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The Interplay Between Implicit Bias and Benign Overfitting in Two-Layer Linear Networks

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Abstract

The recent success of neural network models has shone light on a rather surprising statistical phenomenon: statistical models that perfectly fit noisy data can generalize well to unseen test data. Understanding this phenomenon of *benign overfitting* has attracted intense theoretical and empirical study. In this paper, we consider interpolating two-layer linear neural networks trained with gradient flow on the squared loss and derive bounds on the excess risk when the covariates satisfy sub-Gaussianity and anti-concentration properties, and the noise is independent and sub-Gaussian. By leveraging recent results that characterize the implicit bias of this estimator, our bounds emphasize the role of both the quality of the initialization as well as the properties of the data covariance matrix in achieving low excess risk.

Keywords: implicit bias, generalization, benign overfitting, interpolation, neural networks, regression

1. Introduction

Understanding benign overfitting—the phenomenon where statistical models predict well on test data despite perfectly fitting noisy training data (see, e.g., Zhang et al., 2017; Belkin et al., 2019; Bartlett et al., 2021; Belkin, 2021)—has recently attracted intense attention. One line of work has focused on understanding this phenomenon in relatively simple models such as linear regression (Kobak et al., 2020; Hastie et al., 2022; Bartlett et al., 2020; Muthukumar et al., 2020; Negrea et al., 2020; Chinot and Lerasle, 2020; Wu and Xu, 2020; Tsigler and Bartlett, 2020; Bunea et al., 2020; Chinot et al., 2020; Koehler et al., 2021) including with random features (Hastie et al., 2022; Yang et al., 2020; Li et al., 2021), linear classification (Montanari et al., 2019; Chatterji and Long, 2021; Liang and Sur, 2020; Muthukumar et al., 2021; Hsu et al., 2021; Deng et al., 2022; Wang and Thrampoulidis, 2021), kernel regression (Liang and Rakhlin, 2020; Mei and Montanari, 2019; Liang et al., 2020) and simplicial nearest neighbor methods (Belkin et al., 2018).

A complementary line of work (Soudry et al., 2018; Ji and Telgarsky, 2019; Gunasekar et al., 2017; Nacson et al., 2019; Gunasekar et al., 2018b,a; Yun et al., 2021; Azulay et al.,

2021) has formalized the argument (Neyshabur et al., 2015) that, even when no explicit regularization is used in training these models, there is nevertheless implicit regularization encoded in the choice of the optimization method, loss function and initialization. They argue that this implicit bias is critical in determining the generalization properties of the learnt model.

Recently, Azulay et al. (2021) characterized the implicit bias of gradient flow applied to two-layer linear neural networks with the squared loss. More concretely, the setting is as follows. Given n data points $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^p \times \mathbb{R}$, let $\mathbf{y} := (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$ and $X := (x_1, \ldots, x_n)^\top \in \mathbb{R}^{n \times p}$. They studied two-layer linear networks, with m hidden units, and weights $a \in \mathbb{R}^m$ and $W \in \mathbb{R}^{m \times p}$, that map an input $x \in \mathbb{R}^p$ to the scalar

$$a^\top W x.$$

Let $\theta = a^\top W \in \mathbb{R}^p$ denote the standard parameterization of the resulting linear map. A two-layer linear network with parameters $\{a, W\}$ is said to be *balanced* if

$$aa^\top - WW^\top = 0.$$

Azulay et al. (2021) showed in Proposition 1 that, starting from a balanced initial point $(a(0), W(0))$, if the gradient flow converges to a solution that perfectly fits the data, then the solution can be characterized as follows:

$$\hat{\theta} \in \operatorname*{arg\,min}_{\theta \in \mathbb{R}^p} \|\theta\|^{3/2} - \frac{\theta(0)^\top \theta}{\sqrt{\|\theta(0)\|}}, \qquad \text{s.t.,} \;\; \mathbf{y} = X\theta. \tag{1}$$

In this paper, we study the generalization properties of this solution in the overparameterized regime, where such interpolation is possible. We prove upper bounds on the excess risk and show that it depends both on the properties of the eigenstructure of population covariance matrix—as in the case of the minimum ℓ_2-norm interpolant (ordinary least squares) (Bartlett et al., 2020; Tsigler and Bartlett, 2020)—and also on the quality of the initialization $\theta(0)$. In particular, we show that to drive the excess risk to zero, it suffices if the number of samples is large relative to the trace of the population covariance matrix and also that the number of "small" eigenvalues is large relative to n. Our bounds also show that the excess risk can be smaller as a rescaling of $\theta(0)$ gets closer to the optimal linear predictor.

An overview of the techniques that drive our analysis is as follows. We begin by showing that the predictor $\hat{\theta}$ can be viewed as a perturbation of the ordinary least squares solution in the subspace orthogonal to the row span of X. To characterize this perturbation we find that it is important to derive upper and lower bounds on $\mathrm{Tr}((XX^\top)^{-1})$. To do this, as done in past work, we instead bound the trace of the "tail" of the matrix—the submatrix formed by the many low variance directions—and show that it not only concentrates but also provides a good approximation for the trace of the inverse of the entire matrix $\mathrm{Tr}((XX^\top)^{-1})$.

Along the way we derive a new multiplicative high-probability lower bound on the least singular value of a non-isotropic rectangular random matrix (Lemma 15). We could not find such a result in the literature. The most closely related work that we know of (see Rudelson and Vershynin, 2010, and references therein), characterizing the "hard edge" of a random matrix, has focused on the most difficult case of isotropic square matrices.

The remainder of the paper is organized as follows. In Section 2 we introduce notation and definitions. In Section 3 we present our results. We provide a proof of our main result, Theorem 5, in Section 4 and prove our lower bound in Section 5. We conclude with a discussion in Section 6.

2. Preliminaries

This section includes notational conventions and a description of the setting.

2.1 Notation

Given a vector v, let $\|v\|$ denote its Euclidean norm. Given a matrix M, let $\|M\|$ denote its Frobenius norm and $\|M\|_{op}$ denote its operator norm. For any $j \in \mathbb{N}$, we denote the set $\{1, \ldots, j\}$ by $[j]$. Given a symmetric matrix $M \in \mathbb{R}^{p\times p}$ we let $\mu_1(M) \geq \ldots \geq \mu_p(M)$ denote its eigenvalues. We let I_p denote the identity matrix in p dimensions. Given any vector $v \in \mathbb{R}^p$, we let $v_{1:j} \in \mathbb{R}^p$ denote the vector obtained by zeroing out the last $p-j$ coordinates of v and let $v_{j+1:p} \in \mathbb{R}^p$ denote the vector obtained by zeroing out the first j coordinates. Given a symmetric positive semidefinite matrix $M \in \mathbb{R}^{p\times p}$, let $M_{1:j} \in \mathbb{R}^{p\times p}$ be the matrix formed by zeroing out the last $p-j$ rows and columns of M, and let $M_{j+1:p} \in \mathbb{R}^{p\times p}$ be the matrix formed by zeroing out the first j rows and columns. We let $\|v\|_M := \sqrt{v^\top M v}$ denote the matrix norm of v with respect to the matrix M. We use the standard "big Oh notation" (see, e.g., Cormen et al., 2009). We will use $c, c', c_1, \ldots$ to denote positive absolute constants, which may take different values in different contexts.

2.2 The setting

Throughout the paper we assume that $p > n$. Although we assume throughout that the input dimension p is finite, it is straightforward to extend our results to infinite p.

For random $(x, y) \in \mathbb{R}^p \times \mathbb{R}$, let

$$\theta^\star \in \operatorname*{arg\,min}_{\theta\in\mathbb{R}^p} \mathbb{E}\left[(y - x^\top\theta)^2\right]$$

be an arbitrary optimal linear regressor. We assume that x is mean zero and let $\Sigma := \mathbb{E}[xx^\top]$ denote the covariance matrix of the features. Without loss of generality, we will assume that the covariance matrix is diagonal and its eigenvalues are arranged in descending order $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p > 0$. (Note that such a covariance matrix can always be obtained by a rotation and permutation, and the estimator (1) is correspondingly transformed.) Recall that $\mathbf{y} = (y_1, \ldots, y_n)^\top$ is the vector of responses and $X = (x_1, \ldots, x_n)^\top$ is the data matrix. Define $\boldsymbol{\varepsilon} = (y_1 - x_1^\top\theta^\star, \ldots, y_n - x_n^\top\theta^\star)^\top = (\varepsilon_1, \ldots, \varepsilon_n)^\top$ to be the vector of noise.

We make the following assumptions:

(A.1) the samples $(x_1, y_1), \ldots, (x_n, y_n)$ and (x, y) are drawn i.i.d.;

(A.2) the features x and responses y are mean-zero;

(A.3) the features $x = \Sigma^{1/2}u$, where u has components that are independent σ_x^2-sub-Gaussian random variables with σ_x a positive constant, that is, for all $\phi \in \mathbb{R}^p$

$$\mathbb{E}\left[\exp\left(\phi^\top u\right)\right] \le \exp\left(\sigma_x^2\|\phi\|^2/2\right);$$

(A.4) there is an absolute constant c such that, for any unit vector $\phi \in \mathbb{S}^{n-1}$ and any $a \le b \in \mathbb{R}$

$$\mathbb{P}\left[(\Sigma^{-1/2}X^\top\phi)_i \in [a,b]\right] \le c|b-a|$$

for all $i \in [p]$;

(A.5) the difference $y - x^\top\theta^\star$ is σ_y^2-sub-Gaussian, conditionally on x, with σ_y a positive constant, that is, for all $\phi \in \mathbb{R}$

$$\mathbb{E}_y\left[\exp\left(\phi(y - x^\top\theta^\star)\right) \mid x\right] \le \exp\left(\sigma_y^2\phi^2/2\right)$$

(note that this implies that $\mathbb{E}[y \mid x] = x^\top\theta^\star$);

(A.6) for all x, the conditional variance of $y - x^\top\theta^\star$ is

$$\mathbb{E}_y\left[(y - x^\top\theta^\star)^2 \mid x\right] = \sigma^2$$

where σ is a positive constant.

We emphasize that σ_x, σ_y and σ are absolute constants, independent of all other problem parameters (n, p and Σ). All the constants going forward may depend on the value of these constants.

The assumptions stated above are satisfied in the case where u is generated from a mean-zero isotropic log-concave distribution with sub-Gaussian, independent entries and the noise $y - x^\top\theta^\star$ is independent and sub-Gaussian. We note that Assumptions A.1-A.3, A.5-A.6 are standard in the literature of benign overfitting in linear models (see, e.g., Bartlett et al., 2020). We make an additional small-ball probability assumption (Assumption A.4) which allows us to derive a sharper multiplicative lower tail bound for the minimum eigenvalue of the submatrices of X (Lemma 15).

Given the training samples define the excess risk of an estimate $\theta \in \mathbb{R}^p$ to be

$$\mathsf{Risk}(\theta) := \mathbb{E}_{x,y}\left[(y - x^\top\theta)^2 - (y - x^\top\theta^\star)^2\right],$$

where x, y are independent test samples.

Define the shorthand

$$w := \frac{\theta(0)}{\sqrt{\|\theta(0)\|}},$$

so that the estimator described in equation (1) can be written as the solution to a constrained convex program given by

$$\hat{\theta} \in \operatorname*{arg\,min}_{\theta \in \mathbb{R}^p} \|\theta\|^{3/2} - w^\top\theta, \qquad \text{s.t.,}\ \mathbf{y} = X\theta. \tag{2}$$

We let $UDV^\top = X$ be the singular value decomposition of X where $U \in \mathbb{R}^{n\times n}$ and $V \in \mathbb{R}^{p\times p}$ are unitary matrices and $D \in \mathbb{R}^{n\times p}$ is a rectangular diagonal matrix with its eigenvalues in descending order. By Lemma 26, we know that the rank of D is n. We let $D^\dagger \in \mathbb{R}^{p\times n}$ denote the pseudo-inverse of D. Since D has rank n, the bottom $p-n$ rows of $D^\dagger$ are identically zero.

Also define

$$\widetilde{\mathbf{y}} := D^\dagger U^\top \mathbf{y}, \qquad \widetilde{w} := V^\top w \qquad \text{and} \qquad \widetilde{\theta} := V^\top \hat{\theta}. \tag{3}$$

We will use the following definitions of the "effective rank" from Bartlett et al. (2020).

Definition 1 *Given a subset $S \subseteq [p]$, define $s(S) := \sum_{i\in S} \lambda_i$, and define the following ranks of the covariance matrix Σ with eigenvalues $\lambda_1, \ldots, \lambda_p$:*

$$r(S) := \frac{s(S)}{\max_{i\in S} \lambda_i} \qquad \text{and} \qquad R(S) := \frac{s(S)^2}{\sum_{i\in S} \lambda_i^2}.$$

Further given any $j \in [p]$, with some abuse of notation, define $s_j := \sum_{i>j} \lambda_i$ and

$$r_j := \frac{s_j}{\lambda_{j+1}} \qquad \text{and} \qquad R_j := \frac{s_j^2}{\sum_{i>j} \lambda_i^2}.$$

The following lemma (Bartlett et al., 2020, Lemma 5) relates these different effective ranks.

Lemma 2 *For any subset $S \subseteq [p]$ the ranks defined above satisfy the following:*

$$r(S) \leq R(S) \leq r(S)^2.$$

We define the index k below. The value of k shall help determine what we consider the "tail" of the covariance matrix.

Definition 3 *For a large enough constant b (that will be fixed henceforth), define*

$$k := \min\{j \geq 0 : r_j \geq bn\},$$

where the minimum of the empty set is defined as ∞.

Finally we define ψ, which is a rescaling of w.

Definition 4 *Define*

$$\psi := \frac{2\sqrt{\sigma} n^{1/4}}{3 s_k^{1/4}} w = \frac{2\sqrt{\sigma} n^{1/4}}{3 s_k^{1/4}} \frac{\theta(0)}{\sqrt{\|\theta(0)\|}}.$$

3. Main results

In this section we present our main result, Theorem 5, which is an excess risk bound for the estimator $\hat{\theta}$. It is proved in Section 4.

Theorem 5 *Under Assumptions 1-6, there exist constants* $c_0, \dots, c_7$ *such that for any* $\delta \in (e^{-c_0\sqrt{n}}, 1 - c_1 e^{-c_2 n})$*, if* $p \geq c_3(n+k)$*,* $n \geq c_4 \max\{k, s_k\}$ *and* $\|\theta^\star\|, \|w\| \leq c_5$ *then with probability at least* $1 - c_6\delta$

$$\mathsf{Risk}(\hat{\theta}) \leq \mathsf{Bias} + \mathsf{Variance} + \Xi,$$

where

$$\mathsf{Bias} \leq c_7 \left(\|(\theta^\star - \psi)_{1:k}\|^2_{\Sigma^{-1}_{1:k}} \left(\frac{s_k}{n}\right)^2 + \|(\theta^\star - \psi)_{k+1:p}\|^2_{\Sigma_{k+1:p}} \right) \leq \frac{2c_7\|\theta^\star - \psi\|^2 s_k}{n};$$

$$\mathsf{Variance} \leq c_7 \log(1/\delta) \left(\frac{k}{n} + \frac{n}{R_k} \right);$$

$$\Xi \leq c_7 \lambda_1 \|\psi\|^2 \left[\frac{n}{R_k} + \frac{n^2}{r_k^2} + \frac{s_k}{n} + \frac{\log(1/\delta)}{n} + \frac{k^2}{n^2} \right] \max\left\{ \sqrt{\frac{r_0}{n}}, \frac{r_0}{n}, \sqrt{\frac{\log(1/\delta)}{n}} \right\}.$$

Note that Bias goes to zero as $\psi \to \theta^\star$. In the upper bounds on the excess risk for linear models with a standard (one-layer) parameterization (see Tsigler and Bartlett, 2020, Theorem 1), the corresponding term scales with the square of the norm of $\theta^\star$ rather than $(\theta^\star - \psi)$. If one has a "guess" $\widehat{\psi}$ for $\theta^\star$, then—given knowledge of σ, s_k and n—it is possible to set the initialization as follows:

$$\theta(0) = \frac{9\widehat{\psi}\|\widehat{\psi}\|}{4}\sqrt{\frac{s_k}{\sigma^2 n}};$$

which ensures that $\psi = \widehat{\psi}$. Very accurate prior guesses $\widehat{\psi}$ of θ^* are rewarded with a very small value of the Bias term.

Next, we note that the upper bound on $\mathsf{Variance}$ here is identical to the upper bound on the variance for the minimum ℓ_2-norm interpolant (the OLS estimator) (see Bartlett et al., 2020, Theorem 4). The initialization $\theta(0)$ (through ψ) only affects the conditional bias of the estimator here, but leaves the conditional variance the same as the OLS solution. This is because, as we will show below in Lemma 11, $\hat{\theta}$ can be expressed as a perturbation to the OLS estimator in the subspace orthogonal to the row span of X. It turns out that the variance only depends on behavior of $\hat{\theta}$ in the subspace spanned by the data, where $\hat{\theta}$ and the OLS solution are identical.

As mentioned, $\hat{\theta}$ is a perturbation of the OLS estimator. In particular, it is perturbed by $\alpha^\star \mathsf{Proj}^{\perp}_{X}(w)$, where $\mathsf{Proj}^{\perp}_{X}(w)$ is the projection of w onto the subspace orthogonal to the row span of X and $\alpha^\star$ is a scalar random variable that depends on the data. We shall demonstrate in Lemma 13 that, under the setting specified by the theorem, $\alpha^\star$ concentrates around $\frac{2\sqrt{\sigma}n^{1/4}}{3s_k^{1/4}}$. The final term in the excess risk bound, Ξ, corresponds to the fluctuation of $\alpha^\star$. We might think of $\theta(0)$ (and hence w) as being constructed from ψ and an estimate of α^*; from this point of view, Ξ accounts for the contribution to the excess risk arising from the error in estimating $\alpha^\star$. Next we derive sufficient conditions for the excess risk to go to zero as $n, p \to \infty$. Consider the case where λ_1, $\|\theta^\star\|$, $\|\psi\|$ and $\log(1/\delta)$ are all bounded by constants. (In the case of $\|\psi\|$, this can be achieved by appropriately scaling $\theta(0)$.) For Bias to go to zero it suffices if

$$\frac{s_k}{n} \to 0.$$

For $\mathsf{Variance}$ to decrease to zero it suffices if

$$\frac{k}{n} \to 0 \quad \text{and} \quad \frac{n}{R_k} \to 0.$$

Finally, for Ξ to approach zero it suffices for

$$\frac{r_0}{n} \to 0$$

which also implies the condition $\frac{s_k}{n} \to 0$ needed to control the Bias term. (To see that $\frac{r_0}{n} \to 0$ suffices, recall that we have assumed that $\lambda_1, \log(1/\delta)$ and $\|\psi\|$ are constants. Further, the quantity in the square brackets of our bound on Ξ is at most a constant, which can be seen as follows. The definition of r_k implies that $r_k \geq bn$, and Lemma 2 gives $R_k \geq r_k$. Finally, we have assumed that $n \geq c \max\{k, s_k\}$.) To summarize, if $\frac{k}{n}, \frac{r_0}{n}, \frac{n}{R_k} \to 0$, the excess risk of this estimator approaches zero. Some discussion and examples of when this condition is satisfied are given in (Bartlett et al., 2020; Tsigler and Bartlett, 2020).

