NON-ASYMPTOTIC UPPER BOUNDS FOR THE RECONSTRUCTION ERROR OF PCA

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Abstract. We analyse the reconstruction error of principal component analysis (PCA) and prove non-asymptotic upper bounds for the corresponding excess risk. These bounds unify and improve existing upper bounds from the literature. In particular, they give oracle inequalities under relative eigenvalue conditions. The bounds reveal that the excess risk differs considerably from usually considered subspace distances based on canonical angles. Our approach relies on the analysis of empirical spectral projectors combined with concentration inequalities for weighted empirical covariance operators and empirical eigenvalues.

1. Introduction

Principal component analysis (PCA) is one of the simplest and most widely used dimension reduction procedures. Variants like functional PCA or kernel PCA can be included in the standard multivariate setting by allowing for general Hilbert spaces \( \mathcal{H} \). PCA is commonly derived by minimising the reconstruction error \( \mathbb{E}[\|X - PX\|^2] \) over all orthogonal projections \( P \) of rank \( d \), where \( X \) is an \( \mathcal{H} \)-valued random variable and \( d \) is a given dimension. Replacing the population covariance \( \Sigma \) by an empirical covariance \( \hat{\Sigma} \), PCA computes the orthogonal projection \( \hat{P}_{\leq d} \) onto the eigenspace of the \( d \) leading eigenvalues of \( \hat{\Sigma} \). Put differently, \( \hat{P}_{\leq d} \) minimises the empirical reconstruction error and it is natural to measure its performance by the excess risk \( \mathcal{E}^{PCA}_{d} \), that is by the difference between the reconstruction errors of \( \hat{P}_{\leq d} \) and the overall minimiser \( P_{\leq d} \). It is easy to see that \( \mathcal{E}^{PCA}_{d} = \langle \Sigma, P_{\leq d} - \hat{P}_{\leq d} \rangle \) holds with respect to the Hilbert-Schmidt scalar product.

Bounds for the reconstruction error can be derived using the theory of empirical risk minimisation (ERM). This has been pursued by Shawe-Taylor et al. [27,26] and Blanchard, Bousquet, and Zwald [6]. In [26], a slow \( n^{-1/2} \)-rate is derived, while in [6], it is shown that the convergence rate of the excess risk can typically be faster than \( n^{-1/2} \).

Classical results for PCA provide limit theorems for the empirical eigenvalues and eigenvectors when the sample size \( n \) tends to infinity, see e.g. Anderson [2] and Dauxois, Pousse and Romain [10]. Generalisations, such

2010 Mathematics Subject Classification. Primary 62H25; secondary 15A42, 60F10.

Key words and phrases. Principal component analysis, Reconstruction error, Excess risk, Spectral projectors, Concentration inequalities.
as stochastic expansions, are derived in Hall and Hosseini-Nasab [11] and Jirak [12]. In view of high-dimensional applications, empirical spectral projectors (such as $\hat{P}_{\leq d}$) are often studied when the distance to the population spectral projectors is measured in operator or Hilbert-Schmidt norm, see e.g. Zwald and Blanchard [32], Nadler [25], Mas and Ruymgaart [23], and Koltchinskii and Lounici [16, 19, 18]. A different line of research imposes sparsity constraints to tackle high-dimensional PCA with a focus on spiked covariance models, see e.g. Vu and Lei [30] and Cai, Ma, and Wu [8, 9]. In most cases the analysis of empirical spectral projectors is based on methods from perturbation theory for linear operators. Non-asymptotic bounds often use the Davis-Kahan $\sin \Theta$ theorem and variants of it [32, 30, 8]. Asymptotically more precise results are often based on first or higher order expansions for empirical spectral projectors, see [23, 16, 19, 18].

In this paper, we further study the excess risk of PCA. We show that ERM techniques lead to a slow $n^{-1/2}$-rate and a fast $n^{-1}$-rate, depending on the size of the spectral gap $\lambda_d - \lambda_{d+1}$. While these bounds clarify existing results, we observe that the basic inequality of ERM prevents us from deriving optimal bounds in simple cases due to the asymmetry between the empirical and population risk functions. By the weighting with $\Sigma$, the excess risk is small if all eigenvalues are nearby. In the extreme isotropic case $\Sigma = \sigma^2 I$, the excess risk satisfies $\mathcal{E}_d^{\text{PCA}} = 0$. The main innovation of this paper are therefore new techniques to obtain non-asymptotic upper bounds for the excess risk which explore the dichotomous dependence of the excess risk on the spectral gaps $\lambda_j - \lambda_k$ with $j \leq d$ and $k > d$. The underlying difficulty is that we have to deal with empirical spectral projectors without spectral gap conditions. For that reason, methods from perturbation theory for linear operators are replaced by an algebraic projector-based calculus, resulting in two completely different methods to bound the excess risk. Moreover, to combine these two methods, empirical eigenvalue concentration inequalities are established, taking into account the local eigenvalue structure.

