We have

$$
\begin{aligned}
\|R_\circ\mathbf{1}_{\mathbb{T}_{s-1}}\|_2 &\leqslant \frac{29+8\sqrt{2}}{32}\kappa^3\nu^2(\widetilde{\eta}_p\beta)^2\tau_{s-1} + 4C_T\kappa^5\nu(\widetilde{\eta}_p\beta)^3 + 2C_T^2\kappa^6\nu(\widetilde{\eta}_p\beta)^4 \\
&\leqslant \frac{29+8\sqrt{2}}{32}\kappa^3\nu^2(\widetilde{\eta}_p\beta)^2(\kappa^2-1)^{1/2}\beta^{1/2-3\varepsilon} + 4C_T\kappa^5\nu(\widetilde{\eta}_p\beta)^3 + 2C_T^2\kappa^6\nu(\widetilde{\eta}_p\beta)^4 \\
&\leqslant \frac{29+8\sqrt{2}}{32}\kappa^4\nu^2(\widetilde{\eta}_p\beta)^2\beta^{1/2-3\varepsilon} + 4C_T\kappa^5\nu(\widetilde{\eta}_p\beta)^3 + 2C_T^2\kappa^6\nu(\widetilde{\eta}_p\beta)^4.
\end{aligned}
$$

Write $E_{22} := \sum_{s=N_{1/2-3\varepsilon}}^{n} \mathcal{L}^{2(n-s)}\mathrm{E}\{R_\circ\mathbf{1}_{\mathbb{T}_{s-1}}\}$ for which we have

$$
\begin{aligned}
\|E_{22}\|_2 &\leqslant \sum_{s=N_{1/2-3\varepsilon}}^{n} \|\mathcal{L}\|_2^{2(n-s)}\mathrm{E}\{\|R_\circ\mathbf{1}_{\mathbb{T}_{s-1}}\|_2\} \\
&\leqslant \frac{1}{\beta\gamma[2-\beta\gamma]}\mathrm{E}\{\|R_\circ\mathbf{1}_{\mathbb{T}_{s-1}}\|_2\} \\
&\leqslant \frac{1}{3-\sqrt{2}}\gamma^{-1}\kappa^4\nu\widetilde{\eta}_p^2\beta\left(\frac{29+8\sqrt{2}}{32}\nu\beta^{1/2-3\varepsilon} + 4C_T\kappa(\widetilde{\eta}_p\beta) + 2C_T^2\kappa^2(\widetilde{\eta}_p\beta)^2\right) \\
&\leqslant \frac{1}{3-\sqrt{2}}\left(\frac{29+8\sqrt{2}}{32} + 4C_T\kappa\widetilde{\eta}_p\beta^{1/2+3\varepsilon} + 2C_T^2\kappa^2\widetilde{\eta}_p^2\beta^{3/2+3\varepsilon}\right)\gamma^{-1}\kappa^4\nu^2\widetilde{\eta}_p^2\beta^{3/2-3\varepsilon}.
\end{aligned}
$$

(8) $\mathrm{E}\{\widetilde{J}_3 \circ \widetilde{J}_3\} = \sum_{s=1}^n \mathcal{L}^{2(n-s)} \mathrm{E}\{E_T^{(s-1)} \mathbf{1}_{\mathbb{Q}_K} \circ E_T^{(s-1)} \mathbf{1}_{\mathbb{Q}_K}\}$. Also, by (A.3),

$$\begin{aligned}\|\mathrm{E}\{\widetilde{J}_3 \circ \widetilde{J}_3\}\|_2 &\leqslant \sum_{s=1}^n \|\mathcal{L}\|_2^{2(n-s)} \mathrm{E}\{\|E_T^{(s-1)} \mathbf{1}_{\mathbb{Q}_K}\|_2^2\} \\ &\leqslant \sum_{s=1}^n (1-\beta\gamma)^{2(n-s)} [C_T \nu^{1/2} (\widetilde{\eta}_p \beta)^2 \kappa^3]^2 \\ &\leqslant \frac{C_T^2 \nu (\widetilde{\eta}_p \beta)^4 \kappa^6}{\beta\gamma[2-\beta\gamma]} \leqslant \frac{1}{3-\sqrt{2}} C_T^2 \nu \widetilde{\eta}_p^4 \gamma^{-1} \kappa^6 \beta^3.\end{aligned}$$