To develop intuition, we consider a special case of Theorem 5 defined as follows.

Definition 6 **((k, ε)-spike model)** *For $\varepsilon > 0$ and $k \in \mathbb{N}$, a (k, ε)-spike model is a setting where the eigenvalues of Σ are $\lambda_1 = \ldots = \lambda_k = 1$ and $\lambda_{k+1} = \ldots = \lambda_p = \varepsilon$.*

Instantiating Theorem 5 in the case of the (k, ε)-spike model, and removing some dominated terms, yields the following corollary.

Corollary 7 *Under Assumptions 1-6, there exist constants $c_0, \ldots, c_8$ such that in the (k, ε)-spike model for any $\delta \in (e^{-c_0\sqrt{n}}, 1 - c_1 e^{-c_2 n})$, if $p > c_3(n + k)$, $n \geq c_4 \max\{k, \varepsilon p\}$ and $\|\theta^\star\|, \|w\| \leq c_5$ then with probability at least $1 - c_6\delta$*

$$\mathsf{Risk}(\hat{\theta}) \leq \mathsf{Bias} + \mathsf{Variance} + \Xi,$$

where

$$\mathsf{Bias} \leq c_7 \left(\|(\theta^\star - \psi)_{1:k}\|^2 \left(\frac{\varepsilon p}{n}\right)^2 + \varepsilon \|(\theta^\star - \psi)_{k+1:p}\|^2 \right) \leq c_8 \|\theta^\star - \psi\|^2 \left(\frac{\varepsilon p}{n}\right);$$

$$\mathsf{Variance} \leq c_7 \log(1/\delta) \left(\frac{k}{n} + \frac{n}{p}\right);$$

$$\Xi \leq c_7 \lambda_1 \|\psi\|^2 \left[\frac{n}{p} + \frac{\varepsilon p}{n} + \frac{\log(1/\delta)}{n} + \frac{k^2}{n^2}\right] \max\left\{\sqrt{\frac{k + \varepsilon p}{n}}, \sqrt{\frac{\log(1/\delta)}{n}}\right\}.$$

Again, in the case where λ_1, $\|\psi\|$ and $\log(1/\delta)$ are bounded by constants, a sufficient condition for the excess risk to decrease to zero is when $\frac{\varepsilon p}{n}, \frac{k}{n}, \frac{n}{p} \to 0$.

Next we establish a lower bound. It is proved in Section 5.

Proposition 8 *If $a(0)$ and $W(0)$ are chosen randomly, independent of X and $\mathbf{y}$, so that the distribution of $a(0)^\top W(0)$ is symmetric about the origin, then*

$$\mathbb{E}_{a(0),W(0),X,\mathbf{y}}[\mathsf{Risk}(\hat{\theta})] \geq \mathbb{E}\left[\theta^{\star\top} B\theta^\star\right] + \sigma^2 \mathbb{E}\left[\mathrm{Tr}(C)\right],$$

where

$$\begin{aligned} B &:= \left(I - X^\top (XX^\top)^{-1} X\right) \Sigma \left(I - X^\top (XX^\top)^{-1} X\right) \quad \text{and} \\ C &:= (XX^\top)^{-1} X \Sigma X^\top (XX^\top)^{-1}. \end{aligned}$$

Remark 9 *For the distribution of $a(0)^\top W(0)$ to be symmetric about the origin, it suffices that $a(0)$ and $W(0)$ are chosen independently, and that either the distribution of $a(0)$ is symmetric about the origin, or the distribution of $W(0)$ is.*

Remark 10 *Bartlett et al. (2020) proved that $\mathbb{E}[\mathrm{Tr}(C)] \geq c\left(\frac{k}{n} + \frac{n}{R_k}\right)$ for a constant c. Tsigler and Bartlett (2020) proved a lower bound on $\mathbb{E}[\theta^{\star\top} B\theta^\star]$ under the assumption that the signs of the components of $\theta^\star$ are chosen uniformly at random. For the case that $\psi = 0$, their lower bound matches the upper bound on* Bias *from Theorem 5 of this paper under the assumptions of that theorem. However, there is a gap in the upper and lower bounds when $\psi \neq 0$.*

4. Proof details

The proof of Theorem 5 is built up in parts. First, in Lemma 11 we show that $\hat{\theta}$ can be viewed as a random perturbation of the ordinary least squares (OLS) solution in the subspace orthogonal to the row span of X. In Lemma 12, we show that the excess risk can be decomposed into two terms, one that can bounded above by $\mathsf{Variance}$ and the other that is upper bounded by $\mathsf{Bias} + \Xi$. The next piece is Lemma 13 which is crucial in helping us characterize the perturbation to the OLS solution. To do this we first present concentration inequalities in Section 4.1, then we establish upper and lower bounds on $\mathrm{Tr}((XX^\top)^{-1})$ in Section 4.2, and finally prove Lemma 13 in Section 4.3. We finish by combining all of these elements to prove the theorem in Section 4.4. Throughout this section we assume that the assumptions made in Theorem 5 are in force.

A note about constants. As mentioned earlier, we will not always provide specific constants. The constants $c_1, c_2, \ldots$ in our proofs are independent of the problem parameters, but they can depend on one another. It will not be hard to verify, however, that the constraints on their values are satisfiable. When we write "c_i is large enough", this should be understood to be relative to the constants previously introduced in the proof not including b, the constant used in the definition of r_k. Loosely speaking, b is chosen last: it should be taken to be large relative to all other constants.

We begin with the following lemma that provides a closed-form formula for $\hat{\theta}$ as a perturbation of the ordinary least squares solution.

Lemma 11 *The solution $\hat{\theta}$ can be expressed as follows:*

$$\hat{\theta} = \hat{\theta}_{\mathsf{OLS}} + \alpha^\star (I - X^\top (XX^\top)^{-1} X) w,$$

where $\hat{\theta}_{\mathsf{OLS}} = X^\top \left(XX^\top\right)^{-1}\mathbf{y}$ *is the ordinary least squares solution (minimum* ℓ_2*-norm interpolant) and*

$$\alpha^\star = \sqrt{\frac{8\|\widetilde{w}_{n+1:p}\|^2 + \sqrt{64\|\widetilde{w}_{n+1:p}\|^4 + 1296\|\widetilde{\mathbf{y}}\|^2}}{81}}. \tag{4}$$

where $\widetilde{w}$ *and* $\widetilde{\mathbf{y}}$ *are defined in* (3)*.*

Proof Recall that $X = UDV^\top$ is the singular value decomposition of X. Therefore,

$$\begin{aligned}
&\hat{\theta} \in \operatorname*{arg\,min}_{\theta\in\mathbb{R}^p} \|\theta\|^{3/2} - w^\top\theta, \qquad \text{s.t., } \mathbf{y} = X\theta \\
\iff &\hat{\theta} \in \operatorname*{arg\,min}_{\theta\in\mathbb{R}^p} \|\theta\|^{3/2} - w^\top\theta, \qquad \text{s.t., } D^\dagger U^\top \mathbf{y} = D^\dagger U^\top X\theta \\
\iff &\hat{\theta} \in \operatorname*{arg\,min}_{\theta\in\mathbb{R}^p} \|\theta\|^{3/2} - w^\top\theta, \qquad \text{s.t., } \widetilde{\mathbf{y}} = D^\dagger U^\top X\theta \\
\iff &V^\top\hat{\theta} \in \operatorname*{arg\,min}_{\theta\in\mathbb{R}^p} \|V^\top\theta\|^{3/2} - (w^\top V)V^\top\theta, \qquad \text{s.t., } \widetilde{\mathbf{y}} = D^\dagger U^\top XV(V^\top\theta) \\
&\qquad\qquad\text{(since the Euclidean norm is rotation invariant and } VV^\top = I_p) \\
\iff &\widetilde{\theta} \in \operatorname*{arg\,min}_{\theta\in\mathbb{R}^p} \|\theta\|^{3/2} - \widetilde{w}^\top\theta, \qquad \text{s.t., } \widetilde{\mathbf{y}} = D^\dagger U^\top XV\theta.
\end{aligned}$$

Since the bottom $p-n$ rows of $D^\dagger$ are identically zero, the vector $\widetilde{\mathbf{y}}$ can be written $(\widetilde{\mathbf{y}}_1, \ldots, \widetilde{\mathbf{y}}_n, 0, \ldots, 0)^\top$. Since the SVD of $X = UDV^\top$ we have that

$$D^\dagger U^\top XV\theta = D^\dagger U^\top UDV^\top V\theta = D^\dagger D\theta = \begin{bmatrix} I_n & 0 \\ 0 & 0 \end{bmatrix}\theta.$$

Hence, for the constraint to be satisfied, the first n coordinates of $\widetilde{\theta}$ are required to be equal to $(\widetilde{\mathbf{y}}_1, \ldots, \widetilde{\mathbf{y}}_n)$, and the remaining coordinates of $\widetilde{\theta}$ can be anything. That is, the constraints are satisfied when $\widetilde{\theta} = (\widetilde{\mathbf{y}}_1, \ldots, \widetilde{\mathbf{y}}_n, 0, \ldots, 0)^\top + \phi$, for some $\phi \in \mathbb{R}^p$ with its first n coordinates all equal to zero.

To find this optimal vector $\phi^\star$ we can now proceed to solve the following *unconstrained* optimization problem:

$$\phi^\star \in \operatorname*{arg\,min}_{\phi\in\mathbb{R}^p} \left(\|\widetilde{\theta}_{1:n}\|^2 + \|\phi\|^2\right)^{3/4} - \sum_{j=n+1}^{p} \widetilde{w}_j\phi_j.$$

Since the first term in the objective function above is rotationally invariant, it must be the case that the minimizer has the form $\phi^\star = \alpha^\star\widetilde{w}_{n+1:p}$, for some $\alpha^\star > 0$. That is, it is positively aligned with the tail of the vector $\widetilde{w}$. (If $\phi^\star$ was not in the span of $\widetilde{w}_{n+1:p}$, removing the projection of $\phi^\star$ in the subspace orthogonal to this direction would improve the norm without affecting the second term, and if $\phi^\star \cdot \widetilde{w}_{n+1:p} < 0$, then $-\phi^\star$ would be a better solution than $\phi^\star$.) In particular, we have

$$\widetilde{w}_{n+1:p} = 0 \Rightarrow \phi^\star = 0.$$

Otherwise, $\phi^\star = \alpha^\star \widetilde{w}_{n+1:p}$ for the solution $\alpha^\star$ of the following one-dimensional problem:

$$\alpha^\star \in \operatorname*{arg\,min}_{\alpha>0} \left(\|\widetilde{\theta}_{1:n}\|^2 + \alpha^2 \|\widetilde{w}_{n+1:p}\|^2 \right)^{3/4} - \alpha \|\widetilde{w}_{n+1:p}\|^2.$$

To simplify notation, let $\rho := \|\widetilde{\theta}_{1:n}\|^2$ and $\zeta := \|\widetilde{w}_{n+1:p}\|^2 > 0$. The first derivative of the objective function is as follows:

$$\frac{d}{d\alpha}\left[\left(\rho + \zeta\alpha^2\right)^{3/4} - \alpha\zeta \right] = \frac{3\zeta\alpha}{2\left(\rho + \zeta\alpha^2\right)^{1/4}} - \zeta.$$

Setting this first derivative equal to zero we get that

$$\begin{aligned}
& \frac{3\zeta\alpha}{2\left(\rho + \zeta\alpha^2\right)^{1/4}} - \zeta = 0 \\
\iff & \frac{3\alpha}{2\left(\rho + \zeta\alpha^2\right)^{1/4}} - 1 = 0 \\
\iff & \frac{3\alpha}{2} = \left(\rho + \zeta\alpha^2\right)^{1/4} \\
\iff & \frac{81\alpha^4}{16} = \rho + \zeta\alpha^2 \qquad \text{(because } \alpha > 0 \text{ at the optimum)} \\
\iff & 81\alpha^4 - 16\zeta\alpha^2 - 16\rho = 0.
\end{aligned}$$

We can view this as a quadratic equation in α^2, so

$$\alpha^2 = \frac{16\zeta \pm \sqrt{256\zeta^2 + 5184\rho}}{162} = \frac{16\zeta\left(1 \pm \sqrt{1 + \frac{81\rho}{4\zeta^2}}\right)}{162},$$

but the solution with the negative sign can be ignored since α^2 must be positive. Taking square roots we get that

$$\alpha = \pm\sqrt{\frac{8\zeta\left(1 + \sqrt{1 + \frac{81\rho}{4\zeta^2}}\right)}{81}}.$$

Again, we drop the negative solution since we know that $\alpha > 0$ at the optimum. Thus we find that

$$\widetilde{\theta} = \widetilde{\mathbf{y}} + \alpha^\star \widetilde{w}_{n+1:p}$$

for

$$\begin{aligned}
\alpha^\star = \sqrt{\frac{8\zeta\left(1 + \sqrt{1 + \frac{81\rho}{4\zeta^2}}\right)}{81}} &= \sqrt{\frac{8\|\widetilde{w}_{n+1:p}\|^2\left(1 + \sqrt{1 + \frac{81\|\widetilde{\theta}_{1:n}\|^2}{4\|\widetilde{w}_{n+1:p}\|^4}}\right)}{81}} \\
&= \sqrt{\frac{8\|\widetilde{w}_{n+1:p}\|^2 + \sqrt{64\|\widetilde{w}_{n+1:p}\|^4 + 1296\|\widetilde{\theta}_{1:n}\|^2}}{81}} \\
&= \sqrt{\frac{8\|\widetilde{w}_{n+1:p}\|^2 + \sqrt{64\|\widetilde{w}_{n+1:p}\|^4 + 1296\|\widetilde{\mathbf{y}}\|^2}}{81}}.
\end{aligned}$$

Recall that by definition $\widetilde{\theta} = V^\top \hat{\theta}$, $\widetilde{\mathbf{y}} = D^\dagger U^\top \mathbf{y}$ and $\widetilde{w} = V^\top w$ and hence

$$\begin{aligned}\hat{\theta} &= V\widetilde{\mathbf{y}} + \alpha^\star V \widetilde{w}_{n+1:p} \\ &= VD^\dagger U^\top \mathbf{y} + \alpha^\star V \widetilde{w}_{n+1:p} \\ &= X^\top \left(XX^\top\right)^{-1} \mathbf{y} + \alpha^\star V \widetilde{w}_{n+1:p} \\ &= \hat{\theta}_{\mathsf{OLS}} + \alpha^\star V \widetilde{w}_{n+1:p} \\ &= \hat{\theta}_{\mathsf{OLS}} + \alpha^\star V \begin{bmatrix} 0_{n\times n} & 0_{n\times(p-n)} \\ 0_{(p-n)\times n} & I_{p-n}\end{bmatrix} V^\top w.\end{aligned}$$

Recall that the SVD of X is $UDV^\top$, and the last $(p-n)$ columns of D are zero. Thus, the last $(p-n)$ rows of $V^\top$ span the null space of X.

Furthermore, $(I_p - X^\top(XX^\top)^{-1}X)$ represents the projection onto this null space of X. This can be seen as follows. First, any member u of this null space is mapped to itself (since $Xu = 0$). On the other hand, for each row x of X, $(I_p - X^\top(XX^\top)^{-1}X)x^\top = 0$, as

$$(I_p - X^\top(XX^\top)^{-1}X)X^\top = 0.$$

Recalling that the last $(p-n)$ rows of $V^\top$ span the null space of X, we have

$$V \begin{bmatrix} 0_{n\times n} & 0_{n\times(p-n)} \\ 0_{(p-n)\times n} & I_{p-n}\end{bmatrix} V^\top = I_p - X^\top(XX^\top)^{-1}X.$$

This wraps up our proof. ■

Armed with this formula for $\hat{\theta}$ we can now bound the excess risk.

Lemma 12 *The excess risk of $\hat{\theta}$ satisfies*

$$\mathsf{Risk}(\hat{\theta}) \le c(\theta^\star - \alpha^\star w)^\top B(\theta^\star - \alpha^\star w) + c\log(1/\delta)\mathrm{Tr}(C)$$

with probability at least $1-\delta$ over $\boldsymbol{\varepsilon}$, where

$$\begin{aligned}&B := \left(I - X^\top(XX^\top)^{-1}X\right)\Sigma\left(I - X^\top(XX^\top)^{-1}X\right) \quad \textit{and} \\ &C := (XX^\top)^{-1}X\Sigma X^\top(XX^\top)^{-1}.\end{aligned}$$

Proof Since $\varepsilon = y - x^\top\theta$ is conditionally mean-zero given x,

$$\begin{aligned}\mathsf{Risk}(\hat{\theta}) &= \mathbb{E}_{x,y}\left[(y - x^\top\hat{\theta})^2\right] - \mathbb{E}_{x,y}\left[(y - x^\top\theta^\star)^2\right] \\ &= \mathbb{E}_{x,y}\left[(y - x^\top\theta^\star + x^\top(\theta^\star - \hat{\theta}))^2\right] - \mathbb{E}_{x,y}\left[(y - x^\top\theta^\star)^2\right] \\ &= \mathbb{E}_x\left[\left(x^\top(\theta^\star - \hat{\theta})\right)^2\right].\end{aligned}$$

Using the formula of $\hat{\theta}$ from Lemma 11, and because $\mathbf{y} = X\theta^\star + \boldsymbol{\varepsilon}$ we find that

$$\begin{aligned}\mathsf{Risk}(\hat{\theta}) &= \mathbb{E}_x\left[\left(x^\top\left(I - X^\top(XX^\top)^{-1}X\right)(\theta^\star - \alpha^\star w) - x^\top X^\top(XX^\top)^{-1}\boldsymbol{\varepsilon}\right)^2\right] \\ &\le 2\mathbb{E}_x\left[\left(x^\top\left(I - X^\top(XX^\top)^{-1}X\right)(\theta^\star - \alpha^\star w)\right)^2\right] + 2\mathbb{E}_x\left[\left(x^\top X^\top(XX^\top)^{-1}\boldsymbol{\varepsilon}\right)^2\right] \\ &= 2(\theta^\star - \alpha^\star w)^\top B(\theta^\star - \alpha^\star w) + 2\boldsymbol{\varepsilon}^\top C\boldsymbol{\varepsilon}.\end{aligned}$$

Now by (Bartlett et al., 2020, Lemma 19) we find that $2\boldsymbol{\varepsilon}^\top C\boldsymbol{\varepsilon} \le c'\sigma_y^2\log(1/\delta)\mathrm{Tr}(C) \le c\log(1/\delta)\mathrm{Tr}(C)$ with probability at least $1-\delta$. This completes the proof. ■

The following lemma provides upper and lower bounds on the value of $\alpha^\star$ that are tight up to the leading constant when p is large relative to $n+k$ and when n is sufficiently large relative to k and $s_k = \sum_{j>k}\lambda_j$.