The paper is organised as follows. Section 2 formalises the setting, provides some preliminary results using ERM techniques, and presents our main new bounds for the excess risk. The bounds are illustrated for covariance operators satisfying standard eigenvalue decay assumptions. Section 3 develops our main tools, including empirical projector expansions, a deterministic error decomposition for $\mathcal{E}_d^{\text{PCA}}$, and spectral concentration inequalities. The proofs of our main bounds are given in Section 4. Finally, in the appendix, we present some complementary results which can be obtained by a linear expansion of $\hat{P}_{\leq d}$.

2. Main results

2.1. The reconstruction error of PCA. Let $X$ be a centered random variable taking values in a separable Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ of dimension $p \in \mathbb{N} \cup \{+\infty\}$ and let $\|\cdot\|$ denote the norm on $\mathcal{H}$ defined by $\|u\| = \sqrt{\langle u, u \rangle}$. 

2.1. **Assumption.** Suppose that $X$ is sub-Gaussian, meaning that $\mathbb{E}[\|X\|^2]$ is finite and that there is a constant $C_1$ with
\[
\|\langle X, u \rangle\|_{\psi_2} := \sup_{k \geq 1} k^{-1/2} \mathbb{E}[|\langle X, u \rangle|^k]^{1/k} \leq C_1 \mathbb{E}[\langle X, u \rangle^2]^{1/2}
\]
for all $u \in \mathcal{H}$.

The covariance operator of $X$ is denoted by $\Sigma = \mathbb{E}[X \otimes X]$. By the spectral theorem there exists a sequence $\lambda_1 \geq \lambda_2 \geq \cdots > 0$ of positive eigenvalues (which is either finite or converges to zero) together with an orthonormal system of eigenvectors $u_1, u_2, \ldots$ such that $\Sigma$ has the spectral representation
\[
\Sigma = \sum_{j \geq 1} \lambda_j P_j,
\]
with rank-one projectors $P_j = u_j \otimes u_j$, where $(u \otimes v)x = \langle v, x \rangle u$, $x \in \mathcal{H}$. Note that the choice of $u_j$ and $P_j$ is non-unique in case of multiple eigenvalues $\lambda_j$.

Without loss of generality we shall assume that the eigenvectors $u_1, u_2, \ldots$ form an orthonormal basis of $\mathcal{H}$ such that $\sum_{j \geq 1} P_j = I$. We write
\[
P_{\leq d} = \sum_{j \leq d} P_j, \quad P_{> d} = I - P_{\leq d} = \sum_{k > d} P_k
\]
for the orthogonal projections onto the linear subspace spanned by the first $d$ eigenvectors of $\Sigma$, and onto its orthogonal complement.

Let $X_1, \ldots, X_n$ be $n$ independent copies of $X$ and let
\[
\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n X_i \otimes X_i
\]
be the sample covariance. Again, there exists a sequence $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \cdots \geq 0$ of eigenvalues together with an orthonormal basis of eigenvectors $\hat{u}_1, \hat{u}_2, \ldots$ such that we can write
\[
\hat{\Sigma} = \sum_{j \geq 1} \hat{\lambda}_j \hat{P}_j \text{ with } \hat{P}_j = \hat{u}_j \otimes \hat{u}_j
\]
and
\[
\hat{P}_{\leq d} = \sum_{j \leq d} \hat{P}_j, \quad \hat{P}_{> d} = I - \hat{P}_{\leq d} = \sum_{k > d} \hat{P}_k.
\]