Appendix A.3 Proof of Lemma 6.1

The proof is the same as that for the case $p = 1$ by Kummer's solutions of the hypergeometric differential equation (see, e.g., [20, Subsection 3.8]). Let the eigenvalues of T be $\mu_1, \ldots, \mu_m$. Since ${}_2F_1(a, b; c; T)$ is defined on the spectrum of T, it is a function of $\mu_1, \ldots, \mu_m$. When treated as such, by [23, Theorem 7.5.5], ${}_2F_1(a, b; c; T)$ is the unique solution of partial differential equations,

$$\begin{aligned}&\mu_i(1-\mu_i)\frac{\partial^2 F}{\partial \mu_i^2} + \left(c - \frac{m-1}{2} - \left(a+b+1-\frac{m-1}{2}\right)\mu_i + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i} \frac{\mu_i(1-\mu_i)}{\mu_i-\mu_j}\right)\frac{\partial F}{\partial \mu_i} \\ &\quad - \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i} \frac{\mu_j(1-\mu_j)}{\mu_i-\mu_j}\frac{\partial F}{\partial \mu_j} - abF = 0 \end{aligned} \tag{A.7}$$

subject to the conditions that F is a symmetric function of $\mu_1, \ldots, \mu_m$, analytic at $(\mu_1, \ldots, \mu_m) = (0, \ldots, 0)$, and $F(0, \ldots, 0) = 1$.

We claim that $\widetilde{F}(\mu_1, \ldots, \mu_m) := {}_2F_1(a, b; a+b-c+\frac{m+1}{2}; I-T)$ satisfies (A.7). In fact, letting $\widetilde{\mu}_i = 1-\mu_i$ for $1 \leqslant i \leqslant m$ which are the eigenvalues of $I-T$, we have

$$\begin{aligned}&\mu_i(1-\mu_i)\frac{\partial^2 \widetilde{F}}{\partial \mu_i^2} + \left(c - \frac{m-1}{2} - \left(a+b+1-\frac{m-1}{2}\right)\mu_i + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i} \frac{\mu_i(1-\mu_i)}{\mu_i-\mu_j}\right)\frac{\partial \widetilde{F}}{\partial \mu_i} \\ &\quad - \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i} \frac{\mu_j(1-\mu_j)}{\mu_i-\mu_j}\frac{\partial \widetilde{F}}{\partial \mu_j} - ab\widetilde{F} \\ &\quad = (1-\widetilde{\mu}_i)\widetilde{\mu}_i \frac{\partial^2 \widetilde{F}}{\partial \widetilde{\mu}_i^2} + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i} \frac{(1-\widetilde{\mu}_j)\widetilde{\mu}_j}{(1-\widetilde{\mu}_i)-(1-\widetilde{\mu}_j)}\frac{\partial \widetilde{F}}{\partial \widetilde{\mu}_j} - ab\widetilde{F} \\ &\qquad - \left(c - \frac{m-1}{2} - \left(a+b+1-\frac{m-1}{2}\right)(1-\widetilde{\mu}_i) + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i} \frac{(1-\widetilde{\mu}_i)\widetilde{\mu}_i}{(1-\widetilde{\mu}_i)-(1-\widetilde{\mu}_j)}\right)\frac{\partial \widetilde{F}}{\partial \widetilde{\mu}_i} \\ &\quad = (1-\widetilde{\mu}_i)\widetilde{\mu}_i \frac{\partial^2 \widetilde{F}}{\partial \widetilde{\mu}_i^2} - \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i} \frac{(1-\widetilde{\mu}_j)\widetilde{\mu}_j}{\widetilde{\mu}_i-\widetilde{\mu}_j}\frac{\partial \widetilde{F}}{\partial \widetilde{\mu}_j} - ab\widetilde{F} \\ &\qquad + \left(-c + \frac{m+1}{2} + a + b - \frac{m-1}{2} - \left(a+b+1-\frac{m-1}{2}\right)\widetilde{\mu}_i + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i} \frac{(1-\widetilde{\mu}_i)\widetilde{\mu}_i}{\widetilde{\mu}_i-\widetilde{\mu}_j}\right)\frac{\partial \widetilde{F}}{\partial \widetilde{\mu}_i} \\ &\quad = 0,\end{aligned}$$

where the last equality holds because $\widetilde{F}(\mu_1, \ldots, \mu_m) = {}_2F_1(a, b; a+b-c+\frac{m+1}{2}; I-T)$ satisfies a version of (A.7) after substitutions: $\mu_i \to \widetilde{\mu}_i$ for all i and $c \to a+b-c+\frac{m+1}{2}$.