Lemma 13 *There are constants $c_0, \ldots, c_5$ such that for any $\delta \in (e^{-c_0\sqrt{n}}, 1)$, if $p \ge c_1(n+k)$, $n \ge c_2\max\{k, s_k\}$ and $\|\theta^\star\|, \|w\| \le c_3$ then with probability at least $1 - c_4\delta$,*

$$\left|\frac{\alpha^\star}{\frac{2\sqrt{\sigma}n^{1/4}}{3s_k^{1/4}}} - 1\right| \le c_5\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{s_k}{n}} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n}\right].$$

Lemma 13 is proved over the next few subsections. As might be expected, for $\alpha^\star$ to reliably fall within a small interval, X must be well conditioned in some sense. We begin by establishing bounds on the singular values of submatrices of X in Sections 4.1, whose proofs are provided Appendix B. In Section 4.2, we show that the $\mathrm{Tr}((XX^\top)^{-1})$ is concentrated. Armed with these bounds, we build up our analysis of $\alpha^\star$ in stages in Section 4.3.

4.1 Bounds on the extreme singular values of submatrices of X

In this subsection, we will derive bounds on the largest and smallest singular value of a submatrix of X. Given a subset S of $[p]$, let $X_S \in \mathbb{R}^{n\times|S|}$ be a submatrix of X where only the columns with indices in S are included.

With this in place, we are now ready to prove our concentration results. We prove this lemma in Appendix B.1.

Lemma 14 *There exists a positive absolute constant c such that, for any subset $S \subseteq [p]$ and any $t \ge 0$, with probability at least $1 - 2e^{-t}$, for all $j \in \{1, \ldots, \min(n, |S|)\}$*

$$\left|\mu_j(X_S X_S^\top) - s(S)\right| \le cs(S)\left(\frac{t+n}{r(S)} + \sqrt{\frac{t+n}{R(S)}}\right).$$

This lemma provides an additive lower bound on the minimum singular value of submatrices of X. Next, we will provide a sharper multiplicative bound on the smallest singular value of such matrices. Its proof can be found in Appendix B.2.

Lemma 15 *There exist absolute positive constants $c_0, \ldots, c_3$ such that given any subset $S \subseteq [p]$ if, $r(S) \geq c_0 n$ then for all $t < c_1 < 1$*

$$\mathbb{P}\left[\mu_n(X_S X_S^\top) \leq t \cdot s(S)\right] \leq (c_2 t)^{c_3 \cdot r(S)}.$$

This sharper multiplicative bound provides a much more refined lower tail probability estimate for the minimum eigenvalue than the previous additive bound in Lemma 14, especially when t is close to zero. This is useful in our analysis to control $\mathbb{E}[\mathrm{Tr}(XX^\top)^{-1}]$ which is in turn used to establish Lemma 16 that bounds $\mathrm{Tr}((XX^\top)^{-1})$.

4.2 Concentration of $\mathrm{Tr}((XX^\top)^{-1})$

In this subsection we shall prove the following lemma which shows that $\mathrm{Tr}((XX^\top)^{-1})$ concentrates.

Lemma 16 *There are positive constants $c_0, \ldots, c_4$ such that, if $p \geq c_0(n+k)$ then with probability at least $1 - c_1 e^{-c_2 n}$*

$$\left|\mathrm{Tr}\left((XX^\top)^{-1}\right) - \frac{n}{s_k}\right| \leq \frac{c_3 n}{s_k}\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \frac{k}{n} + e^{-c_4\sqrt{n}}\right].$$

The proof of Lemma 16 in turn requires some lemmas. To state them, we need some additional notation and definitions.

Recall that we have assumed without loss of generality that Σ is diagonal. Let $\lambda_1 \geq \ldots \geq \lambda_p$ be the elements of its diagonal, and define the random vectors

$$z_i := \frac{Xe_i}{\sqrt{\lambda_i}} \in \mathbb{R}^n.$$

These random vectors z_i have entries that are independent, σ_x^2-sub-Gaussian random variables (see Bartlett et al., 2020, Lemma 8). Note that we can write the matrix

$$XX^\top = \sum_{i=1}^{p} \lambda_i z_i z_i^\top.$$

Definition 17 *Define the shorthand $A := XX^\top$, and define*

$$H := \sum_{i=1}^{k} \lambda_i z_i z_i^\top \qquad \text{and} \qquad T := \sum_{i=k+1}^{p} \lambda_i z_i z_i^\top.$$

Therefore $A = H + T$.

To prove Lemma 16 we shall prove the following four results:

- in Lemma 18, we show that $\mathrm{Tr}(A^{-1})$ is close to the $\mathrm{Tr}(T^{-1})$ with high probability;
- in Lemma 19, we show that $\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right]$ is well approximated by $\mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]$;

- in Lemma 20, we show that $\mathrm{Tr}(T^{-1})$ is close to its expectation with high probability;

- finally, in Lemma 21, we establish upper and lower bounds on $\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right]$ that match up to leading constants.

By using these four results and the triangle inequality we shall demonstrate that $\mathrm{Tr}(A^{-1})$ is close to n/s_k with high probability and prove Lemma 16. Throughout this subsection we shall assume that the dimension $p \geq c_0(n+k)$, for a sufficiently large constant c_0. Under this condition, Lemma 26 implies that the tail matrix T is full-rank and invertible.

4.2.1 $\mathrm{Tr}(A^{-1})$ is close to $\mathrm{Tr}(T^{-1})$

We begin by showing that $\mathrm{Tr}(A^{-1})$ is close to $\mathrm{Tr}(T^{-1})$ with high probability.

Lemma 18 *There exist positive constants $c_0, \ldots, c_3$ such that, for all $\beta < c_0 < 1$, with probability at least $1 - 2\exp(-r_k/\beta^2) - (c_1\beta)^{c_2 \cdot r_k}$,*

$$\left|\mathrm{Tr}(A^{-1}) - \mathrm{Tr}(T^{-1})\right| \leq \frac{c_3 k}{\beta^4 s_k}.$$

Proof Recall that $A = XX^\top = \sum_{i=1}^k \lambda_i z_i z_i^\top + \sum_{i=k+1}^p \lambda_i z_i z_i^\top = H + T$. Let $u_1, \ldots, u_k \in \mathbb{R}^n$ be an orthonormal basis for the row span of H, and let $u_1, \ldots, u_n$ be an extension to a basis for $\mathbb{R}^n$. Write $U = [u_1, \ldots, u_n] = [E; F]$, where E is $n \times k$. Thus

$$\begin{aligned}
\mathrm{Tr}(A^{-1}) &\overset{(i)}{=} \mathrm{Tr}\left(U^\top A^{-1} U\right) \\
&= \mathrm{Tr}\left(\left[U^\top A U\right]^{-1}\right) \\
&= \mathrm{Tr}\left(\left[U^\top (H+T) U\right]^{-1}\right) \\
&= \mathrm{Tr}\left(\left[U^\top H U + U^\top T U\right]^{-1}\right) \\
&= \mathrm{Tr}\left(\left[\begin{pmatrix} E^\top H E & E^\top H F \\ F^\top H E & F^\top H F \end{pmatrix} + U^\top T U\right]^{-1}\right) \\
&\overset{(ii)}{=} \mathrm{Tr}\left(\left[\begin{pmatrix} E^\top H E & 0 \\ 0 & 0 \end{pmatrix} + U^\top T U\right]^{-1}\right) \\
&= \mathrm{Tr}\left(\left[\begin{pmatrix} E^\top \\ 0 \end{pmatrix} H \begin{pmatrix} E & 0 \end{pmatrix} + U^\top T U\right]^{-1}\right),
\end{aligned}$$

where (i) follows since U is a unitary matrix, (ii) follows since the columns of F are outside the span of H. Continuing, we apply the Sherman-Morrison-Woodbury identity to get that

$$\begin{aligned}
&\mathrm{Tr}(A^{-1})\\
&= \mathrm{Tr}\left(\left[U^\top T U\right]^{-1}\right)\\
&\quad - \mathrm{Tr}\left(\left[U^\top T U\right]^{-1}\begin{pmatrix}E^\top\\ 0\end{pmatrix}\left[H^\dagger + (E \quad 0)\left[U^\top T U\right]^{-1}\begin{pmatrix}E^\top\\ 0\end{pmatrix}\right]^{-1}(E \quad 0)\left[U^\top T U\right]^{-1}\right)\\
&= \mathrm{Tr}\left(T^{-1}\right)\\
&\quad - \mathrm{Tr}\left(U^\top T^{-1} U\begin{pmatrix}E^\top\\ 0\end{pmatrix}\left[H^\dagger + (E \quad 0)\,U^\top T^{-1} U\begin{pmatrix}E^\top\\ 0\end{pmatrix}\right]^{-1}(E \quad 0)\,U^\top T^{-1} U\right)\\
&\overset{(i)}{=} \mathrm{Tr}\left(T^{-1}\right) - \mathrm{Tr}\left(U^\top T^{-1} E E^\top\left[H^\dagger + E E^\top T^{-1} E E^\top\right]^{-1} E E^\top T^{-1} U\right)\\
&= \mathrm{Tr}\left(T^{-1}\right) - \mathrm{Tr}\left(T^{-1} E E^\top\left[H^\dagger + E E^\top T^{-1} E E^\top\right]^{-1} E E^\top T^{-1}\right), \qquad (5)
\end{aligned}$$

where (i) follows since $(E;0)U^\top = (E;0)(E;F)^\top = EE^\top$. Now

$$\begin{aligned}
0 &\le \mathrm{Tr}\left(T^{-1} E E^\top\left[H^\dagger + E E^\top T^{-1} E E^\top\right]^{-1} E E^\top T^{-1}\right)\\
&\le \mathrm{Tr}\left(T^{-1} E E^\top\left(E E^\top T^{-1} E E^\top\right)^{-1} E E^\top T^{-1}\right)\\
&= \mathrm{Tr}\left(T^{-1} E E^\top\left(E E^\top\right)^\dagger T\left(E E^\top\right)^\dagger E E^\top T^{-1}\right), \qquad (6)
\end{aligned}$$

where the second inequality holds because

$$\begin{aligned}
&H^\dagger \succeq 0\\
&\Rightarrow \left(E E^\top T^{-1} E E^\top\right)^{-1} - \left(H^\dagger + E E^\top T^{-1} E E^\top\right)^{-1} \succeq 0\\
&\Rightarrow T^{-1} E E^\top\left(\left(E E^\top T^{-1} E E^\top\right)^{-1} - \left(H^\dagger + E E^\top T^{-1} E E^\top\right)^{-1}\right) E E^\top T^{-1} \succeq 0\\
&\Rightarrow T^{-1} E E^\top\left(E E^\top T^{-1} E E^\top\right)^{-1} E E^\top T^{-1} \succeq T^{-1} E E^\top\left(\left(H^\dagger + E E^\top T^{-1} E E^\top\right)^{-1}\right) E E^\top T^{-1}
\end{aligned}$$

along with the fact that, for any symmetric positive semi-definite matrices Q and S such that $Q \succeq S$, for all i, $\mu_i(Q) \ge \mu_i(S) \ge 0$.

Thus combining equations (5) and (6) we get that

$$\left|\mathrm{Tr}(A^{-1}) - \mathrm{Tr}\left(T^{-1}\right)\right| \le \left|\mathrm{Tr}\left(T^{-1} E E^\top\left(E E^\top\right)^\dagger T\left(E E^\top\right)^\dagger E E^\top T^{-1}\right)\right|.$$

The rank of $T^{-1}EE^\top \left(EE^\top\right)^\dagger T \left(EE^\top\right)^\dagger EE^\top T^{-1}$ is at most k, so

$$\begin{aligned}\left|\mathrm{Tr}(A^{-1}) - \mathrm{Tr}\left(T^{-1}\right)\right| &\le k \left\| T^{-1}EE^\top \left(EE^\top\right)^\dagger T \left(EE^\top\right)^\dagger EE^\top T^{-1} \right\|_{op} \\ &\le k\|T^{-1}\|_{op}^2 \|EE^\top (EE^\top)^\dagger\|_{op}^2 \|T\|_{op} \\ &\le \frac{k\mu_1(T)}{\mu_n(T)^2}. \end{aligned} \tag{7}$$

Next by invoking Lemma 14, for any $t > 2n$, with probability at least $1 - 2e^{-t}$

$$\begin{aligned}\mu_1(T) &\le s_k \left[1 + c\left(\frac{t+n}{r_k} + \sqrt{\frac{t+n}{R_k}}\right)\right] \\ &\le s_k \left[1 + 3c\left(\frac{t}{r_k} + \sqrt{\frac{t}{R_k}}\right)\right] \\ &\le c' s_k \left[1 + \left(\frac{t}{r_k} + \sqrt{\frac{t}{R_k}}\right)\right]. \end{aligned}$$

Recall that $r_k \ge bn$ by the definition of the index k in Definition 3. Given a $\beta < c_0 < 1$, where c_0 is small enough, set $t = \min\{r_k, R_k\}/\beta^2 = r_k/\beta^2$ (since $r_k \le R_k$ by Lemma 2) to get that

$$\mu_1(T) \le c' s_k \left[1 + \left(\frac{1}{\beta^2} + \frac{1}{\beta}\right)\right]$$

with probability at least $1 - 2\exp(-r_k/\beta^2)$. Next, note that $p - k \ge \sum_{j>k} \lambda_j/\lambda_{k+1} = r_k \ge bn$. Therefore, by Lemma 15, for any $\beta < c_0 < 1$,

$$\mathbb{P}\left[\mu_n(T) \le \beta s_k\right] \le (c_1\beta)^{c_2 \cdot r_k}.$$

Combining the last two inequalities we find that, for any $\beta < c_0 < 1$

$$\frac{\mu_1(T)}{\mu_n(T)^2} \le \frac{c'}{s_k}\left[\frac{1 + \left(\frac{1}{\beta^2} + \frac{1}{\beta}\right)}{\beta^2}\right] \le \frac{c_3}{\beta^4 s_k}$$

with probability at least $1 - 2\exp(-r_k/\beta^2) - (c_1\beta)^{c_2\cdot r_k}$. Combined with inequality (7) this completes our proof. ■

4.2.2 $\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right]$ is close to $\mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]$

Next, we show that $\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right]$ is close to $\mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]$.

Lemma 19 *There exists a positive constant c_0 such that*

$$\left|\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right] - \mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]\right| \le \frac{c_0 k}{s_k}.$$

Proof Given any β define

$$\omega = \frac{ck}{\beta^4 s_k} = \frac{ck}{\beta^4 r_k \lambda_{k+1}}.$$

By Lemma 18 for any $\omega > \frac{c_1 k}{s_k}$, where c_1 is a large enough constant

$$\mathbb{P}\left[\left|\mathrm{Tr}(A^{-1}) - \mathrm{Tr}(T^{-1})\right| > \omega\right] \le 2\exp\left(-c' r_k^{3/2}\sqrt{\frac{\lambda_{k+1}}{k}}\sqrt{\omega}\right) + \left(\frac{c'' k}{\omega s_k}\right)^{\frac{c_2 \cdot r_k}{4}}.$$

Thus

$$\begin{aligned}
&\left|\mathbb{E}[\mathrm{Tr}(A^{-1})] - \mathbb{E}[\mathrm{Tr}(T^{-1})]]\right| \\
&\qquad \le \mathbb{E}\left[\left|\mathrm{Tr}(A^{-1}) - \mathrm{Tr}(T^{-1})\right|\right] \\
&\qquad = \int_0^\infty \mathbb{P}\left[\left|\mathrm{Tr}(A^{-1}) - \mathrm{Tr}(T^{-1})\right| > \omega\right]\, \mathrm{d}\omega \\
&\qquad = \int_0^{\frac{c_1 k}{s_k}} \mathbb{P}\left[\left|\mathrm{Tr}(A^{-1}) - \mathrm{Tr}(T^{-1})\right| > \omega\right]\, \mathrm{d}\omega + \int_{\frac{c_1 k}{s_k}}^\infty \mathbb{P}\left[\left|\mathrm{Tr}(A^{-1}) - \mathrm{Tr}(T^{-1})\right| > \omega\right]\, \mathrm{d}\omega \\
&\qquad \le \frac{c_1 k}{s_k} + \underbrace{\int_{\frac{c_1 k}{s_k}}^\infty 2\exp\left(-c' r_k^{3/2}\sqrt{\frac{\lambda_{k+1}}{k}}\sqrt{\omega}\right)\, \mathrm{d}\omega}_{=:\spadesuit} + \underbrace{\int_{\frac{c_1 k}{s_k}}^\infty \left(\frac{c'' k}{\omega s_k}\right)^{\frac{c_2 \cdot r_k}{4}}\, \mathrm{d}\omega}_{=:\clubsuit}. \qquad (8)
\end{aligned}$$

First we control $\spadesuit$ as follows:

$$\begin{aligned}
\spadesuit &= \int_{\frac{c_1 k}{s_k}}^\infty 2\exp\left(-c' r_k^{3/2}\sqrt{\frac{\lambda_{k+1}}{k}}\sqrt{\omega}\right)\, \mathrm{d}\omega \\
&= 4\exp\left(-c_3 r_k\right)\frac{c_3 r_k + 1}{\left(c' r_k^{3/2}\sqrt{\frac{\lambda_{k+1}}{k}}\right)^2} \qquad \left(\text{since } \int \exp(-\sqrt{z}) = -2e^{-\sqrt{z}}(\sqrt{z}+1) + c\right) \\
&= \frac{4k}{s_k}\left[\exp\left(-c_3 r_k\right)\frac{c_3 r_k + 1}{\left(c' r_k\right)^2}\right] \qquad (\text{since } s_k = r_k \lambda_{k+1}) \\
&\le \frac{c_4 k}{s_k}. \qquad (9)
\end{aligned}$$

Next we control $\clubsuit$ as follows

$$\begin{aligned}
\clubsuit = \int_{\frac{c_1 k}{s_k}}^\infty \left(\frac{c'' k}{\omega s_k}\right)^{\frac{c_2 \cdot r_k}{4}}\, \mathrm{d}\omega &= \left(\frac{c'' k}{s_k}\right)^{\frac{c_2 \cdot r_k}{4}} \int_{\frac{c_1 k}{s_k}}^\infty \left(\frac{1}{\omega}\right)^{\frac{c_2 \cdot r_k}{4}}\, \mathrm{d}\omega \\
&= \left(\frac{c'' k}{s_k}\right)^{\frac{c_2 \cdot r_k}{4}} \times \frac{1}{\frac{c_2 \cdot r_k}{4} - 1} \times \left(\frac{s_k}{c_1 k}\right)^{\frac{c_2 \cdot r_k}{4} - 1} \\
&= \frac{c_5 k}{s_k}\left((c'')^{\frac{c_2 \cdot r_k}{4}} \times \frac{4}{c_2 \cdot r_k - 4} \times \left(\frac{1}{c_1}\right)^{\frac{c_2 \cdot r_k}{4} - 1}\right) \\
&\le \frac{c_5 k}{s_k} \qquad (10)
\end{aligned}$$

where the last inequality follows because the constant c_1 large enough and because $r_k \geq bn$ for a large enough constant b. Combining inequalities (8), (9) and (10) we conclude that

$$\left|\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right] - \mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]\right| \leq \frac{c_1 k}{s_k} + \frac{c_4 k}{s_k} + \frac{c_5 k}{s_k} \leq \frac{c_0 k}{s_k},$$

wrapping up the proof. ■

4.2.3 $\mathrm{Tr}(T^{-1})$ concentrates around its mean

Finally, we shall show that $\mathrm{Tr}(T^{-1})$ is close to its expectation $\mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]$ with high probability.