For linear operators $S, T : \mathcal{H} \to \mathcal{H}$ we make use of trace and adjoint $\text{tr}(S), S^*$ to define the Hilbert-Schmidt or Frobenius norm and scalar product
\[
\|S\|_2^2 = \text{tr}(S^*S), \quad \langle S, T \rangle = \text{tr}(S^*T)
\]
as well as the operator norm $\|S\|_\infty = \max_{u \in \mathcal{H}, \|u\|=1} \|Su\|$. For covariance operators $\Sigma$ this gives $\|\Sigma\|_\infty = \lambda_1$ and $\|\Sigma\|_2^2 = \sum_{j \geq 1} \lambda_j^2$. Under Assumption 2.1 $\Sigma$ is a trace class operator (see e.g. [20, Theorem III.2.3]) and all
quantities are well defined. In addition, for \( r \geq 1 \), we use the abbreviations \( \text{tr}_{>r}(\Sigma) \) and \( \text{tr}_{\geq r}(\Sigma) \) for \( \sum_{j>r} \lambda_j \) and \( \sum_{j \geq r} \lambda_j \), respectively.

Introducing the class

\[
P_d = \{ P : \mathcal{H} \to \mathcal{H} \mid P \text{ is orthogonal projection of rank } d \},
\]

the (population) reconstruction error of \( P \in P_d \) is defined by

\[
R(P) = \mathbb{E}[\|X - PX\|^2] = \langle \Sigma, I - P \rangle.
\]

The fundamental idea behind PCA is that \( P \leq d \) satisfies

\[
P \leq d \in \arg\min_{P \in P_d} R(P), \quad R(P \leq d) = \text{tr}_{>d}(\Sigma).
\]

(2.1)

Similarly, the empirical reconstruction error of \( P \in P_d \) is defined by

\[
R_n(P) = \frac{1}{n} \sum_{i=1}^{n} \|X_i - PX_i\|^2 = \langle \hat{\Sigma}, I - P \rangle,
\]

and we have

\[
\hat{P} \leq d \in \arg\min_{P \in P_d} R_n(P).
\]

(2.2)

The excess risk of the PCA projector \( \hat{P} \leq d \) is thus given by

\[
\mathcal{E}_{d}^{\text{PCA}} := R(\hat{P} \leq d) - R(P \leq d) = \langle \Sigma, P \leq d - \hat{P} \leq d \rangle.
\]

(2.3)

By (2.1) the excess risk \( \mathcal{E}_{d}^{\text{PCA}} \) defines a non-negative loss function in the decision-theoretic sense for the estimator \( \hat{P} \leq d \) under the parameter \( \Sigma \). Our main objective is to find non-asymptotic bounds for \( \mathbb{E}[\mathcal{E}_{d}^{\text{PCA}}] \), the decision-theoretic risk.

Throughout the paper, \( c \) and \( C \) are constants depending only on \( C_1 \) from Assumption 2.1. The constants \( c, C \) may change from line to line. Sometimes we make \( C \) more explicit by using the additional constant \( C_2 > 0 \) which is the smallest constant such that

\[
\mathbb{E}[\|P_j(\Sigma - \hat{\Sigma})P_k\|^2] \leq C_2 \delta \lambda_j \lambda_k / n
\]

(2.4)

with \( \delta = 1 \) if \( j \neq k \) and \( \delta = 2 \) otherwise. Note that we always have \( C_2 \leq 16C_1^4 \) and that for \( X \) Gaussian we have equality in (2.4) with \( C_2 = 1 \).

2.2. ERM-bounds for the excess risk. A natural approach to derive upper bounds for the excess risk is to follow the standard theory of empirical risk minimisation (ERM). The important basic inequality in ERM is

\[
0 \leq \langle \Sigma, P \leq d - \hat{P} \leq d \rangle \leq \langle \Sigma - \hat{\Sigma}, P \leq d - \hat{P} \leq d \rangle = \langle \Delta, P \leq d - \hat{P} \leq d \rangle
\]

(2.5)

with

\[
\Delta = \Sigma - \hat{\Sigma},
\]

which follows from the variational characterisations in (2.1) and (2.2). This route has been taken by Blanchard, Bousquet, and Zwald [6], who applied sophisticated arguments from empirical process theory, based on Bartlett, Bousquet, and Mendelson [3]. Let us derive some simple non-asymptotic
expectation bounds from (2.5), which will set the stage for more refined results later.