$\widehat{F}(\mu_1, \ldots, \mu_m) := \det(T)^{\frac{m+1}{2}-c} {}_2F_1(a-c+\frac{m+1}{2}, b-c+\frac{m+1}{2}; m+1-c; T)$ satisfies (A.7), too. Set $t = \frac{m+1}{2} - c$ and write $G(\mu_1, \ldots, \mu_m) = {}_2F_1(a+t, b+t; c+2t; T)$. We have

$$\frac{\partial \widehat{F}}{\partial \mu_i} = \frac{t}{\mu_i}\det(T)^t G + \det(T)^t \frac{\partial G}{\partial \mu_i},$$

$$\frac{\partial^2 \widehat{F}}{\partial \mu_i^2} = \frac{t(t-1)}{\mu_i^2}\det(T)^t G + 2\frac{t}{\mu_i}\det(T)^t\frac{\partial G}{\partial \mu_i} + \det(T)^t\frac{\partial^2 G}{\partial \mu_i^2},$$

and thus

$$\begin{aligned}
&\mu_i(1-\mu_i)\frac{\partial^2 \widehat{F}}{\partial \mu_i^2} + \left(c - \frac{m-1}{2} - \left(a+b+1-\frac{m-1}{2}\right)\mu_i + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_i(1-\mu_i)}{\mu_i-\mu_j}\right)\frac{\partial \widehat{F}}{\partial \mu_i}\\
&\quad - \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_j(1-\mu_j)}{\mu_i-\mu_j}\frac{\partial \widehat{F}}{\partial \mu_j} - ab\widehat{F}\\
&\quad = \mu_i(1-\mu_i)\left(\frac{t(t-1)}{\mu_i^2}\det(T)^t G + 2\frac{t}{\mu_i}\det(T)^t\frac{\partial G}{\partial \mu_i} + \det(T)^t\frac{\partial^2 G}{\partial \mu_i^2}\right)\\
&\qquad + \left(c - \frac{m-1}{2} - \left(a+b+1-\frac{m-1}{2}\right)\mu_i + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_i(1-\mu_i)}{\mu_i-\mu_j}\right)\left(\frac{t}{\mu_i}\det(T)^t G + \det(T)^t\frac{\partial G}{\partial \mu_i}\right)\\
&\qquad - \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_j(1-\mu_j)}{\mu_i-\mu_j}\left(\frac{t}{\mu_i}\det(T)^t G + \det(T)^t\frac{\partial G}{\partial \mu_i}\right) - ab\det(T)^t G\\
&\quad = \det(T)^t\Bigg\{\mu_i(1-\mu_i)\frac{\partial^2 G}{\partial \mu_i^2} - \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_j(1-\mu_j)}{\mu_i-\mu_j}\frac{\partial G}{\partial \mu_j}\\
&\qquad + \left(2\mu_i(1-\mu_i)\frac{t}{\mu_i} + c - \frac{m-1}{2} - \left(a+b+1-\frac{m-1}{2}\right)\mu_i + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_i(1-\mu_i)}{\mu_i-\mu_j}\right)\frac{\partial G}{\partial \mu_i}\\
&\qquad + \Bigg[\mu_i(1-\mu_i)\frac{t(t-1)}{\mu_i^2} + \left(c - \frac{m-1}{2} - \left(a+b+1-\frac{m-1}{2}\right)\mu_i + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_i(1-\mu_i)}{\mu_i-\mu_j}\right)\frac{t}{\mu_i}\\
&\qquad - \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_j(1-\mu_j)}{\mu_i-\mu_j}\frac{t}{\mu_j} - ab\Bigg]G\Bigg\}\\
&\quad = \det(T)^t\Bigg\{\mu_i(1-\mu_i)\frac{\partial^2 G}{\partial \mu_i^2} - \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_j(1-\mu_j)}{\mu_i-\mu_j}\frac{\partial G}{\partial \mu_j}\\
&\qquad + \left(2(1-\mu_i)t + c - \frac{m-1}{2} - \left(a+b+1-\frac{m-1}{2}\right)\mu_i + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_i(1-\mu_i)}{\mu_i-\mu_j}\right)\frac{\partial G}{\partial \mu_i}\\
&\qquad + \left[\frac{t(t-1)}{\mu_i} - t(t-1) + \left(c - \frac{m-1}{2}\right)\frac{t}{\mu_i} - \left(a+b+1-\frac{m-1}{2}\right)t + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}(-1)t - ab\right]G\Bigg\}\\
&\quad = \det(T)^t\Bigg\{\mu_i(1-\mu_i)\frac{\partial^2 G}{\partial \mu_i^2} - \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_j(1-\mu_j)}{\mu_i-\mu_j}\frac{\partial G}{\partial \mu_j}\\
&\qquad + \left(2t + c - \frac{m-1}{2} - \left(2t+a+b+1-\frac{m-1}{2}\right)\mu_i + \frac{1}{2}\sum_{1\leqslant j\leqslant m}^{j\neq i}\frac{\mu_i(1-\mu_i)}{\mu_i-\mu_j}\right)\frac{\partial G}{\partial \mu_i}\\
&\qquad - [t^2 + (a+b)t + ab]G\Bigg\}\\
&\quad = 0,
\end{aligned}$$