Lemma 20 *There exists a positive constant c_0 such that with probability at least $1 - 2e^{-n}$,*

$$\left|\mathrm{Tr}(T^{-1}) - \mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]\right| \leq \frac{c_0 n}{s_k}\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k}\right].$$

Proof We use a symmetrization argument:

$$\begin{aligned}\left|\mathrm{Tr}(T^{-1}) - \mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]\right| = \left|\sum_{i=1}^{n} \frac{1}{\mu_i(T)} - \mathbb{E}\left[\frac{1}{\mu_i(T)}\right]\right| &\leq \sum_{i=1}^{n}\left|\frac{1}{\mu_i(T)} - \mathbb{E}\left[\frac{1}{\mu_i(T)}\right]\right| \\ &= \sum_{i=1}^{n}\left|\frac{1}{\mu_i(T)} - \mathbb{E}_{T'}\left[\frac{1}{\mu_i(T')}\right]\right|,\end{aligned}$$

where in the equation above the matrices T and T' are independent and identically distributed. Thus

$$\begin{aligned}\left|\mathrm{Tr}(T^{-1}) - \mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]\right| \leq \sum_{i=1}^{n}\left|\mathbb{E}_{T'}\left[\frac{1}{\mu_i(T)} - \frac{1}{\mu_i(T')}\right]\right| &\leq \sum_{i=1}^{n}\mathbb{E}_{T'}\left[\left|\frac{1}{\mu_i(T)} - \frac{1}{\mu_i(T')}\right|\right] \\ &= \sum_{i=1}^{n}\mathbb{E}_{T'}\left[\frac{|\mu_i(T') - \mu_i(T)|}{\mu_i(T)\mu_i(T')}\right].\end{aligned} \tag{11}$$

By Lemma 14, with probability at least $1 - 2e^{-n}$, for all $i \in [n]$,

$$s_k\left[1 - c_1\left(\frac{n}{r_k} + \sqrt{\frac{n}{R_k}}\right)\right] \leq \mu_i(T) \leq s_k\left[1 + c_1\left(\frac{n}{r_k} + \sqrt{\frac{n}{R_k}}\right)\right]. \tag{12}$$

We will assume that the event described above, which controls the singular values of T, occurs going forward. (This determines the success probability in the statement of the lemma.) The game plan now is to evaluate the expectation with respect to T' in equation (11) by integrating tail bounds. Since (12) holds,

$$\begin{aligned}
&\left|\mu_i(T)-\mu_i(T')\right| \\
&= \max\{\mu_i(T)-\mu_i(T'), \mu_i(T')-\mu_i(T)\} \\
&\le \max\left\{ s_k\left[1+c_1\left(\frac{n}{r_k}+\sqrt{\frac{n}{R_k}}\right)\right]-\mu_i(T'),\right. \\
&\qquad\qquad \left.\mu_i(T')-s_k\left[1-c_1\left(\frac{n}{r_k}+\sqrt{\frac{n}{R_k}}\right)\right]\right\} \\
&\le \max\left\{ s_k\left[1+c_1\left(\frac{n}{r_k}+\sqrt{\frac{n}{R_k}}\right)\right]-s_k\left[1-c_2\left(\frac{t+n}{r_k}+\sqrt{\frac{t+n}{R_k}}\right)\right],\right. \\
&\qquad \left. s_k\left[1+c_2\left(\frac{t+n}{r_k}+\sqrt{\frac{t+n}{R_k}}\right)\right]-s_k\left[1-c_1\left(\frac{n}{r_k}+\sqrt{\frac{n}{R_k}}\right)\right]\right\} \\
&\qquad\qquad\qquad\qquad \text{(by Lemma 14)} \\
&\le c_3 s_k\left(\frac{t+n}{r_k}+\sqrt{\frac{t+n}{R_k}}\right), \qquad (13)
\end{aligned}$$

with probability $1-2e^{-t}$.

Next, by Lemma 15, we know that for all $\beta < c_4 < 1$

$$\mathbb{P}\left[\mu_n(T') \le \beta s_k\right] \le (c_5\beta)^{c_6\cdot r_k}. \qquad (14)$$

Combining equations (13) and (14), and because condition (12) holds, we get that

$$\mathbb{P}\left[\exists\, i\in[n] \;:\; \frac{|\mu_i(T)-\mu_i(T')|}{\mu_i(T)\mu_i(T')} \ge \frac{c_3\left(\frac{t+n}{r_k}+\sqrt{\frac{t+n}{R_k}}\right)}{\beta s_k\left[1-c_1\left(\frac{n}{r_k}+\sqrt{\frac{n}{R_k}}\right)\right]}\right] \le 2e^{-t}+(c_5\beta)^{c_6\cdot r_k}.$$

Now since $r_k \ge bn$ for a large enough constant b by the definition of k, and since $R_k > r_k$ by Lemma 2, we can simplify the denominator in the equation above to get that

$$\mathbb{P}\left[\exists\, i\in[n] \;:\; \frac{|\mu_i(T)-\mu_i(T')|}{\mu_i(T)\mu_i(T')} \ge \frac{c_7\left(\frac{t+n}{r_k}+\sqrt{\frac{t+n}{R_k}}\right)}{\beta s_k}\right] \le 2e^{-t}+(c_5\beta)^{c_6\cdot r_k}.$$

Setting $t = n/\beta$ yields

$$\mathbb{P}\left[\exists\, i\in[n] \;:\; \frac{|\mu_i(T)-\mu_i(T')|}{\mu_i(T)\mu_i(T')} \ge \frac{c_7\left(\frac{n(\beta+1)}{\beta r_k}+\sqrt{\frac{n(\beta+1)}{\beta R_k}}\right)}{\beta s_k}\right] \le 2e^{-n/\beta}+(c_5\beta)^{c_6\cdot r_k}.$$

Now since $\beta < c_4 < 1$, we find that

$$\begin{aligned}
&\mathbb{P}\left[\exists\, i\in[n] \;:\; \frac{|\mu_i(T)-\mu_i(T')|}{\mu_i(T)\mu_i(T')} \ge \frac{c_8}{s_k}\max\left\{\frac{n}{\beta^2 r_k}, \frac{\sqrt{n}}{\beta^{3/2}\sqrt{R_k}}\right\}\right] \\
&\qquad\qquad\qquad\qquad\qquad\qquad \le 2e^{-n/\beta}+(c_5\beta)^{c_6\cdot r_k}. \qquad (15)
\end{aligned}$$

For every β define

$$\omega := \frac{c_8}{s_k}\max\left\{\frac{n}{\beta^2 r_k}, \frac{\sqrt{n}}{\beta^{3/2}\sqrt{R_k}}\right\}.$$

Inverting the map from β to ω yields

$$\beta(\omega) = \begin{cases} \left(\frac{c_8\sqrt{n}}{\omega\sqrt{R_k}s_k}\right)^{2/3} & \text{if } \omega \leq \omega_\tau := \frac{c_8}{s_k}\left(\frac{r_k^3}{R_k^2 n}\right), \\ \sqrt{\frac{c_8 n}{\omega r_k s_k}} & \text{otherwise.} \end{cases} \tag{16}$$

Let ω_0 be such that $\beta(\omega_0) = c_4$, and define

$$\omega_- := \min\{\omega_0, \omega_\tau\} \quad \text{and} \quad \omega_+ := \max\{\omega_0, \omega_\tau\}.$$

Applying inequality (15) we have that, for all $\omega \in (\omega_-, \omega_\tau]$

$$\begin{aligned} &\mathbb{P}\left[\exists\, i \in [n] \;:\; \frac{|\mu_i(T) - \mu_i(T')|}{\mu_i(T)\mu_i(T')} \geq \omega\right] \\ &\qquad \leq 2\exp\left(-c_9\left(\omega n\sqrt{R_k}s_k\right)^{2/3}\right) + \left(\frac{c_{10}\sqrt{n}}{\omega\sqrt{R_k}s_k}\right)^{c_{11}\cdot r_k}, \end{aligned} \tag{17}$$

and for $\omega > \omega_+$, we have

$$\mathbb{P}\left[\exists\, i \in [n] \;:\; \frac{|\mu_i(T) - \mu_i(T')|}{\mu_i(T)\mu_i(T')} \geq \omega\right] \leq 2\exp\left(-c_{12}\left(\omega n r_k s_k\right)^{1/2}\right) + \left(\frac{c_{13} n}{\omega r_k s_k}\right)^{c_{14}\cdot r_k}. \tag{18}$$

Thus

$$\begin{aligned} \mathbb{E}_{T'}\left[\frac{|\mu_i(T') - \mu_i(T)|}{\mu_i(T)\mu_i(T')}\right] &= \int_0^\infty \mathbb{P}\left[\frac{|\mu_i(T') - \mu_i(T)|}{\mu_i(T)\mu_i(T')} \geq \omega\right]\, \mathrm{d}\omega \\ &= \int_0^{\omega_0} \mathbb{P}\left[\frac{|\mu_i(T') - \mu_i(T)|}{\mu_i(T)\mu_i(T')} \geq \omega\right]\, \mathrm{d}\omega \\ &\qquad + \int_{\omega_-}^{\omega_\tau} \mathbb{P}\left[\frac{|\mu_i(T') - \mu_i(T)|}{\mu_i(T)\mu_i(T')} \geq \omega\right]\, \mathrm{d}\omega \\ &\qquad + \int_{\omega_+}^{\infty} \mathbb{P}\left[\frac{|\mu_i(T') - \mu_i(T)|}{\mu_i(T)\mu_i(T')} \geq \omega\right]\, \mathrm{d}\omega \\ &\leq \omega_0 + \underbrace{\int_{\omega_-}^{\omega_\tau} \mathbb{P}\left[\frac{|\mu_i(T') - \mu_i(T)|}{\mu_i(T)\mu_i(T')} \geq \omega\right]\, \mathrm{d}\omega}_{=:\spadesuit} \\ &\qquad + \underbrace{\int_{\omega_+}^{\infty} \mathbb{P}\left[\frac{|\mu_i(T') - \mu_i(T)|}{\mu_i(T)\mu_i(T')} \geq \omega\right]\, \mathrm{d}\omega}_{=:\clubsuit}. \end{aligned} \tag{19}$$

Let us perform each of these two integrals ♠ and ♣ separately.

First,

$$\begin{aligned}
&\spadesuit\\
&= \int_{\omega_-}^{\omega_\tau} \mathbb{P}\left[\frac{|\mu_i(T')-\mu_i(T)|}{\mu_i(T)\mu_i(T')} \geq \omega\right] \mathrm{d}\omega\\
&\leq \int_{\omega_-}^{\omega_\tau}\left[2\exp\left(-c_9\left(\omega n\sqrt{R_k}s_k\right)^{2/3}\right)+\left(\frac{c_{10}\sqrt{n}}{\omega\sqrt{R_k}s_k}\right)^{c_{11}\cdot r_k}\right]\mathrm{d}\omega \qquad \text{(by inequality (17))}\\
&\leq \mathbb{I}[\omega_- < \omega_\tau]\int_{\omega_-}^{\infty}\left[2\exp\left(-c_9\left(\omega n\sqrt{R_k}s_k\right)^{2/3}\right)+\left(\frac{c_{10}\sqrt{n}}{\omega\sqrt{R_k}s_k}\right)^{c_{11}\cdot r_k}\right]\mathrm{d}\omega.
\end{aligned}$$

Now, for $\zeta := c_9\left(n\sqrt{R_k}s_k\right)^{2/3}$, we have that

$$\begin{aligned}
&2\int_{\omega_-}^{\infty}\exp\left(-c_9\left(\omega n\sqrt{R_k}s_k\right)^{2/3}\right)\mathrm{d}\omega\\
&= 2\int_{\omega_-}^{\infty}\exp\left(-\zeta\omega^{2/3}\right)\mathrm{d}\omega\\
&= \frac{3\omega_-^{1/3}\exp(-\zeta\omega_-^{2/3})}{\zeta}+\frac{3\sqrt{\pi}\left(1-\mathsf{erf}\left(\sqrt{\zeta}\omega_-^{1/3}\right)\right)}{2\zeta^{3/2}}\\
&\qquad\qquad\qquad\qquad \text{(since } \textstyle\int \exp(-z^{2/3}) = \frac{3}{4}\left(\sqrt{\pi}\mathsf{erf}(z^{1/3})-2e^{-z^{2/3}}z^{1/3}\right)+c\text{)}\\
&\leq \frac{3\omega_-^{1/3}\exp(-\zeta\omega_-^{2/3})}{\zeta}+\frac{3\exp(-\zeta\omega_-^{2/3})}{2\zeta^2\omega_-^{1/3}}\\
&= \frac{c_{15}\exp\left(-c_9\left(n\sqrt{R_k}s_k\right)^{2/3}\omega_-^{2/3}\right)}{(n\sqrt{R_k}s_k)^{2/3}}\left(\omega_-^{1/3}+\frac{1}{\left(n\sqrt{R_k}s_k\right)^{2/3}\omega_-^{1/3}}\right). \qquad (20)
\end{aligned}$$

Continuing our work of bounding $\spadesuit$, we have that

$$\begin{aligned}
\int_{\omega_-}^{\infty}\left(\frac{c_{10}\sqrt{n}}{\omega\sqrt{R_k}s_k}\right)^{c_{11}\cdot r_k}\mathrm{d}\omega &= \left(\frac{c_{10}\sqrt{n}}{\sqrt{R_k}s_k}\right)^{c_{11}\cdot r_k}\int_{\omega_-}^{\infty}\left(\frac{1}{\omega}\right)^{c_{11}\cdot r_k}\mathrm{d}\omega\\
&= \left(\frac{c_{10}\sqrt{n}}{\sqrt{R_k}s_k}\right)^{c_{11}\cdot r_k}\times\frac{1}{c_{11}\cdot r_k-1}\left(\frac{1}{\omega_-}\right)^{c_{11}\cdot r_k-1}\\
&\leq c_{16}\left(\frac{c_{10}\sqrt{n}}{\sqrt{R_k}s_k}\right)^{c_{11}\cdot r_k}\left(\frac{1}{\omega_-}\right)^{c_{11}\cdot r_k-1}, \qquad (21)
\end{aligned}$$

where the last inequality follows since $r_k \geq bn$ for a large enough constant b. By combining inequalities (20) and (21) we get the following bound on the integral $\spadesuit$:

$$\begin{aligned}
\spadesuit \leq \mathbb{I}[\omega_- < \omega_\tau]&\frac{c_{15}\exp\left(-c_9\left(n\sqrt{R_k}s_k\right)^{2/3}\omega_-^{2/3}\right)}{(n\sqrt{R_k}s_k)^{2/3}}\left(\omega_-^{1/3}+\frac{1}{\left(n\sqrt{R_k}s_k\right)^{2/3}\omega_-^{1/3}}\right)\\
&+\mathbb{I}[\omega_- < \omega_\tau]c_{16}\left(\frac{c_{10}\sqrt{n}}{\sqrt{R_k}s_k}\right)^{c_{11}\cdot r_k}\left(\frac{1}{\omega_-}\right)^{c_{11}\cdot r_k-1}. \qquad (22)
\end{aligned}$$

Let us now bound $\clubsuit$

$$\begin{aligned}\clubsuit &= \int_{\omega_+}^{\infty} \mathbb{P}\left[\frac{|\mu_i(T') - \mu_i(T)|}{\mu_i(T)\mu_i(T')} \geq \omega\right] \mathrm{d}\omega \\ &\leq \int_{\omega_+}^{\infty} \left[2\exp\left(-c_{12}\left(\omega n r_k s_k\right)^{1/2}\right) + \left(\frac{c_{13} n}{\omega r_k s_k}\right)^{c_{14}\cdot r_k}\right] \mathrm{d}\omega \qquad \text{(applying inequality (18)).}\end{aligned}$$

For $\zeta' := c_{12}\left(n r_k s_k\right)^{1/2}$, we have

$$\begin{aligned}&2\int_{\omega_+}^{\infty} \exp\left(-c_{12}\left(\omega n r_k s_k\right)^{1/2}\right) \mathrm{d}\omega \\ &\qquad = 2\int_{\omega_+}^{\infty} \exp\left(-\zeta' \omega^{1/2}\right) \mathrm{d}\omega \\ &\qquad = \frac{4\exp(-\zeta'\sqrt{\omega_+})(\zeta'\sqrt{\omega_+}+1)}{\zeta'^2} \qquad \left(\text{since } \textstyle\int \exp(-\sqrt{z}) = -2e^{-\sqrt{z}}(\sqrt{z}+1) + c\right) \\ &\qquad = \frac{c_{17}\exp\left(-c_{12}\left(n r_k s_k \omega_+\right)^{1/2}\right)\left[c_{12}\left(n r_k s_k \omega_+\right)^{1/2} + 1\right]}{n r_k s_k}. \qquad (23)\end{aligned}$$

We continue to bound the other integral in $\clubsuit$ as follows

$$\int_{\omega_+}^{\infty} \left(\frac{c_{13} n}{\omega r_k s_k}\right)^{c_{14}\cdot r_k} \mathrm{d}\omega \leq c_{18}\left(\frac{c_{13} n}{r_k s_k}\right)^{c_{14}\cdot r_k}\left(\frac{1}{\omega_+}\right)^{c_{14}\cdot r_k - 1}, \qquad (24)$$

where the bound follows by mirroring the logic used to arrive at inequality (21) above. Therefore, combining inequalities (23) and (24) we get that

$$\begin{aligned}\clubsuit \leq &\frac{c_{17}\exp\left(-c_{12}\left(n r_k s_k \omega_+\right)^{1/2}\right)\left[c_{12}\left(n r_k s_k \omega_+\right)^{1/2} + 1\right]}{n r_k s_k} \\ &\qquad + c_{18}\left(\frac{c_{13} n}{r_k s_k}\right)^{c_{14}\cdot r_k}\left(\frac{1}{\omega_+}\right)^{c_{14}\cdot r_k - 1}. \qquad (25)\end{aligned}$$

Having controlled both $\spadesuit$ and $\clubsuit$ in (22) and (25) respectively, by using the decomposition in (19) we find that

$$\begin{aligned}&\mathbb{E}_{T'}\left[\frac{|\mu_i(T') - \mu_i(T)|}{\mu_i(T)\mu_i(T')}\right] \\ &\quad \leq \omega_0 + \mathbb{I}[\omega_- < \omega_\tau]\frac{c_{15}\exp\left(-c_9\left(n\sqrt{R_k}s_k\right)^{2/3}\omega_-^{2/3}\right)}{(n\sqrt{R_k}s_k)^{2/3}}\left(\omega_-^{1/3} + \frac{1}{\left(n\sqrt{R_k}s_k\right)^{2/3}\omega_-^{1/3}}\right) \\ &\qquad + \mathbb{I}[\omega_- < \omega_\tau] c_{16}\left(\frac{c_{10}\sqrt{n}}{\sqrt{R_k}s_k}\right)^{c_{11}\cdot r_k}\left(\frac{1}{\omega_-}\right)^{c_{11}\cdot r_k - 1} \\ &\qquad + \frac{c_{17}\exp\left(-c_{12}\left(n r_k s_k \omega_+\right)^{1/2}\right)\left[c_{12}\left(n r_k s_k \omega_+\right)^{1/2} + 1\right]}{n r_k s_k} \\ &\qquad + c_{18}\left(\frac{c_{13} n}{r_k s_k}\right)^{c_{14}\cdot r_k}\left(\frac{1}{\omega_+}\right)^{c_{14}\cdot r_k - 1}. \qquad (26)\end{aligned}$$

We now consider two cases.