2.2. Proposition. We have

$$
E_{PCA}^d \leq \min \left( \sqrt{2d} \| \Delta \|_2, \frac{2\| \Delta \|^2}{\lambda_d - \lambda_{d+1}} \right)
$$

with the convention $x/0 := \infty$. With Assumption 2.1

$$
E[E_{PCA}^d] \leq \min \left( \frac{\sqrt{4C_d^2 \text{tr}(\Sigma)}}{\sqrt{n}}, \frac{4C_d^2 \text{tr}(\Sigma)^2}{n(\lambda_d - \lambda_{d+1})} \right) \tag{2.6}
$$

(2.6) follows, where $C_d$ is the constant in (2.4).

2.3. Remark. The excess risk is thus bounded by a global $n^{-1/2}$-rate as well as by a fast local $n^{-1}$-rate which depends on the spectral gap $\lambda_d - \lambda_{d+1}$. For (2.6) to hold only (2.4) is required instead of the full Assumption 2.1.

Proof of Proposition 2.2. From (2.5) we obtain

$$
(E_{PCA}^d)^2 \leq \| \Delta \|^2 \| P_{\leq d} - \hat{P}_{\leq d} \|^2 \tag{2.7}
$$

by the Cauchy-Schwarz inequality. Since orthogonal projectors are idempotent and self-adjoint, we have $\langle P_{\leq d}, \hat{P}_{\leq d} \rangle = \| P_{\leq d} \hat{P}_{\leq d} \|^2 \geq 0$, and thus

$$
\| P_{\leq d} - \hat{P}_{\leq d} \|^2 = 2(1 - \langle P_{\leq d}, \hat{P}_{\leq d} \rangle) \leq 2d.
$$

Insertion into (2.7) yields the first part of the bound. The second part of the bound follows from a short recursion argument. Indeed, we have

$$
\| P_{\leq d} - \hat{P}_{\leq d} \|^2 \leq \frac{2E_{PCA}^d}{\lambda_d - \lambda_{d+1}},
$$

which is a variant of the Davis-Kahan inequality and follows by simple projector calculus, see Lemma 2.5 and (2.19) below. We obtain

$$
(E_{PCA}^d)^2 \leq \| \Delta \|^2 \frac{2E_{PCA}^d}{\lambda_d - \lambda_{d+1}}.
$$

This yields the second part of the bound. Finally, the expectation bound (2.6) follows from inserting (2.4).

The global rate can be improved by using the variational characterisation of partial traces again. In the case $\Sigma = I + xP_{\leq d}$, for instance, the global rate $p\sqrt{d/n}$ of Proposition 2.2 is improved to $d\sqrt{p/n}$. The latter is optimal for $d \leq p/2$ and for the spectral gap $x = \sqrt{p/n}$, see the lower bound (2.17) below.

2.4. Proposition. Grant Assumption 2.1. Then we have

$$
E[E_{PCA}^d] \leq C \sum_{j \leq d} \max \left( \frac{\lambda_j \text{tr}_{\geq j}(\Sigma)}{n}, \frac{\text{tr}_{\geq j}(\Sigma)}{n} \right).
$$
Proof. Using (2.5), we have
\[
\mathcal{E}_{d}^{\text{PCA}} \leq \langle \Delta, P_{\leq d} \rangle + \langle -\Delta, \hat{P}_{\leq d} \rangle \leq \langle \Delta, P_{\leq d} \rangle + \sup_{P \in P_{d}} \langle -\Delta, P \rangle.
\]

Letting \( \lambda_1(-\Delta) \geq \lambda_2(-\Delta) \geq \cdots > 0 \) be the (finite) sequence of positive eigenvalues of \(-\Delta = \hat{\Sigma} - \Sigma\), we have (compare to (2.1), (2.2))
\[
\sup_{P \in P_{d}} \langle -\Delta, P \rangle \leq \sum_{j \leq d} \lambda_j(-\Delta).
\]

Moreover, by the min-max characterisation of eigenvalues (see e.g. [20, Chapter 28]), we get
\[
\sum_{j \leq d} \lambda_j(-\Delta) \leq \sum_{j \leq d} \lambda_1(P_{\geq j}(-\Delta)P_{\geq j}) \leq \sum_{j \leq d} \|P_{\geq j} \Delta P_{\geq j}\|_\infty.
\]

Thus, noting that \( \mathbb{E}[(\Delta, P_{\leq d})] = 0 \), we conclude that
\[
\mathbb{E}\mathcal{E}_{d}^{\text{PCA}} \leq \mathbb{E} \left[ \sup_{P \in P_{d}} \langle -\Delta, P \rangle \right] \leq \sum_{j \leq d} \mathbb{E}\|P_{\geq j} \Delta P_{\geq j}\|_\infty. \tag{2.8}
\]