where the last equality holds because $G(\mu_1,\ldots,\mu_m) = {}_2F_1(a+t, b+t; c+2t; T)$ satisfies a version of (A.7) after substitutions: $a \to a+t$, $b \to b+t$ and $c \to c+2t$.

Similarly $\widetilde{\widetilde{F}}(\mu_1,\ldots,\mu_m) := \det(I-T)^{c-a-b}{}_2F_1(c-b, c-a; c-a-b+\frac{m+1}{2}; I-T)$ satisfies (A.7). Thus, any linear combination of $\widetilde{F}$ and $\widetilde{\widetilde{F}}$, such as the right-hand side of (6.1), also satisfies (A.7). It can be verified that the combination is symmetric with respect to $\mu_1, \ldots, \mu_m$, and analytic at $T = 0$. Therefore, by the uniqueness and $F(0) = 1$, similarly to the discussion in [20, Subsection 3.9], we have (6.1).

Appendix A.4 Complementary calculation in the proof of Lemma 6.2

Here in defining g_d, although $\Gamma_p(-\frac{p}{2})$ and $\Gamma_p(\frac{1}{2})$ may be ∞, by analytic continuation, $\Gamma_p(-\frac{p}{2})/\Gamma_p(\frac{1}{2})$ is well defined because

$$\begin{aligned}\frac{\Gamma_p(-\frac{p}{2}+\epsilon)}{\Gamma_p(\frac{1}{2}+\epsilon)} &= \prod_{i=1}^{p} \frac{\Gamma(-\frac{p}{2}-\frac{i-1}{2}+\epsilon)}{\Gamma(\frac{1}{2}-\frac{i-1}{2}+\epsilon)} \\ &= \begin{cases} \displaystyle\prod_{i=1}^{p}\prod_{j=1}^{(p-1)/2} \frac{1}{\frac{-i}{2}-j+1+\epsilon} & \text{for odd } p, \\ \displaystyle\frac{\Gamma(\frac{1-2p}{2}+\epsilon)}{\Gamma(\frac{1}{2}+\epsilon)} \prod_{i=1}^{p-1}\prod_{j=1}^{p/2} \frac{1}{\frac{-i-1}{2}-j+1+\epsilon} & \text{for even } p \end{cases} \\ &\xrightarrow{\epsilon\to 0} \left\{ \begin{aligned} &\prod_{i=1}^{p}\prod_{j=1}^{(p-1)/2} \frac{-2}{i+2j-2}, \\ &\prod_{k=1}^{p} \frac{1}{\frac{-1}{2}-k+1} \prod_{i=1}^{p-1}\prod_{j=1}^{p/2} \frac{-2}{i+2j-1} \end{aligned} \right\} = \prod_{i=1}^{2\lfloor p/2\rfloor+1} \prod_{j=1}^{\lfloor p/2\rfloor} \frac{-2}{i+2j-2}.\end{aligned}$$