Case 1: ($\omega_0 < \omega_\tau$). In this case, using the fact that $\beta(\omega_0) = c_4$ and the formula for β in equation (16) we get that

$$\omega_0 = \frac{c_8\sqrt{n}}{c_4^{3/2}\sqrt{R_k}s_k} = \frac{c_{19}\sqrt{n}}{\sqrt{R_k}s_k},$$

and that

$$\begin{aligned}\omega_- &= \min\{\omega_0, \omega_\tau\} = \omega_0 = \frac{c_8\sqrt{n}}{c_4^{3/2}\sqrt{R_k}s_k},\\ \omega_+ &= \max\{\omega_0, \omega_\tau\} = \omega_\tau = \frac{c_8 r_k^3}{R_k^2 n s_k}.\end{aligned}$$

Also note that in this case since,

$$\omega_0 = \frac{c_8\sqrt{n}}{c_4^{3/2}\sqrt{R_k}s_k} < \frac{c_8 r_k^3}{R_k^2 n s_k} = \omega_\tau \quad \Rightarrow R_k \leq \frac{c_4 r_k^2}{n}$$

and so $\omega_+ \geq \frac{c_8 n}{c_4^2 r_k s_k}$.

Thus, substituting the above values of ω_0, ω_- in inequality (26), and, because the RHS of this inequality is a decreasing function in ω_+ (since the function $z \mapsto \exp(-z)(z+1)$ is a decreasing function for all positive z), replacing ω_+ with the above lower bound, we find that

$$\begin{aligned}&\mathbb{E}_{T'}\left[\frac{|\mu_i(T') - \mu_i(T)|}{\mu_i(T)\mu_i(T')}\right]\\ &\quad\leq \frac{c_{19}\sqrt{n}}{\sqrt{R_k}s_k} + \frac{c_{20}\exp(-c_{21}n)}{\sqrt{nR_k}s_k} + \frac{c_{20}\exp(-c_{21}n)}{n^{3/2}\sqrt{R_k}s_k}\\ &\qquad\qquad + \frac{c_{16}c_8\sqrt{n}}{c_4^{3/2}\sqrt{R_k}s_k}\left(\frac{c_{10}c_4^{3/2}}{c_8}\right)^{c_{11}\cdot r_k} + \frac{c_{22}\exp(-c_{23}n)}{r_k s_k} + \frac{c_{18}c_8 n}{c_4^2 r_k s_k}\left(\frac{c_{13}c_4^2}{c_8}\right)^{c_{14}\cdot r_k}\\ &\quad\overset{(i)}{\leq} \frac{c_{19}\sqrt{n}}{\sqrt{R_k}s_k} + \frac{c_{20}\exp(-c_{21}n)}{\sqrt{nR_k}s_k} + \frac{c_{20}\exp(-c_{21}n)}{n^{3/2}\sqrt{R_k}s_k} + \frac{c_{16}c_8\sqrt{n}}{c_4^{3/2}\sqrt{R_k}s_k} + \frac{c_{22}\exp(-c_{23}n)}{r_k s_k} + \frac{c_{18}c_8 n}{c_4^2 r_k s_k}\\ &\quad\leq \frac{c_{24}\sqrt{n}}{\sqrt{R_k}s_k} + \frac{c_{25}n}{r_k s_k},\end{aligned}$$

where (i) follows since c_4 is small enough. This combined with inequalities (11) and (12) proves the lemma in this case.

Case 2: ($\omega_0 \geq \omega_\tau$). In this case, using the fact that $\beta(\omega_0) = c_4$ and the formula for β in equation (16) we get that

$$\omega_0 = \frac{c_8 n}{c_4^2 r_k s_k}$$

and that

$$\begin{aligned}\omega_- &= \min\{\omega_0, \omega_\tau\} = \omega_\tau,\\ \omega_+ &= \max\{\omega_0, \omega_\tau\} = \omega_0 = \frac{c_8 n}{c_4^2 r_k s_k}.\end{aligned}$$

Now by applying inequality (26) we get that

$$\begin{aligned}\mathbb{E}_{T'}\left[\frac{|\mu_i(T')-\mu_i(T)|}{\mu_i(T)\mu_i(T')}\right] &\le \frac{c_8 n}{c_4^2 r_k s_k}+\frac{c_{26}\exp(-c_{27}n)}{r_k s_k}+\frac{c_{28}n}{r_k s_k}\left(\frac{c_{13}c_4^2}{c_8}\right)^{c_{14}\cdot r_k}\\ &\overset{(i)}{\le} \frac{c_8 n}{c_4^2 r_k s_k}+\frac{c_{26}\exp(-c_{27}n)}{r_k s_k}+\frac{c_{28}n}{r_k s_k}\le\frac{c_{29}n}{r_k s_k},\end{aligned}$$

where (i) follows since c_4 is small enough. Again, combining this inequality with inequalities (11) and (12) proves the lemma in this second case. ■

4.2.4 Bounds on $\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right]$

To characterize $\mathrm{Tr}\left(A^{-1}\right)$ in terms of relevant problem parameters we will need to establish upper and lower bounds that are tight up to the leading constant on its expectation.

Lemma 21 *There are positive constants c_0 and c_1 such that*

$$\left|\mathbb{E}\left[\mathrm{Tr}\left(A^{-1}\right)\right]-\frac{n}{s_k}\right|\le\frac{c_0 n}{s_k}\left[\sqrt{\frac{n}{R_k}}+\frac{n}{r_k}+\frac{k}{n}+e^{-c_1\sqrt{n}}\right].$$

Proof By Lemma 19 we know that

$$\mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]-\frac{ck}{s_k}\le\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right]\le\mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]+\frac{ck}{s_k}. \tag{27}$$

Thus, we shall instead upper and lower bound $\mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]$.

The lower bound: By definition

$$\mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]=\mathbb{E}\left[\sum_{i=1}^{n}\frac{1}{\mu_i(T)}\right]\ge\mathbb{E}\left[\frac{n}{\frac{1}{n}\sum_{i=1}^{n}\mu_i(T)}\right]\qquad\text{(by the AM-HM inequality).} \tag{28}$$

By Bernstein's inequality (see Theorem 31) we know that with probability at least $1-2e^{-t}$,

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^{n}\mu_i(T)&=\frac{1}{n}\mathrm{Tr}(T)\\ &=\frac{1}{n}\sum_{i>k}\lambda_i\mathrm{Tr}(z_i z_i^\top)\\ &=\frac{1}{n}\sum_{i>k}\lambda_i\|z_i\|^2\\ &\le\sum_{i>k}\lambda_i+c_2\max\left\{t\lambda_{k+1},\sqrt{t\sum_{i>k}\lambda_i^2}\right\}\\ &=s_k\left[1+c_2\max\left\{\frac{t}{r_k},\sqrt{\frac{t}{R_k}}\right\}\right]\qquad(\text{since } s_k=\textstyle\sum_{j>k}\lambda_j)\\ &\le s_k\left[1+c_2\max\left\{\frac{t}{\sqrt{R_k}},\sqrt{\frac{t}{R_k}}\right\}\right],\end{aligned}$$

since $r_k \geq \sqrt{R_k}$ by Lemma 2. Setting $t = \sqrt{n}$ implies that

$$\frac{1}{n}\sum_{i=1}^{n}\mu_i(T) \leq s_k\left[1 + 2c_2\sqrt{\frac{n}{R_k}}\right]$$

with probability at least $1 - 2e^{-\sqrt{n}}$. Thus by inequality (28)

$$\begin{aligned}
\mathbb{E}\left[\mathrm{Tr}(T^{-1})\right] &\geq \frac{n}{s_k\left(1 + 2c_2\sqrt{\frac{n}{R_k}}\right)}\mathbb{P}\left[\frac{1}{n}\sum_{i=1}^{n}\mu_i(T) \leq s_k\left[1 + 2c_2\sqrt{\frac{n}{R_k}}\right]\right] \\
&\geq \frac{n}{s_k}\left[\frac{1 - 2e^{-\sqrt{n}}}{1 + 2c_2\sqrt{\frac{n}{R_k}}}\right]. \qquad (29)
\end{aligned}$$

Combined with the lower bound in inequality (27) we find that

$$\begin{aligned}
\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right] &\geq \frac{n}{s_k}\left[\frac{1 - 2e^{-\sqrt{n}}}{1 + 2c_2\sqrt{\frac{n}{R_k}}}\right] - \frac{c_1 k}{s_k} \\
&\geq \frac{n}{s_k}\left[1 - \frac{2c_2\sqrt{\frac{n}{R_k}} + 2e^{-\sqrt{n}}}{1 + 2c_2\sqrt{\frac{n}{R_k}}} - \frac{c_1 k}{n}\right] \\
&\geq \frac{n}{s_k}\left[1 - c_0\left(\sqrt{\frac{n}{R_k}} + \frac{k}{n} + e^{-\sqrt{n}}\right)\right] \qquad \text{(since } R_k \geq r_k \geq bn\text{)}. \qquad (30)
\end{aligned}$$

This proves the desired lower bound.

The upper bound: To obtain the upper bound we shall bound

$$\mathbb{E}\left[\mathrm{Tr}(T^{-1})\right] = \mathbb{E}\left[\sum_{i=1}^{n}\frac{1}{\mu_i(T)}\right] \leq n\mathbb{E}\left[\frac{1}{\mu_n(T)}\right]. \qquad (31)$$

We will upper bound the expected value of $1/\mu_n(T)$ again by integrating tail bounds. We have

$$\begin{aligned}\mathbb{E}\left[\frac{1}{\mu_n(T)}\right] &= \int_0^\infty \mathbb{P}\left[\frac{1}{\mu_n(T)} \geq \omega\right] \mathrm{d}\omega \\ &= \int_0^\infty \mathbb{P}\left[\mu_n(T) \leq \frac{1}{\omega}\right] \mathrm{d}\omega \\ &= \underbrace{\int_0^{\frac{1}{s_k\left[1-c_3\left(\frac{n+\eta}{r_k}+\sqrt{\frac{n+\eta}{R_k}}\right)\right]}} \mathbb{P}\left[\mu_n(T) \leq \frac{1}{\omega}\right] \mathrm{d}\omega}_{=:\clubsuit} \\ &\qquad + \underbrace{\int_{\frac{1}{s_k\left[1-c_3\left(\frac{n+\eta}{r_k}+\sqrt{\frac{n+\eta}{R_k}}\right)\right]}}^{\frac{1}{c_4 s_k}} \mathbb{P}\left[\mu_n(T) \leq \frac{1}{\omega}\right] \mathrm{d}\omega}_{=:\spadesuit} \\ &\qquad + \underbrace{\int_{\frac{1}{c_4 s_k}}^\infty \mathbb{P}\left[\mu_n(T) \leq \frac{1}{\omega}\right] \mathrm{d}\omega}_{=:\blacklozenge}, \qquad (32)\end{aligned}$$

where

- c_3 is the constant c from Lemma 14,
- c_4 is smaller than the constant c_1^2 in Lemma 15, and
- η is small enough such that it satisfies $c_4 \leq 1 - c_3\left(\frac{n+\eta}{r_k} + \sqrt{\frac{n+\eta}{R_k}}\right)$.

Below we will set η to scale linearly with n, thus, this condition will be satisfied since $R_k \geq r_k \geq bn$ for a large enough value of b.

The first term $\clubsuit$ is positive because η scales linearly with n and $R_k \geq r_k \geq bn$ for suitably large b, and so it can be bounded as follows:

$$\clubsuit \leq \frac{1}{s_k\left[1-c_3\left(\frac{n+\eta}{r_k}+\sqrt{\frac{n+\eta}{R_k}}\right)\right]}. \qquad (33)$$

Next, consider the term $\spadesuit$. Here we will use the additive concentration inequality (Lemma 14). By Lemma 14 we know that with probability at most $2e^{-t}$

$$\begin{aligned}\mu_n(T) &\leq s_k\left[1 - c_3\left(\frac{t+n}{r_k} + \sqrt{\frac{t+n}{R_k}}\right)\right] \\ &\leq s_k\left[1 - c_3\left(\frac{t+n}{r_k} + \sqrt{\frac{t+n}{r_k}}\right)\right] \qquad \text{(since } r_k \leq R_k \text{ by Lemma 2)} \\ &\leq s_k\left[1 - 2c_3 \max\left\{\frac{t+n}{r_k}, \sqrt{\frac{t+n}{r_k}}\right\}\right]. \qquad (34)\end{aligned}$$

Also, the integral term $\spadesuit$ is positive, because c_4 is chosen to be small enough, η scales linearly with n, and $R_k \geq r_k \geq bn$ for suitably large b. Thus,

$$\begin{aligned}
\spadesuit &= \int_{\frac{1}{s_k\left[1-c_3\left(\frac{n+\eta}{r_k}+\sqrt{\frac{n+\eta}{R_k}}\right)\right]}}^{\frac{1}{c_4 s_k}} \mathbb{P}\left[\mu_n(T) \leq \frac{1}{\omega}\right] \, \mathrm{d}\omega \\
&\leq \int_{\frac{1}{s_k\left[1-c_5\sqrt{\frac{n+\eta}{r_k}}\right]}}^{\frac{1}{c_4 s_k}} \mathbb{P}\left[\mu_n(T) \leq \frac{1}{\omega}\right] \, \mathrm{d}\omega \\
&\leq 2\int_{\frac{1}{s_k\left[1-c_5\sqrt{\frac{n+\eta}{r_k}}\right]}}^{\frac{1}{c_4 s_k}} \exp\left[-r_k \min\left\{\frac{\left(1-\frac{1}{\omega s_k}\right)}{2c_3}, \frac{\left(1-\frac{1}{\omega s_k}\right)^2}{4c_3^2}\right\} + n\right] \, \mathrm{d}\omega \\
&\qquad \text{(applying inequality (34), and by setting } 1/\omega \text{ equal to the RHS of (34) and solving for } t\text{)} \\
&\leq 2e^n \int_{\frac{1}{s_k\left[1-c_5\sqrt{\frac{n+\eta}{r_k}}\right]}}^{\frac{1}{c_4 s_k}} \exp\left[-c_6 r_k \left(1-\frac{1}{\omega s_k}\right)^2\right] \, \mathrm{d}\omega,
\end{aligned}$$

where the last inequality follows since $\omega > 1/s_k$ and therefore the term in the round bracket is always smaller than 1. Thus, we get that

$$\spadesuit \leq 2e^n \int_{\frac{1}{s_k\left[1-c_5\sqrt{\frac{n+\eta}{r_k}}\right]}}^{\frac{1}{c_4 s_k}} \exp\left[-c_6 r_k \left(1-\frac{1}{\omega s_k}\right)^2\right] \, \mathrm{d}\omega.$$

Now we set $\eta = c_7 n$, for a large enough constant c_7, and perform a change of variables, redefining $1 - \frac{1}{\omega s_k} \to \bar{\omega}$, to get

$$\begin{aligned}
\spadesuit &\leq \frac{2e^n}{s_k} \int_{c_5\sqrt{\frac{(c_7+1)n}{r_k}}}^{1-c_4} \frac{\exp\left(-c_6 r_k \bar{\omega}^2\right)}{(1-\bar{\omega})^2} \, \mathrm{d}\bar{\omega} \\
&\leq \frac{2\exp\left(-c_8 n\right)}{s_k} \int_{c_5\sqrt{\frac{(c_7+1)n}{r_k}}}^{1-c_4} \frac{1}{(1-\bar{\omega})^2} \, \mathrm{d}\omega \\
&= \frac{2\exp\left(-c_8 n\right)}{s_k} \left[\frac{1}{1-c_5\sqrt{\frac{(c_7+1)n}{r_k}}} - \frac{1}{c_4}\right] \\
&\overset{(i)}{\leq} \frac{c_9 \exp\left(-c_8 n\right)}{s_k},
\end{aligned} \tag{35}$$

where (i) holds because $r_k \geq bn$ for a large value of b.

Finally, we turn our attention to the term ♦. By using Lemma 15 we know that

$$\begin{aligned}
\blacklozenge &= \int_{\frac{1}{c_4 s_k}}^{\infty} \mathbb{P}\left[\mu_n(T) \le \frac{1}{\omega}\right] \,\mathrm{d}\omega \\
&\le \int_{\frac{1}{c_4 s_k}}^{\infty} \left(\frac{c_{10}}{\omega s_k}\right)^{c_{11} r_k} \,\mathrm{d}\omega \\
&= \frac{1}{c_4 s_k (c_{11} r_k - 1)} \left(c_4 c_{10}\right)^{c_{11} r_k} \le \frac{c_{12}}{r_k s_k}, \qquad (36)
\end{aligned}$$

where the last inequality follows since $r_k \ge bn$ and because c_4 is chosen to be small enough.