Finally, we apply the moment bound for sample covariance operators obtained by Koltchinskii and Lounici [17]. Consider \( X' = P_{\geq j}X, X'_i = P_{\geq j}X_i \) which again satisfy Assumption 2.1 (with the same constant \( C_1 \)) and lead to the covariance and sample covariance
\[
\Sigma' = P_{\geq j}\Sigma P_{\geq j}, \quad \hat{\Sigma}' = P_{\geq j}\hat{\Sigma} P_{\geq j}, \tag{2.9}
\]

Since \( \Sigma' \) has trace \( tr_{\geq j}(\Sigma) \) and operator norm \( \lambda'_1 = \lambda_j \), [17, Theorem 4] applied to \( \Delta' = \Sigma' - \hat{\Sigma}' \) gives
\[
\mathbb{E}\|P_{\geq j} \Delta P_{\geq j}\|_\infty \leq C \max \left( \sqrt{\frac{\lambda_j tr_{\geq j}(\Sigma)}{n}}, \frac{tr_{\geq j}(\Sigma)}{n} \right),
\]

where \( C \) is a constant depending only on \( C_1 \). Summing over \( j \) gives the second claim. \( \square \)

The bounds in Propositions 2.2 and 2.4 exhibit nicely the interplay between the global \( n^{-1/2} \)-rate and the local \( n^{-1} \)-rate. At first glance, it is surprising that the bounds derived via the basic ERM-inequality may nevertheless be suboptimal. For the simple isotropic case \( \Sigma = \sigma^2 I \) with \( \mathcal{E}_{d}^{\text{PCA}} = 0 \) they only provide an upper bound of order \( d\sqrt{p/n} \). The reason is an asymmetry with the risk \( \langle \hat{\Sigma}, P_{\leq d} - P_{\leq d} \rangle \) with the population and empirical versions exchanged, which may be much larger than the excess risk.

For the lower bound model \( \Sigma = I + xP_{\leq d} \) with \( n = 500, p = 40, \) and \( d = 15 \), Figure 1 displays the expectation (obtained from accurate Monte Carlo simulations) of the upper bound from the basic inequality (2.5) (dashed-dotted line) and the upper bound (2.8), used for proving Proposition 2.4 (dotted line), compared to the expected excess risk (solid line). In addition, Figure 1 displays the upper bound obtained in the next Section 2.4 with
2.3. New bounds for the excess risk. All results presented are proved in Section 4 below. The following representation of the excess risk is fundamental for the new bounds.

2.5. Lemma. For any $\mu \in \mathbb{R}$ we have

$$E_{d}^{PCA} = \sum_{j \leq d} (\lambda_j - \mu)\langle P_j, \hat{P}_{>d} \rangle + \sum_{k > d} (\mu - \lambda_k)\langle P_k, \hat{P}_{\leq d} \rangle.$$ 

It turns out that the two risk parts exhibit a different behaviour and we shall bound them separately. Therefore, we introduce

$$E_{\leq d}^{PCA}(\mu) = \sum_{j \leq d} (\lambda_j - \mu)\langle P_j, \hat{P}_{>d} \rangle, \quad E_{>d}^{PCA}(\mu) = \sum_{k > d} (\mu - \lambda_k)\langle P_k, \hat{P}_{\leq d} \rangle.$$ 

Usually, we shall choose $\mu \in [\lambda_{d+1}, \lambda_d]$ such that all terms are positive, but sometimes it pays off to choose a different value. Our first main result is as follows.

2.6. Theorem. Grant Assumption 2.1 and let $\mu \in [\lambda_{d+1}, \lambda_d]$. Then for all $r = 0, \ldots, d$ we have

$$E[|E_{\leq r}^{PCA}(\mu)|] \leq C \sum_{j \leq r} (\lambda_j - \mu) \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2} + \sum_{j=r+1}^{d \land (r+p-d)} (\lambda_j - \mu).$$

Figure 1. Expected excess risk (solid) and its upper bounds from (2.5) (dashed-dotted), (2.8) (dotted), and (2.16) (dashed) as functions of the spectral gap.

$C = 1.1$, taking into account Remark 3.4 (dashed line). This new upper bound captures correctly the small excess risk for small spectral gaps $x$. 