Also,

$$\frac{\Gamma_p(\frac{p}{2})}{\Gamma_p(\frac{p+1}{2})} = \prod_{i=1}^{p} \frac{\Gamma(\frac{p}{2}-\frac{i-1}{2})}{\Gamma(\frac{p+1}{2}-\frac{i-1}{2})} = \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{p+1}{2})}, \quad \frac{\Gamma_p(\frac{d}{2})}{\Gamma_p(\frac{d+1}{2})} = \prod_{i=1}^{p} \frac{\Gamma(\frac{d}{2}-\frac{i-1}{2})}{\Gamma(\frac{d+1}{2}-\frac{i-1}{2})} = \frac{\Gamma(\frac{d-p+1}{2})}{\Gamma(\frac{d+1}{2})},$$

which implies $f_d = \frac{\Gamma(\frac{1}{2})\Gamma(\frac{d+1}{2})}{\Gamma(\frac{p+1}{2})\Gamma(\frac{d-p+1}{2})}$. We have

$$f_d^{-1} g_d = \frac{\Gamma_p(\frac{p+1}{2})\Gamma_p(\frac{d}{2})\Gamma_p(-\frac{p}{2})}{\Gamma_p(\frac{p}{2})\Gamma_p(\frac{d-p}{2})\Gamma_p(\frac{1}{2})} = \frac{\Gamma(\frac{p+1}{2})\Gamma_p(\frac{d}{2})\Gamma_p(-\frac{p}{2})}{\Gamma(\frac{1}{2})\Gamma_p(\frac{d-p}{2})\Gamma_p(\frac{1}{2})}.$$

Note that

$$\frac{\Gamma_p(\frac{d}{2})}{\Gamma_p(\frac{d-p}{2})} = \prod_{i=1}^{p} \frac{\Gamma(\frac{d}{2}-\frac{i-1}{2})}{\Gamma(\frac{d-p}{2}-\frac{i-1}{2})} = \begin{cases} \displaystyle\frac{\Gamma(\frac{d}{2})}{\Gamma(\frac{d-p}{2})} \prod_{i=1}^{p}\prod_{j=1}^{(p-1)/2} \left(\frac{d-i}{2}-j\right) & \text{for odd } p, \\ \displaystyle\prod_{i=1}^{p}\prod_{j=1}^{p/2} \left(\frac{d-i}{2}-j\right) & \text{for even } p, \end{cases}$$

and by $\lim_{n\to\infty} \frac{\Gamma(n+\alpha)}{\Gamma(n)n^{\alpha}} = 1$ for any α (see, e.g., [20, (16) of Subsection 2.1]),

$$\frac{\Gamma(\frac{d}{2})}{\Gamma(\frac{d-p}{2})} = \begin{cases} \displaystyle\frac{\Gamma(\frac{d-1}{2})(\frac{d-1}{2})^{1/2}[1+\mathrm{o}(1)]}{\Gamma(\frac{d-1}{2})(\frac{d-1}{2})^{(1-p)/2}[1+\mathrm{o}(1)]} & \text{for odd } d, \\ \displaystyle\frac{\Gamma(\frac{d}{2})}{\Gamma(\frac{d}{2})(\frac{d}{2})^{-p/2}[1+\mathrm{o}(1)]} & \text{for even } d \end{cases} = \begin{cases} \left(\dfrac{d-1}{2}\right)^{p/2}[1+\mathrm{o}(1)], \\ \left(\dfrac{d}{2}\right)^{p/2}[1+\mathrm{o}(1)], \end{cases}$$

which implies

$$\frac{\Gamma_p(\frac{d}{2})}{\Gamma_p(\frac{d-p}{2})} = \left(\frac{d}{2}\right)^{p^2/2}[1+\mathrm{o}(1)] \quad \text{as } d\to\infty.$$