By combining inequalities (32), (33), (35) and (36) we conclude that

$$\begin{aligned}
&\mathbb{E}\left[\frac{1}{\mu_n(T)}\right] \\
&\le \frac{1}{s_k\left[1 - c_3\left(\frac{n+\eta}{r_k} + \sqrt{\frac{n+\eta}{R_k}}\right)\right]} + \frac{c_9 \exp\left(-c_8 n\right)}{s_k} + \frac{c_{12}}{r_k s_k} \\
&\le \frac{1}{s_k\left[1 - c_{13}\left(\frac{n}{r_k} + \sqrt{\frac{n}{R_k}}\right)\right]} + \frac{c_9 \exp\left(-c_8 n\right)}{s_k} + \frac{c_{12}}{r_k s_k} \qquad \text{(since } \eta = c_7 n\text{)} \\
&= \frac{1}{s_k}\left[1 + c_{14}\left(\frac{\sqrt{\frac{n}{R_k}} + \frac{n}{r_k}}{1 - c_{13}\left(\sqrt{\frac{n}{R_k}} + \frac{n}{r_k}\right)} + \exp(-c_8 n) + \frac{1}{r_k}\right)\right] \\
&\le \frac{1}{s_k}\left[1 + c_{15}\left(\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \exp(-c_8 n)\right)\right],
\end{aligned}$$

where the last inequality follows since $R_k \ge r_k \ge bn$ with b being large enough. Hence by inequality (31)

$$\begin{aligned}
\mathbb{E}\left[\mathrm{Tr}(T^{-1})\right] &\le \frac{n}{s_k}\left[1 + c_{15}\left(\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \exp(-c_8 n)\right)\right] \\
&\le \frac{n}{s_k}\left[1 + c_{15}\left(\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \exp(-c_8 \sqrt{n})\right)\right],
\end{aligned}$$

which combined with inequality (27) completes our proof. ■

4.2.5 Proof of Lemma 16

As mentioned previously, by using the previous four lemmas we will now show that the trace of A^{-1} is close to n/s_k with high probability. Recall the statement of the lemma from above.

Lemma 16 *There are positive constants $c_0, \ldots, c_4$ such that, if $p \ge c_0(n+k)$ then with probability at least $1 - c_1 e^{-c_2 n}$*

$$\left|\mathrm{Tr}\left((XX^\top)^{-1}\right) - \frac{n}{s_k}\right| \le \frac{c_3 n}{s_k}\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \frac{k}{n} + e^{-c_4\sqrt{n}}\right].$$

Proof Recall that by definition $A = XX^\top$. By an application of the triangle inequality,

$$\begin{aligned}\left|\mathrm{Tr}(A^{-1}) - \frac{n}{s_k}\right| &\leq \left|\mathrm{Tr}(A^{-1}) - \mathrm{Tr}(T^{-1})\right| + \left|\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right] - \mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]\right| \\ &\quad + \left|\mathrm{Tr}(T^{-1}) - \mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]\right| + \left|\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right] - \frac{n}{s_k}\right|. \end{aligned} \tag{37}$$

By Lemma 18 we know that

$$\left|\mathrm{Tr}(A^{-1}) - \mathrm{Tr}(T^{-1})\right| \leq \frac{c_5 k}{s_k} \tag{38}$$

with probability at least

$$1 - 2\exp(-c_6 r_k) - (c_7)^{c_8 r_k} \geq 1 - c_9 \exp(-c_{10} r_k) \geq 1 - c_9 \exp(-c_{11} n),$$

where the last two inequalities follow since $r_k \geq bn$ for some large enough value of b. Next, by Lemma 19 we know that

$$\left|\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right] - \mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]\right| \leq \frac{c_{12} k}{s_k}. \tag{39}$$

By Lemma 20 we get that with probability at least $1 - 2e^{-n}$,

$$\left|\mathrm{Tr}(T^{-1}) - \mathbb{E}\left[\mathrm{Tr}(T^{-1})\right]\right| \leq \frac{c_{13} n}{s_k}\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k}\right]. \tag{40}$$

Finally, by Lemma 21 we know that

$$\left|\mathbb{E}\left[\mathrm{Tr}(A^{-1})\right] - \frac{n}{s_k}\right| \leq \frac{c_{14} n}{s_k}\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \frac{k}{n} + e^{-c_{15}\sqrt{n}}\right]. \tag{41}$$

Combining the (37)-(41) establishes our claim. ■

4.3 Proof of Lemma 13

Armed with Lemmas 14, 15 and 16, we are ready to prove Lemma 13 and establish upper and lower bounds on $\alpha^\star$. This proof is further divided into a series of lemmas.

We prove bounds on $\alpha^\star$ in terms of $\|\widetilde{\mathbf{y}}\|$ and $\|w\|$ in Lemma 22. We in turn bound $\|\widetilde{\mathbf{y}}\|$ in terms of $\|\theta^\star\|$ and $\|D^\dagger U^\top \boldsymbol{\varepsilon}\|$ in Lemma 23. Next, in Lemma 24 we show that, with high probability, $\|D^\dagger U^\top \boldsymbol{\varepsilon}\|$ is close to $\sigma^2 \mathrm{Tr}\left((XX^\top)^{-1}\right)$. Recall that, in Section 4.2, we showed that $\mathrm{Tr}\left((XX^\top)^{-1}\right)$ concentrates around n/s_k.

The next lemma provides an upper and lower bound on $\alpha^\star$.

Lemma 22 *The scaling factor $\alpha^\star$ satisfies the following*

$$\frac{2\|\widetilde{\mathbf{y}}\|^{1/2}}{3} \leq \alpha^\star \leq \frac{2\|\widetilde{\mathbf{y}}\|^{1/2}}{3}\sqrt{\sqrt{1 + \frac{4\|w\|^4}{81\|\widetilde{\mathbf{y}}\|^2}} + \frac{2\|w\|^2}{9\|\widetilde{\mathbf{y}}\|}}.$$

Proof Recall the definition of $\alpha^\star$ from above

$$\alpha^\star = \sqrt{\frac{8\|\widetilde{w}_{n+1:p}\|^2 + \sqrt{64\|\widetilde{w}_{n+1:p}\|^4 + 1296\|\widetilde{\mathbf{y}}\|^2}}{81}}.$$

Note that $\|\widetilde{w}_{n+1:p}\| \geq 0$. This immediately leads to the lower bound. For the upper bound note that $\|\widetilde{w}_{n+1:p}\| \leq \|\widetilde{w}\| = \|V^\top w\| = \|w\|$, since V is a unitary matrix. ■

The following lemma provides high probability upper and lower bounds on the norm of $\widetilde{\mathbf{y}}$.

Lemma 23 *The squared norm of $\widetilde{\mathbf{y}}$ satisfies the following*

$$\|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 \left(1 - \frac{2\|\theta^\star\|}{\|D^\dagger U^\top \boldsymbol{\varepsilon}\|}\right) \leq \|\widetilde{\mathbf{y}}\|^2 \leq \|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 \left(1 + \frac{\|\theta^\star\|}{\|D^\dagger U^\top \boldsymbol{\varepsilon}\|}\right)^2.$$

Proof Recall that $UDV^\top$ is the SVD of X, $\widetilde{\mathbf{y}} = D^\dagger U^\top \mathbf{y}$ and that $\mathbf{y} = X\theta^\star + \boldsymbol{\varepsilon}$. Therefore

$$\begin{aligned}\widetilde{\mathbf{y}} = D^\dagger U^\top (X\theta^\star + \boldsymbol{\varepsilon}) = D^\dagger U^\top (UDV^\top \theta^\star + \boldsymbol{\varepsilon}) &= D^\dagger D V^\top \theta^\star + D^\dagger U^\top \boldsymbol{\varepsilon} \\ &= \begin{bmatrix} I_n \\ 0_{(p-n)\times n} \end{bmatrix} V^\top \theta^\star + D^\dagger U^\top \boldsymbol{\varepsilon}.\end{aligned}$$

Define $\widetilde{\theta}^\star := V^\top \theta^\star$ and so

$$\widetilde{\mathbf{y}} = \widetilde{\theta}^\star_{1:n} + D^\dagger U^\top \boldsymbol{\varepsilon}.$$

Thus,

$$\|\widetilde{\mathbf{y}}\|^2 = \|\widetilde{\theta}^\star_{1:n}\|^2 + \|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 + 2\left(\boldsymbol{\varepsilon}^\top U D^{\dagger\top}\right)\left(\widetilde{\theta}^\star_{1:n}\right).$$

Now since $0 \leq \|\widetilde{\theta}^\star_{1:n}\| \leq \|\widetilde{\theta}^\star\| = \|V^\top \theta^\star\| = \|\theta^\star\|$ we get that

$$\|\widetilde{\mathbf{y}}\|^2 \geq \|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 - 2\|D^\dagger U^\top \boldsymbol{\varepsilon}\|\|\theta^\star\| = \|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 \left(1 - \frac{2\|\theta^\star\|}{\|D^\dagger U^\top \boldsymbol{\varepsilon}\|}\right)$$

and also that

$$\begin{aligned}\|\widetilde{\mathbf{y}}\|^2 &\leq \|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 + 2\|D^\dagger U^\top \boldsymbol{\varepsilon}\|\|\theta^\star\| + \|\theta^\star\|^2 \\ &= \left(\|D^\dagger U^\top \boldsymbol{\varepsilon}\| + \|\theta^\star\|\right)^2 = \|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 \left(1 + \frac{\|\theta^\star\|}{\|D^\dagger U^\top \boldsymbol{\varepsilon}\|}\right)^2,\end{aligned}$$

which establishes our claim. ■

The next result upper and lower bounds $\|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2$ with high probability.

Lemma 24 *For any $t \geq 0$, with probability at least $1 - 2e^{-t}$*

$$\left|\|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 - \sigma^2 \mathrm{Tr}\left((XX^\top)^{-1}\right)\right| \leq c \max\left\{\frac{t}{\mu_n(XX^\top)}, \sqrt{t\sum_{i=1}^n \frac{1}{\mu_i^2(XX^\top)}}\right\}.$$

Proof Let $u_1, \ldots, u_n$ be the columns of U. The matrix U is unitary so each column u_i has unit norm. So

$$\|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 = \sum_{i=1}^n \frac{(u_i^\top \boldsymbol{\varepsilon})^2}{D_{ii}^2} = \sum_{i=1}^n \frac{(u_i^\top \boldsymbol{\varepsilon})^2}{\mu_i(XX^\top)}$$

and

$$\mathbb{E}_{\boldsymbol{\varepsilon}}\left[\|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 \mid X\right] = \sum_{i=1}^n \frac{\mathbb{E}\left[(u_i^\top \boldsymbol{\varepsilon})^2 \mid X\right]}{D_{ii}^2} = \sum_{i=1}^n \frac{\sigma^2}{D_{ii}^2} = \sigma^2 \mathrm{Tr}\left((XX^\top)^{-1}\right).$$

Since the components are $\boldsymbol{\varepsilon}$ are independent, σ_y^2-sub-Gaussian random variables, with variance σ^2, by invoking the Hanson-Wright inequality (see Rudelson and Vershynin, 2013, Theorem 1) we infer that

$$\begin{aligned}\left|\|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 - \sigma^2 \mathrm{Tr}((XX^\top)^{-1})\right| &= \left|\boldsymbol{\varepsilon}^\top \left(UD^{\dagger\top}D^\dagger U^\top\right)\boldsymbol{\varepsilon} - \sigma^2\mathrm{Tr}((XX^\top)^{-1})\right| \\ &\le c_1\sigma_y^2 \max\left\{\frac{t}{\mu_n(XX^\top)}, \sqrt{t \cdot \sum_{i=1}^n \frac{1}{\mu_i^2(XX^\top)}}\right\} \\ &= c\max\left\{\frac{t}{\mu_n(XX^\top)}, \sqrt{t \cdot \sum_{i=1}^n \frac{1}{\mu_i^2(XX^\top)}}\right\}\end{aligned}$$

with probability at least $1 - 2e^{-t}$, completing the proof. ■

With these lemmas in place we are now ready to prove Lemma 13. We restate it here.

Lemma 13 *There are constants* $c_0, \ldots, c_5$ *such that for any* $\delta \in (e^{-c_0\sqrt{n}}, 1)$*, if* $p \ge c_1(n+k)$*,* $n \ge c_2 \max\{k, s_k\}$ *and* $\|\theta^\star\|, \|w\| \le c_3$ *then with probability at least* $1 - c_4\delta$*,*

$$\left|\frac{\alpha^\star}{\frac{2\sqrt{\sigma}n^{1/4}}{3s_k^{1/4}}} - 1\right| \le c_5\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{s_k}{n}} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n}\right].$$

Proof Using Lemma 16, with probability at least $1 - c_6e^{-c_7n}$,

$$\left|\mathrm{Tr}(XX^{-1}) - \frac{n}{s_k}\right| \le \frac{c_8n}{s_k}\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \frac{k}{n} + e^{-c_9\sqrt{n}}\right]. \tag{42}$$

Next, by Lemma 14, with probability at least $1 - 2e^{-\sqrt{n}}$, for all $i \in [n]$

$$\begin{aligned}\mu_i(XX^\top) &\ge s_k\left[1 - c_{10}\left(\frac{n+\sqrt{n}}{r_k} + \sqrt{\frac{n+\sqrt{n}}{R_k}}\right)\right] \\ &\ge s_k\left[1 - c_{11}\left(\frac{n}{r_k} + \sqrt{\frac{n}{r_k}}\right)\right] && \text{(since } R_k \ge r_k \text{ by Lemma 2)} \\ &\ge c_{12}s_k && \text{(since } r_k \ge bn\text{)}.\end{aligned}$$

This, combined with Lemma 24, tells us that for any $\delta \in (e^{-c_0\sqrt{n}}, 1)$ with probability at least $1 - c_{13}\delta$

$$\begin{aligned}\left| \|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 - \sigma^2 \mathrm{Tr}((XX^\top)^{-1}) \right| &\leq c_{14} \max\left\{ \frac{\log(2/\delta)}{s_k}, \frac{\sqrt{n\log(2/\delta)}}{s_k} \right\} \\ &\leq \frac{c_{14}\sqrt{n\log(2/\delta)}}{s_k}.\end{aligned}$$

Combining this with inequality (42) and recalling that σ^2 is a constant, we infer that, with probability at least $1 - c_3\delta$,

$$\begin{aligned}\left| \|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 - \frac{\sigma^2 n}{s_k} \right| &\leq \frac{c_{15}n}{s_k}\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + e^{-c_9\sqrt{n}} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n} \right] \\ &\leq \frac{c_{16}n}{s_k}\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n} \right] && (43) \\ &\leq \frac{c_{17}n}{s_k}, && (44)\end{aligned}$$

where the last inequality follows since $R_k \geq r_k \geq bn$, $n \geq c_2 k$ and since $\delta \geq e^{-c_0\sqrt{n}}$.

We shall assume that condition (43) holds going forward. (This determines the success probability in the statement of the lemma.) Now since $r_k \geq bn$ and $n \geq c_2 \max\{k, s_k\}$ for a large enough constants b and c_2, by invoking Lemma 23, we find that

$$\begin{aligned}\|\widetilde{\mathbf{y}}\|^2 &\leq \|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 \left(1 + \frac{\|\theta^\star\|}{\|D^\dagger U^\top \boldsymbol{\varepsilon}\|}\right)^2 \\ &= \|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 \left(1 + \frac{\|\theta^\star\|^2}{\|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2} + \frac{2\|\theta^\star\|}{\|D^\dagger U^\top \boldsymbol{\varepsilon}\|}\right) \\ &\overset{(i)}{\leq} \frac{\sigma^2 n}{s_k}\left[1 + c_{16}\left(\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n}\right)\right] \\ &\qquad\qquad \times \left(1 + c_{18}\left(\frac{\|\theta^\star\|^2 s_k}{n} + \frac{\|\theta^\star\|\sqrt{s_k}}{\sqrt{n}}\right)\right) \\ &\overset{(ii)}{\leq} \frac{\sigma^2 n}{s_k}\left[1 + c_{16}\left(\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n}\right)\right]\left(1 + c_{19}\sqrt{\frac{s_k}{n}}\right) && (45) \\ &\leq \frac{c_{20}n}{s_k}, && (46)\end{aligned}$$

where (i) follows by applying inequalities (43) and (44), and also because σ^2 is a constant. The second inequality (ii) follows since $\|\theta^\star\| \leq c_3$ and because $n \geq c_2 s_k$. Also, by Lemma 23, we get that

$$\begin{aligned}
\|\widetilde{\mathbf{y}}\|^2 &\geq \|D^\dagger U^\top \boldsymbol{\varepsilon}\|^2 \left(1 - \frac{2\|\theta^\star\|}{\|D^\dagger U^\top \boldsymbol{\varepsilon}\|}\right) \\
&\geq \frac{\sigma^2 n}{s_k}\left[1 - c_{16}\left(\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n}\right)\right]\left(1 - c_{21}\sqrt{\frac{s_k}{n}}\right) \qquad (47) \\
&\geq \frac{c_{22} n}{s_k}, \qquad (48)
\end{aligned}$$

where the last two inequalities follow by repeating the logic from the previous equation block.

Now recall that, by Lemma 22,

$$\frac{2\|\widetilde{\mathbf{y}}\|^{1/2}}{3} \leq \alpha^\star \leq \frac{2\|\widetilde{\mathbf{y}}\|^{1/2}}{3}\sqrt{\sqrt{1 + \frac{4\|w\|^4}{81\|\widetilde{\mathbf{y}}\|^2}} + \frac{2\|w\|^2}{9\|\widetilde{\mathbf{y}}\|}}. \qquad (49)$$

Using the lower bound in the equation above combining with inequality (47) we find that

$$\alpha^\star \geq \frac{2\sqrt{\sigma} n^{1/4}}{3 s_k^{1/4}}\left[1 - c_{16}\left(\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n}\right)\right]\left(1 - c_{23}\sqrt{\frac{s_k}{n}}\right),$$

and since $n \geq c_2 s_k$ for a large enough constant c_2,

$$\frac{\alpha^\star}{\frac{2\sqrt{\sigma} n^{1/4}}{3 s_k^{1/4}}} - 1 \geq -c_{24}\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{s_k}{n}} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n}\right]. \qquad (50)$$

Now for the upper bound, since $\|w\| \leq c_3$, by using (48) we have that $\|w\|^2/\|\widetilde{\mathbf{y}}\| \leq 1/20$, since $n > c_2 s_k$, where c_2 is large enough. Thus, by (49),

$$\begin{aligned}
\alpha^\star &\leq \frac{2\|\widetilde{\mathbf{y}}\|^{1/2}}{3}\left(1 + \frac{c_{25}\|w\|}{\|\widetilde{\mathbf{y}}\|^{1/2}}\right) \\
&\leq \frac{2\sqrt{\sigma} n^{1/4}}{3 s_k^{1/4}}\left[1 + c_{26}\left(\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n}\right)\right]\left(1 + c_{27}\sqrt{\frac{s_k}{n}}\right)
\end{aligned}$$

and so

$$\frac{\alpha^\star}{\frac{2\sqrt{\sigma} n^{1/4}}{3 s_k^{1/4}}} - 1 \leq c_{28}\left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{s_k}{n}} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n}\right].$$

This combined with (50) completes the proof. ■

4.4 Proof of Theorem 5

Let us first restate the theorem.