Moreover, if \( d \leq n/(16C_d^2) \), then for all \( l = d + 1, \ldots, p + 1 \) we have

\[
\mathbb{E}[\mathcal{E}^{\text{PCA}}_{>d}(\mu)] \leq C \sum_{k \geq l} (\mu - \lambda_k) \frac{\lambda_k \text{tr}(\Sigma)}{n(\lambda_d - \lambda_k)^2} + \sum_{k=(d+1)\lor(l-d)}^{l-1} (\mu - \lambda_k) + R
\]

with remainder term \( R = (\mu - \lambda_p)e^{-n/(32C_3^2)} \) and \( C = 8C_2 + 8C_3^2 \), where \( C_2 \) and \( C_3 \) are given in (2.4) and (3.19), respectively. For \( p = \infty \) we understand \( \lambda_p = 0 \) and \( l \in \{k \in \mathbb{N} \mid k \geq d+1\} \cup \{+\infty\} \) and for \( l = p = \infty \) we understand \( \sum_{k=(d-1)\lor(d+1)}^{l-1} (\mu - \lambda_k) = d\mu \).

Bounds of the same order can be derived for \( L^p \)-norms of \( \mathcal{E}^{\text{PCA}}_{\leq d} \) with a constant \( C \) depending additionally on \( p \), see e.g. Lemma 4.4 for the additional arguments needed in the case \( p = 2 \).

Using that for \( \mu \in [\lambda_{d+1}, \lambda_d] \) the terms \( \lambda_j - \mu \) (resp. \( \mu - \lambda_k \)) can be upper bounded by \( \lambda_j - \lambda_{d+1} \) (resp. \( \lambda_d - \lambda_k \)) and that \( \lambda \mapsto \lambda/(\lambda - \lambda_{d+1})^2 \) is decreasing for \( \lambda > \lambda_{d+1} \) (resp. \( \lambda \mapsto \lambda/(\lambda_d - \lambda)^2 \) is increasing for \( \lambda < \lambda_d \)), we obtain the following corollary.

2.7. Corollary. Grant Assumption 2.1 and let \( \mu \in [\lambda_{d+1}, \lambda_d] \). Then we have

\[
\mathbb{E}[\mathcal{E}^{\text{PCA}}_{\leq d}(\mu)] \leq \sum_{j \leq d} \min \left( \frac{C \lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})}, \lambda_j - \lambda_{d+1} \right).
\]

Moreover, if \( d \leq n/(16C_d^2) \), then

\[
\mathbb{E}[\mathcal{E}^{\text{PCA}}_{>d}(\mu)] \leq \sum_{k \geq d} \min \left( C \frac{\lambda_k \text{tr}(\Sigma)}{n(\lambda_d - \lambda_k)}, \lambda_d - \lambda_k \right) + (\lambda_d - \lambda_p)e^{-n/(32C_3^2)}.
\]

Summing up the inequalities in Theorem 2.6 leads to an upper bound for \( \mathbb{E}[\mathcal{E}^{\text{PCA}}_{d}] \) which improves the local bound of Proposition 2.2 and gives the value 0 in the isotropic case \( \Sigma = \sigma^2 I \). Furthermore, global bounds emerge as trade-off between the arguments of the minima in the upper bound. More precisely, we have:

2.8. Corollary. Grant Assumption 2.1 and suppose \( d \leq n/(16C_d^2) \). Then we have the local bound

\[
\mathbb{E}[\mathcal{E}^{\text{PCA}}_d] \leq C \sum_{j \leq d; \lambda_j > \lambda_{d+1}} \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})} + C \sum_{k \geq d; \lambda_k < \lambda_d} \frac{\lambda_k \text{tr}(\Sigma)}{n(\lambda_d - \lambda_k)} + \lambda_d e^{-n/(32C_3^2)}
\]

and the global bound

\[
\mathbb{E}[\mathcal{E}^{\text{PCA}}_d] \leq \sum_{j \leq d} \sqrt{\frac{C\lambda_j \text{tr}(\Sigma)}{n}} + \sqrt{\frac{Cd \text{tr}_{>d}(\Sigma) \text{tr}(\Sigma)}{n}}. \tag{2.10}
\]