Theorem 5 *Under Assumptions 1-6, there exist constants* $c_0, \dots, c_7$ *such that for any* $\delta \in (e^{-c_0\sqrt{n}}, 1 - c_1 e^{-c_2 n})$*, if* $p \geq c_3(n+k)$*,* $n \geq c_4 \max\{k, s_k\}$ *and* $\|\theta^\star\|, \|w\| \leq c_5$ *then with probability at least* $1 - c_6\delta$

$$\mathsf{Risk}(\hat{\theta}) \leq \mathsf{Bias} + \mathsf{Variance} + \Xi,$$

where

$$\begin{aligned}\mathsf{Bias} &\leq c_7 \left(\|(\theta^\star - \psi)_{1:k}\|^2_{\Sigma^{-1}_{1:k}} \left(\frac{s_k}{n}\right)^2 + \|(\theta^\star - \psi)_{k+1:p}\|^2_{\Sigma_{k+1:p}} \right) \leq \frac{2c_7 \|\theta^\star - \psi\|^2 s_k}{n};\\ \mathsf{Variance} &\leq c_7 \log(1/\delta) \left(\frac{k}{n} + \frac{n}{R_k} \right);\\ \Xi &\leq c_7 \lambda_1 \|\psi\|^2 \left[\frac{n}{R_k} + \frac{n^2}{r_k^2} + \frac{s_k}{n} + \frac{\log(1/\delta)}{n} + \frac{k^2}{n^2} \right] \max\left\{ \sqrt{\frac{r_0}{n}}, \frac{r_0}{n}, \sqrt{\frac{\log(1/\delta)}{n}} \right\}.\end{aligned}$$

Proof By Lemma 12, we know that

$$\mathsf{Risk}(\hat{\theta}) \leq c_8 (\theta^\star - \alpha^\star w)^\top B (\theta^\star - \alpha^\star w) + c_8 \log(1/\delta) \mathrm{Tr}(C)$$

with probability at least $1 - \delta$, where the matrices

$$\begin{aligned}B &= \left(I - X^\top (XX^\top)^{-1} X\right) \Sigma \left(I - X^\top (XX^\top)^{-1} X\right) \quad \text{and}\\ C &= (XX^\top)^{-1} X \Sigma X^\top (XX^\top)^{-1}.\end{aligned}$$

Recall that $\psi = \frac{2\sqrt{\sigma} n^{1/4} w}{3 s_k^{1/4}}$. Thus, with the same probability

$$\begin{aligned}\mathsf{Risk}(\hat{\theta}) &\leq c_8 \left(\theta^\star - \psi - (\alpha^\star w - \psi)\right)^\top B \left(\theta^\star - \psi - (\alpha^\star w - \psi)\right) + c_8 \log(1/\delta) \mathrm{Tr}(C)\\ &= c_8 \|\theta^\star - \psi - (\alpha^\star w - \psi)\|_B^2 + c_8 \log(1/\delta) \mathrm{Tr}(C)\\ &\leq 2c_8 \|\theta^\star - \psi\|_B^2 + 2c_8 \|\alpha^\star w - \psi\|_B^2 + c_8 \log(1/\delta) \mathrm{Tr}(C)\\ &= \underbrace{2c_8 \left(\theta^\star - \psi\right)^\top B \left(\theta^\star - \psi\right)}_{\text{“Bias”}} + \underbrace{c_8 \log(1/\delta) \mathrm{Tr}(C)}_{\text{“Variance”}} + \underbrace{2c_8 \|B\|_{op} \|\alpha^\star w - \psi\|^2}_{\text{“}\Xi\text{”}}. \qquad (51)\end{aligned}$$

We shall bound each of the three terms in the inequality above to establish the theorem.

Recall the definition of the matrix $T = \sum_{j>k} \lambda_j z_j z_j^\top$ from Definition 17 above. Define $S := \{j : j > k\}$, and let $X_S \in \mathbb{R}^{n \times |S|}$ be the submatrix formed by the last $p - k$ columns of $X \in \mathbb{R}^{n \times p}$. It can be verified that $T = X_S X_S^\top$. By Lemma 14, with probability at least $1 - 2e^{-n} \geq 1 - c_9\delta$, (since $\delta \geq e^{-c_0\sqrt{n}}$)

$$\mu_1(T) \leq c_{10} \sum_{j>k} \lambda_j \quad \text{and} \quad \mu_n(T) \geq c_{11} \sum_{j>k} \lambda_j.$$

Therefore, the condition number of the matrix T is a constant with the same probability. Assuming this bound on the condition number holds we shall bound the first two terms in (51).

Bound on the bias and variance: Since the condition number of T is at most a constant, by invoking (Tsigler and Bartlett, 2020, Theorem 1) we get that with probability at least $1 - c_{12}\delta$

$$\mathsf{Bias} \le c_7 \left(\|(\theta^\star - \psi)_{1:k}\|^2_{\Sigma_{1:k}^{-1}} \left(\frac{s_k}{n}\right)^2 + \|(\theta^\star - \psi)_{k+1:p}\|^2_{\Sigma_{k+1:p}} \right) \tag{52}$$

and

$$\mathsf{Variance} \le c_7 \log(1/\delta) \left(\frac{k}{n} + \frac{n}{R_k} \right). \tag{53}$$

We simplify our upper bound on Bias by noting that under our choice of k as follows:

$$\begin{aligned}
&c_7 \left(\|(\theta^\star - \psi)_{1:k}\|^2_{\Sigma_{1:k}^{-1}} \left(\frac{s_k}{n}\right)^2 + \|(\theta^\star - \psi)_{k+1:p}\|^2_{\Sigma_{k+1:p}} \right) \\
&\quad = c_7 \sum_{i=1}^{p} \left[\mathbb{I}(i \le k)(\theta_i^\star - \psi_i)^2 \frac{s_k^2}{n^2 \lambda_i} + \mathbb{I}(i > k)\lambda_i(\theta_i^\star - \psi_i)^2 \right] \\
&\quad = c_7 \sum_{i=1}^{p} \lambda_i(\theta_i^\star - \psi_i)^2 \left[\mathbb{I}(i \le k)\frac{s_k^2}{n^2 \lambda_i^2} + \mathbb{I}(i > k) \right] \\
&\quad = c_7 \sum_{i=1}^{p} \lambda_i(\theta_i^\star - \psi_i)^2 \frac{(\frac{s_k}{n})^2}{(\frac{s_k}{n})^2 + \lambda_i^2} \left[\mathbb{I}(i \le k) \left(1 + \frac{1}{\lambda_i^2}\left(\frac{s_k}{n}\right)^2 \right) + \mathbb{I}(i > k) \left(1 + \lambda_i^2 \left(\frac{n}{s_k}\right)^2 \right) \right] \\
&\quad \overset{(i)}{\le} c_7 \sum_{i=1}^{p} \lambda_i(\theta_i^\star - \psi_i)^2 \frac{(\frac{s_k}{n})^2}{(\frac{s_k}{n})^2 + \lambda_i^2} \left[\mathbb{I}(i \le k) \left(1 + b^2 \right) + \mathbb{I}(i > k) \left(1 + \lambda_i^2 \left(\frac{n}{s_k}\right)^2 \right) \right] \\
&\quad \le c_7 \sum_{i=1}^{p} \lambda_i(\theta_i^\star - \psi_i)^2 \frac{(\frac{s_k}{n})^2}{(\frac{s_k}{n})^2 + \lambda_i^2} \left[\mathbb{I}(i \le k) \left(1 + b^2 \right) + \mathbb{I}(i > k) \left(1 + \lambda_{k+1}^2 \left(\frac{n}{s_k}\right)^2 \right) \right] \\
&\quad \le c_7 \sum_{i=1}^{p} \lambda_i(\theta_i^\star - \psi_i)^2 \frac{(\frac{s_k}{n})^2}{(\frac{s_k}{n})^2 + \lambda_i^2} \left[\mathbb{I}(i \le k) \left(1 + b^2 \right) + \mathbb{I}(i > k) \left(1 + \left(\frac{n}{r_k}\right)^2 \right) \right] \\
&\quad \overset{(ii)}{\le} c_7 \sum_{i=1}^{p} \lambda_i(\theta_i^\star - \psi_i)^2 \frac{(\frac{s_k}{n})^2}{(\frac{s_k}{n})^2 + \lambda_i^2} \left[\mathbb{I}(i \le k) \left(1 + b^2 \right) + \mathbb{I}(i > k) \left(1 + \frac{1}{b^2} \right) \right] \\
&\quad \le c_{13} \sum_{i=1}^{p} \lambda_i(\theta_i^\star - \psi_i)^2 \frac{(\frac{s_k}{n})^2}{(\frac{s_k}{n})^2 + \lambda_i^2},
\end{aligned}$$

where (i) follows since by definition $k = \min\{j \geq 0 : r_j \geq bn\}$ and so for $i \leq k$, $s_k/\lambda_i \leq s_i/\lambda_i = r_i < bn$. Inequality (ii) follows since $r_k \geq bn$. Continuing we get that

$$\begin{aligned}
&c_7 \left(\|(\theta^\star - \psi)_{1:k}\|^2_{\Sigma^{-1}_{1:k}} \left(\frac{s_k}{n}\right)^2 + \|(\theta^\star - \psi)_{k+1:p}\|^2_{\Sigma_{k+1:p}} \right) \\
&\quad \leq c_{13} \sum_{i=1}^p \lambda_i (\theta^\star - \psi)_i^2 \frac{\left(\frac{s_k}{n}\right)^2}{\left(\frac{s_k}{n}\right)^2 + \lambda_i^2} \\
&\quad = c_{13} \left(\frac{s_k}{n}\right)^2 \sum_{i=1}^p (\theta^\star - \psi)_i^2 \frac{\lambda_i}{\left(\frac{s_k}{n}\right)^2 + \lambda_i^2} \\
&\quad \leq c_{13} \left(\frac{s_k}{n}\right)^2 \|\theta^\star - \psi\|^2 \max_{i \in [p]} \frac{\lambda_i}{\left(\frac{s_k}{n}\right)^2 + \lambda_i^2} \qquad \text{(by Hölder's inequality)} \\
&\quad \leq c_{13} \left(\frac{s_k}{n}\right)^2 \|\theta^\star - \psi\|^2 \max_{\zeta \geq 0} \frac{\zeta}{\left(\frac{s_k}{n}\right)^2 + \zeta^2} = \frac{2c_{13}\|\theta^\star - \psi\|^2 s_k}{n}. \qquad (54)
\end{aligned}$$

Bound on Ξ (the estimation error of $\alpha^\star$): By Lemma 13 with probability at least $1 - c_{14}\delta$

$$\left| \alpha^\star - \frac{2\sqrt{\sigma} n^{1/4}}{3 s_k^{1/4}} \right| \leq c_{15} \frac{2\sqrt{\sigma} n^{1/4}}{3 s_k^{1/4}} \left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{s_k}{n}} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n} \right]$$

and therefore,

$$\begin{aligned}
\|\alpha^\star w - \psi\| &\leq c_{16} \|\psi\| \left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{s_k}{n}} + \sqrt{\frac{\log(2/\delta)}{n}} + \frac{k}{n} \right] \\
&\leq c_{17} \|\psi\| \left[\sqrt{\frac{n}{R_k}} + \frac{n}{r_k} + \sqrt{\frac{s_k}{n}} + \sqrt{\frac{\log(1/\delta)}{n}} + \frac{k}{n} \right] \quad (\text{since } \delta \leq 1 - c_1 e^{-c_2 n}). \qquad (55)
\end{aligned}$$

To control the operator norm of B, we first observe that

$$\begin{aligned}
\|B\|_{op} &= \left\| \left(I - X^\top (XX^\top)^{-1} X\right) \Sigma \left(I - X^\top (XX^\top)^{-1} X\right) \right\|_{op} \\
&= \left\| \left(I - X^\top (XX^\top)^{-1} X\right) \left(\Sigma - \frac{X^\top X}{n}\right) \left(I - X^\top (XX^\top)^{-1} X\right) \right\|_{op} \\
&\leq \left\| I - X^\top (XX^\top)^{-1} X \right\|_{op}^2 \left\| \Sigma - \frac{X^\top X}{n} \right\|_{op} \\
&\leq \left\| \Sigma - \frac{X^\top X}{n} \right\|_{op}.
\end{aligned}$$

Thus, by invoking (Koltchinskii and Lounici, 2017, Theorem 9) we get that with probability at least $1 - \delta$

$$\begin{aligned}
\|B\|_{op} &\leq c_{18} \lambda_1 \max\left\{ \sqrt{\frac{r_0}{n}}, \frac{r_0}{n}, \sqrt{\frac{\log(1/\delta)}{n}}, \frac{\log(1/\delta)}{n} \right\} \\
&\leq c_{18} \lambda_1 \max\left\{ \sqrt{\frac{r_0}{n}}, \frac{r_0}{n}, \sqrt{\frac{\log(1/\delta)}{n}} \right\}, \qquad (56)
\end{aligned}$$

where the second inequality follows since $\delta \geq e^{-c_0\sqrt{n}}$.

Combining inequalities (55) and (56) we get that with probability at least $1 - c_{19}\delta$

$$\begin{aligned} 2c_8\|B\|_{op}\|\alpha^\star w - \psi\|^2 \leq c_{20}\lambda_1\|\psi\|^2 \max\left\{\sqrt{\frac{r_0}{n}}, \frac{r_0}{n}, \sqrt{\frac{\log(1/\delta)}{n}}\right\} \\ \times\left[\frac{n}{R_k} + \frac{n^2}{r_k^2} + \frac{s_k}{n} + \frac{\log(2/\delta)}{n} + \frac{k^2}{n^2}\right]. \end{aligned} \tag{57}$$

Combining inequalities (52), (53), (54) and (57) along with a union bound completes the proof. ■

5. Proof of Proposition 8

Recall the statement of the proposition.

Proposition 25 *If $a(0)$ and $W(0)$ are chosen randomly, independent of X and $\mathbf{y}$, so that the distribution of $a(0)^\top W(0)$ is symmetric about the origin, then*

$$\mathbb{E}_{a(0),W(0),X,\mathbf{y}}[\mathsf{Risk}(\hat{\theta})] \geq \mathbb{E}\left[\theta^{\star\top}B\theta^\star\right] + \sigma^2\mathbb{E}\left[\mathrm{Tr}(C)\right],$$

where

$$\begin{aligned} &B := \left(I - X^\top(XX^\top)^{-1}X\right)\Sigma\left(I - X^\top(XX^\top)^{-1}X\right) \quad \textit{and} \\ &C := (XX^\top)^{-1}X\Sigma X^\top(XX^\top)^{-1}. \end{aligned}$$

Proof In the proof of Lemma 12, we showed that, for all $X, \mathbf{y}$, we have

$$\mathsf{Risk}(\hat{\theta}) = \mathbb{E}_x\left[\left(x^\top\left(I - X^\top(XX^\top)^{-1}X\right)(\theta^\star - \alpha^\star w) - x^\top X^\top(XX^\top)^{-1}\boldsymbol{\varepsilon}\right)^2\right].$$

Expanding the quadratic yields

$$\begin{aligned} \mathsf{Risk}(\hat{\theta}) = \mathbb{E}_x&\left[\left(x^\top\left(I - X^\top(XX^\top)^{-1}X\right)(\theta^\star - \alpha^\star w)\right)^2\right] + \mathbb{E}_x\left[\left(x^\top X^\top(XX^\top)^{-1}\boldsymbol{\varepsilon}\right)^2\right] \\ &+ 2\mathbb{E}_x\left[\left(x^\top\left(I - X^\top(XX^\top)^{-1}X\right)\theta^\star\right)\left(x^\top X^\top(XX^\top)^{-1}\boldsymbol{\varepsilon}\right)\right] \\ &- 2\mathbb{E}_x\left[\left(x^\top\left(I - X^\top(XX^\top)^{-1}X\right)(\alpha^\star w)\right)\left(x^\top X^\top(XX^\top)^{-1}\boldsymbol{\varepsilon}\right)\right]. \end{aligned}$$

Since the distribution of w is symmetric about the origin, and independent of X and $\mathbf{y}$, and since, for fixed X and $\mathbf{y}$, $\alpha^\star$ is determined as a function of w, after conditioning on X and $\mathbf{y}$, the distribution of $\alpha^\star w$ is symmetric about the origin, and therefore has zero mean.

This, along with the fact that $\mathbb{E}[\boldsymbol{\varepsilon}] = 0$, gives

$$\begin{aligned}
\mathbb{E}[\mathsf{Risk}(\hat{\theta})] &= \mathbb{E}\left[\left(x^\top \left(I - X^\top (XX^\top)^{-1}X\right)(\theta^\star - \alpha^\star w)\right)^2\right] + \mathbb{E}_x\left[\left(x^\top X^\top (XX^\top)^{-1}\boldsymbol{\varepsilon}\right)^2\right] \\
&= \mathbb{E}[(\theta^\star - \alpha^* w)^\top B(\theta - \alpha^* w)^\star] + \mathbb{E}\left[\left(x^\top X^\top (XX^\top)^{-1}\boldsymbol{\varepsilon}\right)^2\right] \\
&\geq \mathbb{E}[\theta^{\star\top} B\theta^\star] + \mathbb{E}\left[\left(x^\top X^\top (XX^\top)^{-1}\boldsymbol{\varepsilon}\right)^2\right] \\
&\geq \mathbb{E}[\theta^{\star\top} B\theta^\star] + \sigma^2\mathbb{E}\left[\mathrm{Tr}(C)\right],
\end{aligned}$$

completing the proof. ■

6. Discussion

Despite the fact that parameterizing a linear model using a balanced, two-layer linear network has been shown in previous work to have a substantial effect on the inductive bias of gradient descent (Azulay et al., 2021), it remains compatible with benign overfitting, and the initial weights also encode a potentially useful bias.

While Proposition 8 limits the prospects for improving our upper bounds, there still appears to be a gap between our upper and lower bounds.

Moving beyond the case where the initialization is balanced would be an interesting next step. We briefly note that, for the initial parameters to be balanced, it is necessary for the weight matrix in the first layer $W \in \mathbb{R}^{m\times p}$ to have rank one. In the case where there is a single neuron ($m = 1$), Theorem 2 by (Azulay et al., 2021) characterizes the implicit bias of the final solution learnt by gradient flow on the squared loss. The techniques developed in this paper might perhaps be useful in bounding the excess risk of this solution.

Yet another interesting open question concerns characterizing the implicit bias of gradient flow with the squared loss in the case where a linear model is parameterized using a deeper representation than two layers, building on existing research (Gunasekar et al., 2017, 2018b; Arora et al., 2019; Woodworth et al., 2020; Gissin et al., 2020; Razin and Cohen, 2020; Yun et al., 2021; Azulay et al., 2021; Jagadeesan et al., 2021). It would also be interesting to prove corresponding excess risk bounds for such solutions, and to study the effect of depth on the generalization properties of the resulting models.

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Appendix A. The design matrix has full rank (and more)

Lemma 26 *Under Assumption 4, for any eigenvector v of Σ, and any sample size n, the projection of the rows of X onto the subspace of $\mathbb{R}^p$ orthogonal to v has rank n.*

Proof Assume without loss of generality that Σ is diagonal and $v = (1, 0, 0, \ldots, 0)$. Let $x_1, \ldots, x_n$ denote the rows of X, and let $x'_1, \ldots, x'_n$ be obtained from $x_1, \ldots, x_n$ by replacing each of their first components with 0, thereby projecting them onto the subspace orthogonal to v. It suffices to prove that, almost surely, $x'_1, \ldots, x'_n$ are linearly independent.