For our second main result we impose additional eigenvalue conditions and thus improve the bounds of Theorem 2.6. A main feature is that the full trace of \( \Sigma \) can be replaced by the partial trace \( \text{tr}_{>s}(\Sigma) \), which in the case \( s = d \) coincides with the oracle reconstruction error.
2.9. **Theorem.** Grant Assumption 2.1. Then for all indices $s = 1, \ldots, d$ such that
\[ \frac{\lambda_s}{\lambda_s - \lambda_{d+1}} \sum_{j \leq s} \frac{\lambda_j}{\lambda_j - \lambda_{d+1}} \leq n/(256C_3^2) \] (2.11)
and all $r = 0, \ldots, s$, we have
\[ E[\mathcal{E}_{\leq d}^{PCA}(\lambda_{d+1})] \leq C \sum_{j \leq r} \frac{\lambda_j \text{tr}_{> s}(\Sigma)}{n(\lambda_j - \lambda_{d+1})} + 2 \sum_{r < j \leq d} (\lambda_j - \lambda_{d+1}) + R \]
with $C = 16C_2 + 8C_3^2$ and remainder term given by
\[ R = C \sum_{j \leq r} \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})} e^{-\frac{n(\lambda_j - \lambda_{d+1})^2}{(16C_3^2)^2}}. \]

In the special case $\lambda_{d+1} = \cdots = \lambda_p$, compare the spiked covariance model below, we have $E[\mathcal{E}_{> d}^{PCA}(\lambda_{d+1})] = 0$ and thus Theorem 2.9 yields an upper bound for the whole excess risk. In the general case, we still have the following corollary:

2.10. **Corollary.** Grant Assumption 2.1 and suppose $\lambda_d - \lambda_{d+1} \geq c_1(\lambda_d - \lambda_p)$ with a constant $c_1 > 0$. If Condition (2.11) holds with $s = d$, then we have the local bound
\[ E[\mathcal{E}_{d}^{PCA}] \leq \frac{C}{c_1 n} \left( \text{tr}_{> d}(\Sigma) + \text{tr}(\Sigma)e^{-\frac{n(\lambda_d - \lambda_p)^2}{(C\lambda_d^2)}} \right) \sum_{j \leq d} \frac{\lambda_j}{\lambda_j - \lambda_{d+1}}. \]
Moreover, if $s \leq d$ is the largest number such that (2.11) is satisfied (and $s = 0$ if such a number does not exist), then we have the global bound
\[ E[\mathcal{E}_{d}^{PCA}] \leq \frac{C}{c_1 \sqrt{n}} \left( \sqrt{\text{tr}_{> s}(\Sigma)} + \sqrt{\text{tr}(\Sigma)e^{-\frac{n(\lambda_s - \lambda_p)^2}{(C\lambda_s^2)}}} \right) \sum_{j \leq d} \sqrt{\lambda_j}. \]

Finally, observe that upper bounds for the expectation of the excess risk $E[\mathcal{E}_{d}^{PCA}] \leq r.h.s.$ can be equivalently formulated as exact oracle inequalities $E[R(\hat{P}_{\leq d})] \leq \inf_{P \in \mathcal{P}_d} R(P) + r.h.s.$ If we give up the constant 1 in front of the infimum, Theorem 2.9 also leads to a third type of bound.

2.11. **Corollary.** Grant Assumption 2.1. Then for all indices $s = 1, \ldots, d$ such that (2.11) holds, we have
\[ E[R(\hat{P}_{\leq d})] \leq C \text{tr}_{> s}(\Sigma) + C \text{tr}(\Sigma)e^{-\frac{n(\lambda_s - \lambda_{d+1})^2}{(C\lambda_s^2)}}. \]

If (2.11) holds with $s = d$, then $\text{tr}_{> d}(\Sigma) = \inf_{P \in \mathcal{P}_d} R(P)$ and we obtain a standard oracle inequality with an exponentially small remainder term.

2.4. **Applications.** Let us illustrate our different upper bounds for three main classes of eigenvalue behaviour: exponential decay, polynomial decay, and a simple spiked covariance model. Eigenvalue structures such as exponential or polynomial decay are typically considered in the context of functional data, see e.g. [11, 23, 12], spiked covariance models are often studied in the context of high-dimensional data [13, 8, 30].
**Exponential decay.** Assume for some $\alpha > 0$

$$\lambda_j = e^{-\alpha j}, \quad j \geq 1. \quad (2.12)$$

Then the assumption in Corollary 2.10 is satisfied with $c_1 = 1 - e^{-\alpha}$ and thus by (4.7), we have $\mathcal{E}_d^{PCA} \leq c_1^{-1} \mathcal{E}_{\leq d}^{PCA}(\lambda_{d+1})$. Hence, the first bound in Theorem 2.6 implies

$$\mathbb{E}[\mathcal{E}_d^{PCA}] \leq C \sum_{j \leq d} \min \left( \frac{1}{n}, e^{-\alpha j} \right) \leq C(d \wedge \log n)/n,$$

where $C$ (not the same at each occurrence) is a constant depending only on $C_1$ and $\alpha$. This bound improves the local bound in Proposition 2.2 (which gives $Ce^{\alpha d}/n$) and the bounds in Theorems 3.2 and 3.4 of [6], respectively.