We will prove this by induction. The base case, there $n = 1$, is straightforward. When $n > 1$, by the inductive hypothesis, $x'_1, \ldots, x'_{n-1}$ are linearly independent. Since $p > n$, Assumption 4 implies that the span of $x'_1, \ldots, x'_{n-1}$ has probability 0, so that, almost surely, x'_n is not a member this span, completing the proof. ■

Appendix B. Concentration inequalities

For an excellent reference of sub-Gaussian and sub-exponential concentration inequalities we refer the reader to Vershynin (2018). We begin by defining sub-Gaussian and sub-exponential random variables.

Definition 27 *A random variable ϕ is sub-Gaussian if*

$$\|\phi\|_{\psi_2} := \inf\left\{t > 0 : \mathbb{E}[\exp(\phi^2/t^2)] < 2\right\}$$

is bounded. Further, $\|\phi\|_{\psi_2}$ is defined to be its sub-Gaussian norm.

Definition 28 *A random variable ϕ is said to be sub-exponential if*

$$\|\phi\|_{\psi_1} := \inf\left\{t > 0 : \mathbb{E}[\exp(|\phi|/t) < 2]\right\}$$

is bounded. Further, $\|\phi\|_{\psi_1}$ is defined to be its sub-exponential norm.

Next we state a few well-known facts about sub-Gaussian and sub-exponential random variables.

Lemma 29 (Vershynin 2018, Lemma 2.7.6) *If a random variable ϕ is sub-Gaussian then ϕ^2 is sub-exponential with $\|\phi^2\|_{\psi_1} = \|\phi\|_{\psi_2}^2$.*

Lemma 30 (Vershynin 2018, Lemma 2.7.10) *If a random variable ϕ is sub-exponential then $\phi - \mathbb{E}[\phi]$ is sub-exponential with $\|\phi - \mathbb{E}[\phi]\|_{\psi_1} \leq c\|\phi\|_{\psi_1}$ for some positive constant c.*

We state Bernstein's inequality (see, e.g., Vershynin, 2018, Theorem 2.8.1), a concentration inequality for a sum of independent sub-exponential random variables.

Theorem 31 *For independent mean-zero sub-exponential random variables $\phi_1, \ldots, \phi_m$, for every $\eta > 0$, we have*

$$\mathbb{P}\left[\Big|\sum_{i=1}^{m} \phi_i\Big| \geq \eta\right] \leq 2\exp\left(-c\min\left\{\frac{\eta^2}{\sum_{i=1}^{m}\|\phi_i\|_{\psi_1}^2}, \frac{\eta}{\max_i\|\phi_i\|_{\psi_1}}\right\}\right),$$

where c is a positive absolute constant.

Let us continue by defining an ε-net with respect to the Euclidean distance.

Definition 32 *Let $S \subseteq \mathbb{R}^p$. A subset K is called an ε-net of S if every point in S is within Euclidean distance ε of some point in K.*

The following lemma bounds the size of a $1/4$-net of unit vectors in $\mathbb{R}^p$.

Lemma 33 *Let S be the set of all unit vectors in $\mathbb{R}^p$. Then there exists a $1/4$-net of S of size 9^p.*

Proof Follows immediately by invoking (Vershynin, 2018, Corollary 4.2.13) with $\varepsilon = 1/4$. ■

B.1 Proof of Lemma 14

Let $\Sigma = \sum_{i=1}^p \lambda_i e_i e_i^\top$ be the spectral decomposition of the covariance matrix. Define the random vectors

$$z_i := \frac{Xe_i}{\sqrt{\lambda_i}} \in \mathbb{R}^n.$$

These random vectors z_i have entries that are independent, σ_x^2-sub-Gaussian random variables (see Bartlett et al., 2020, Lemma 8). Note that we can write the matrix

$$X_S X_S^\top = \sum_{i \in S} \lambda_i z_i z_i^\top.$$

Further, its expected value is as follows:

$$\mathbb{E}\left[X_S X_S^\top\right] = \sum_{i\in S} \lambda_i \mathbb{E}\left[z_i z_i^\top\right] = \sum_{i \in S} \mathbb{E}\left[X e_i e_i^\top X^\top\right] = I_n \sum_{i\in S} \lambda_i = I_n s(S).$$

With this in place, we are now ready to prove our concentration results.

Lemma 14 *There exists a positive absolute constant c such that, for any subset $S \subseteq [p]$ and any $t \geq 0$, with probability at least $1 - 2e^{-t}$, for all $j \in \{1, \ldots, \min(n, |S|)\}$*

$$\left|\mu_j(X_S X_S^\top) - s(S)\right| \leq cs(S)\left(\frac{t+n}{r(S)} + \sqrt{\frac{t+n}{R(S)}}\right).$$

Proof We shall prove this bound in the case where the set $S = [p]$. The bound for any other subset S shall follow by exactly the same logic. First, note that by a standard ε-net argument (see, e.g, Bartlett et al., 2020, Lemma 25) to bound the operator norm we can use the following inequality:

$$\left\|XX^\top - I_n \sum_{i=1}^p \lambda_i\right\|_{op} \leq 2 \max_{v_j \in \mathcal{N}_{\frac{1}{4}}} \left|v_j^\top\left(XX^\top - I_n\sum_{i=1}^p \lambda_i\right)v_j\right|, \tag{58}$$

where $\mathcal{N}_{\frac{1}{4}}$ is a 1/4-net of the unit sphere with respect to the Euclidean norm of size at most 9^n. (We know that such a net exists by Lemma 33.) Consider an arbitrary unit vector $v \in \mathbb{S}^{n-1}$. Then

$$v^\top \left(XX^\top - I_n \sum_{i=1}^{p} \lambda_i \right) v = \sum_{i=1}^{p} \lambda_i \left((z_i^\top v)^2 - 1 \right). \tag{59}$$

By Lemmas 29 and 30 we know that the random variables $\lambda_i((z_i^\top v)^2 - 1)$ are $c_1 \lambda_i \sigma_x^2$-sub-exponential, for some positive constant c_1.Therefore we can use Bernstein's inequality (see Theorem 31) to upper bound the sum in equation (59) to get that, with probability at least $1 - 2e^{-t}$,

$$\left| \sum_{i=1}^{p} \lambda_i \left((z_i^\top v)^2 - 1 \right) \right| \le c_2 \sigma_x^2 \max \left\{ \lambda_1 t, \sqrt{t \sum_{j=1}^{p} \lambda_j^2} \right\}. \tag{60}$$

Next by a union bound over all the elements of the cover $\mathcal{N}_{\frac{1}{4}}$ we find that, with probability at least $1 - 2e^{-t}$, for all $v \in \mathcal{N}_{\frac{1}{4}}$,

$$\left| \sum_{i=1}^{p} \lambda_i \left((z_i^\top v)^2 - 1 \right) \right| \le c_2 \sigma_x^2 \max \left\{ \lambda_1 \left(t + n \log(9) \right), \sqrt{\left(t + n \log(9) \right) \sum_{j=1}^{p} \lambda_j^2} \right\}.$$

Hence, by using inequality (58) we get that with probability at least $1 - 2e^{-t}$

$$\begin{aligned} \left\| XX^\top - I_n \sum_{i=1}^{p} \lambda_i \right\|_{op} &\le c_3 \sigma_x^2 \max \left\{ \lambda_1 \left(t + n \log(9) \right), \sqrt{\left(t + n \log(9) \right) \sum_{j=1}^{p} \lambda_j^2} \right\} \\ &\le c_4 \sigma_x^2 \left(\lambda_1 (t + n) + \sqrt{(t + n) \sum_{j=1}^{p} \lambda_j^2} \right). \end{aligned}$$

Recalling that σ_x is assumed to be a positive constant, this implies that the greatest and least eigenvalues of $XX^\top$ are within $c_5 \left(\lambda_1 (t + n) + \sqrt{(t + n) \sum_{j=1}^{p} \lambda_j^2} \right)$ of $\sum_{i=1}^{p} \lambda_i$, which in turn implies

$$\begin{aligned} \left| \mu_j(XX^\top) - \sum_{i=1}^{p} \lambda_i \right| &\le c_5 \left(\lambda_1 (t + n) + \sqrt{(t + n) \sum_{j=1}^{p} \lambda_j^2} \right) \\ &= c_5 \left(\sum_{i=1}^{p} \lambda_i \right) \left(\frac{t + n}{r_0} + \sqrt{\frac{t + n}{R_0}} \right), \end{aligned}$$

completing the proof. ■

B.2 Proof of Lemma 15

We begin by proving an auxiliary lemma that relates the minimum singular value of a matrix to its approximation over an ε-net under the assumption that its operator norm is bounded. Recall that $X_S \in \mathbb{R}^{n\times|S|}$.

Lemma 34 *Let $\mathcal{N}_\varepsilon$ be an ε-net of the unit sphere in $\mathbb{R}^n$ with respect to the Euclidean norm. For any $a, b \geq 0$, if*

$$\inf_{z\in\mathbb{S}^{n-1}} \|X_S^\top z\| \leq a - \varepsilon b \quad \textit{and} \quad \|X_S^\top\|_{op} \leq b$$

then $\inf_{z\in\mathcal{N}_\varepsilon}\|X_S^\top z\| \leq a$.

Proof Let ζ be a function that maps any unit vector z to its nearest neighbor (with respect to the Euclidean norm) in the net $\mathcal{N}_\varepsilon$. Therefore, if $\|X_S^\top\|_{op} \leq b$ then

$$\begin{aligned}
\inf_{z\in\mathbb{S}^{n-1}} \|X_S^\top z\| &= \inf_{z\in\mathbb{S}^{n-1}} \|X_S^\top(z-\zeta(z)) + X_S^\top\zeta(z)\| \\
&\geq \inf_{z\in\mathbb{S}^{n-1}} \|X_S^\top\zeta(z)\| - \inf_{z\in\mathbb{S}^{n-1}} \|X_S^\top(z-\zeta(z))\| \\
&= \inf_{z\in\mathcal{N}_\varepsilon} \|X_S^\top z\| - \inf_{z\in\mathbb{S}^{n-1}} \|X_S^\top(z-\zeta(z))\| \\
&\geq \inf_{z\in\mathcal{N}_\varepsilon} \|X_S^\top z\| - \|X_S^\top\|_{op} \inf_{z\in\mathbb{S}^{n-1}} \|z-\zeta(z)\| \\
&\geq \inf_{z\in\mathcal{N}_\varepsilon} \|X_S^\top z\| - \varepsilon b.
\end{aligned}$$

Further if $\inf_{z\in\mathbb{S}^{n-1}}\|X_S^\top z\| \leq a - \varepsilon b$ then, due to the inequality above, $\inf_{z\in\mathcal{N}_\varepsilon}\|X_S^\top z\| \leq a$ which completes the proof. ■

With this lemma in place let us prove our result.

Lemma 15 *There exist absolute positive constants $c_0, \ldots, c_3$ such that given any subset $S \subseteq [p]$ if, $r(S) \geq c_0 n$ then for all $t < c_1 < 1$*

$$\mathbb{P}\left[\mu_n(X_S X_S^\top) \leq t\cdot s(S)\right] \leq (c_2 t)^{c_3\cdot r(S)}.$$

Proof To reduce notational burden in the proof we shall present a proof in the case where the $S = [p]$, and therefore $X_S = X$. For any other subset S the proof shall proceed in exactly the same manner.

In the proof we shall prove bounds on the smallest singular value of X, $s_{\min}(X)$. This immediately leads to a bound on $\mu_n(XX^\top) = s^2_{\min}(X)$.

Recall that $s_{\min}(X) = s_{\min}(X^\top)$. So we will instead prove a bound on the smallest singular value of $X^\top$ to simplify our calculations. For some parameter $h \geq c_4 \geq 1$ that will be set in the sequel, decompose the probability into

$$\begin{aligned}
&\mathbb{P}\left[s_{\min}(X^\top) \le t\sqrt{\sum_{j=1}^p \lambda_j}\right] \\
&= \mathbb{P}\left[\left\{s_{\min}(X^\top) \le t\sqrt{\sum_{j=1}^p \lambda_j}\right\} \cap \left\{\|X\|_{op} \le h\sqrt{\lambda_1 p}\right\}\right] \\
&\quad + \mathbb{P}\left[\left\{s_{\min}(X^\top) \le t\sqrt{\sum_{j=1}^p \lambda_j}\right\} \cap \left\{\|X\|_{op} > h\sqrt{\lambda_1 p}\right\}\right] \\
&\le \mathbb{P}\left[\left\{s_{\min}(X^\top) \le t\sqrt{\sum_{j=1}^p \lambda_j}\right\} \cap \left\{\|X\|_{op} \le h\sqrt{\lambda_1 p}\right\}\right] + \mathbb{P}\left[\|X\|_{op} > h\sqrt{\lambda_1 p}\right]. \qquad (61)
\end{aligned}$$

Now we will control each of these probabilities separately. First, let us control the second probability

$$\begin{aligned}
\mathbb{P}\left[\|X\|_{op} > h\sqrt{\lambda_1 p}\right] &= \mathbb{P}\left[\|X\Sigma^{-1/2}\Sigma^{1/2}\|_{op} > h\sqrt{\lambda_1 p}\right] \\
&\le \mathbb{P}\left[\|X\Sigma^{-1/2}\|_{op} > h\sqrt{p}\right] \le e^{-c_4 h^2 p}, \qquad (62)
\end{aligned}$$

by invoking Proposition 2.4 by Rudelson and Vershynin (2009).

To control the first probability in inequality (61) we need the following definition. Given a random vector $\xi \in \mathbb{R}^p$ define the Lévy concentration function

$$\mathcal{L}(\xi; t) := \sup_{w \in \mathbb{R}^p} \mathbb{P}\left[\|\xi - w\| \le t\right].$$

Let $\phi \in \mathbb{S}^{n-1}$ be a fixed unit vector. By Assumption 4 we know that for any $a \le b \in \mathbb{R}$:

$$\mathbb{P}\left[(\Sigma^{-1/2}X^\top\phi)_i \in [a,b]\right] \le c|b-a|. \qquad (63)$$

Using this fact we find that for any $i \in [p]$:

$$\begin{aligned}
\mathcal{L}((\Sigma^{-1/2}X^\top\phi)_i\,; 2t) &= \sup_{w\in\mathbb{R}} \mathbb{P}\left[|(\Sigma^{-1/2}X^\top\phi)_i - w| \le 2t\right] \\
&= \sup_{w\in\mathbb{R}} \mathbb{P}\left[(\Sigma^{-1/2}X^\top\phi)_i \in [w-2t, w+2t]\right] \le 4c_5 t.
\end{aligned}$$

Next by invoking Theorem 1.5 in Rudelson and Vershynin (2015) we infer that

$$\mathcal{L}\left(X^\top\phi; 2t\sqrt{\sum_{i=1}^p \lambda_i}\right) \le (ct)^{c' r_0}.$$

This implies that

$$\mathbb{P}\left[\|X^\top \phi\| \le 2t\sqrt{\sum_{i=1}^p \lambda_i}\right] \le \sup_{w\in\mathbb{R}^p} \mathbb{P}\left[\|X^\top \phi - w\| \le 2t\sqrt{\sum_{i=1}^p \lambda_i}\right]$$

$$= \mathcal{L}\left(X^\top \phi; 2t\sqrt{\sum_{i=1}^p \lambda_i}\right) \le (ct)^{c' r_0}. \tag{64}$$

This establishes a *small-ball* probability (anti-concentration) for a fixed unit vector ϕ. We will now proceed by using an ε-net argument. For some $\varepsilon \in \left(0, \frac{2t}{h}\sqrt{\frac{\sum_{i=1}^p \lambda_i}{\lambda_1 p}}\right)$ let $\mathcal{N}_\varepsilon$ be an ε-net of the unit vectors in $\mathbb{R}^n$ with respect to the Euclidean norm of size at most $\left(\frac{2}{\varepsilon}+1\right)^n$ (such a net exists, see, e.g., Corollary 4.2.13 in Vershynin (2018)). By a union bound over the elements of the net

$$\mathbb{P}\left[\min_{\phi\in\mathcal{N}_\varepsilon} \|X^\top \phi\| \le 2t\sqrt{\sum_{i=1}^p \lambda_i}\right] \le (ct)^{c' r_0} \cdot \left(\frac{2}{\varepsilon}+1\right)^n. \tag{65}$$

Next by Lemma 34 we know that

$$\begin{aligned}
&\mathbb{P}\left[\left\{s_{\min}(X^\top) \le 2t\sqrt{\sum_{i=1}^p \lambda_i} - \varepsilon h\sqrt{\lambda_1 p}\right\} \cap \left\{\|X\|_{op} \le h\sqrt{\lambda_1 p}\right\}\right] \\
&= \mathbb{P}\left[\left\{\inf_{z\in\mathbb{S}^{n-1}} \|X^\top z\| \le 2t\sqrt{\sum_{i=1}^p \lambda_i} - \varepsilon h\sqrt{\lambda_1 p}\right\} \cap \left\{\|X\|_{op} \le h\sqrt{\lambda_1 p}\right\}\right] \\
&\le \mathbb{P}\left[\min_{z\in\mathcal{N}_\varepsilon} \|X^\top z\| \le 2t\sqrt{\sum_{i=1}^p \lambda_i}\right] \\
&\le (ct)^{c' r_0} \cdot \left(\frac{2}{\varepsilon}+1\right)^n.
\end{aligned}$$

Setting $\varepsilon = \frac{t}{h}\sqrt{\frac{\sum_{i=1}^p \lambda_i}{\lambda_1 p}} = \frac{t}{h}\sqrt{\frac{r_0}{p}}$ we get that

$$\mathbb{P}\left[\left\{s_{\min}(X^\top) \le t\sqrt{\sum_{i=1}^p \lambda_i}\right\} \cap \left\{\|X\|_{op} \le h\sqrt{\lambda_1 p}\right\}\right] \le (ct)^{c' r_0} \cdot \left(\frac{2h}{t}\sqrt{\frac{p}{r_0}}+1\right)^n.$$

This combined with inequalities (61) and (62) above yields

$$\mathbb{P}\left[s_{\min}(X^\top) \le t\sqrt{\sum_{i=1}^p \lambda_i}\right] \le (ct)^{c' r_0} \cdot \left(\frac{2h}{t}\sqrt{\frac{p}{r_0}}+1\right)^n + e^{-c_4 h^2 p}.$$

Finally set $h = \frac{1}{t}\sqrt{\frac{r_0}{p}}$ to obtain the bound

$$\mathbb{P}\left[s_{\min}(X^\top) \leq t\sqrt{\sum_{i=1}^{p} \lambda_i}\right] \leq (ct)^{c' r_0} \cdot \left(\frac{c''}{t^2}\right)^n + e^{-c_5 r_0/t^2} \overset{(i)}{\leq} (c_2 t)^{c_3 \cdot r_0}$$

where (i) follows since $r_0 > c_0 n$ for a large enough constant c_0 and because $t < c_1$ for a small enough constant c_1. ■

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