Next, we show that this result can be much improved by applying the local bound in Corollary 2.10. Indeed, the left-hand side of Condition (2.11) with $s = d$ can be bounded by $d(1 - e^{-\alpha})^{-2}$. Thus, assuming that this value is smaller than $n/(256C_3^2)$, we can apply the local bound in Corollary 2.10. The main term is bounded by $C(1 - e^{-\alpha})^{-3}e^{-\alpha(d+1)}/n$ and the remainder term by $C(1 - e^{-\alpha})^{-2}n^{-1} \exp(-n(1 - e^{-\alpha})^2/(256C_3^2))$. Thus the local bound in Corollary 2.10 yields that there are constants $c, C > 0$ (depending only on $C_1$ and $\alpha$) such that

$$\mathbb{E}[\mathcal{E}_d^{PCA}] \leq C \frac{de^{-\alpha d}}{n},$$

provided that $d \leq cn$. Noting for the population reconstruction error

$$R(P_{\leq d}) = \sum_{k > d} e^{-\alpha k} = e^{-\alpha} (1 - e^{-\alpha})^{-1} e^{-\alpha d},$$

we see that the excess risk is smaller than the oracle risk, provided that $d \leq cn$.

**Polynomial decay.** Assume for some $\alpha > 1$

$$\lambda_j = j^{-\alpha}, \quad j \geq 1. \quad (2.13)$$

The local bound in Corollary 2.8 and [12, Equation (10)] yield

$$\mathbb{E}[\mathcal{E}_d^{PCA}] \leq C \frac{d \log d}{n}$$

for all $2 \leq d \leq cn$. This already improves the results obtained in [6, Section 5], where a rate strictly between $n^{-1/2}$ and $n^{-1}$ is derived.

Again, for large $d$, this result can be much improved by using Theorem 2.9 and Corollary 2.10. Choosing $s = \lfloor d/2 \rfloor$, there is a constant $c$ depending only on $C_1$ and $\alpha$ such that Condition (2.11) is satisfied if $d \leq cn$. Thus, Corollary 2.11 yields

$$\mathbb{E}[\mathcal{E}^{PCA}] \leq C \operatorname{tr}_{\geq \lfloor d/2 \rfloor}(\Sigma) + Ce^{-n/C} \leq Cd^{-(\alpha-1)} + Ce^{-n/C}, \quad (2.14)$$
provided that \( d \leq cn \). Noting for the population reconstruction error
\[
R(P_{\leq d}) = \sum_{k>d} k^{-\alpha} \geq cd^{-(\alpha-1)},
\]
we see from (2.14) that for \( d \leq cn \) the excess risk is always smaller than a constant times the oracle risk.

On the other hand, from [12, Equation (10)] follows that there is a constant \( c \) depending only on \( C \) such that Condition (2.11) with \( s = d \) is satisfied if \( d^2 \log d \leq cn \). Moreover the condition in Corollary 2.10 is satisfied with \( c_1 = (d + 1)^{-1} \). Hence, the local bound in Corollary 2.10 implies
\[
\mathbb{E}[\mathcal{E}_{d}^{PCA}] \leq C d^{-(\alpha-3)} \frac{\log d}{n} + C d^2 \frac{\log d}{n} e^{-\frac{n}{d^2}} \leq C d^{-(\alpha-3)} \frac{\log d}{n},
\]
provided that \( d^2 \log d \leq cn \). We see that the excess risk is of much smaller order than the oracle risk, as long as \( d^2 \log d \leq cn \). Considering the asymptotic limit in Proposition 2.13 below, we would expect the leading term \( C d^2 \alpha / n \) instead of \( C d^3 \alpha \log d / n \). In Appendix B below we show how such a leading term can be obtained by using linear expansions.

**Spiked covariance model.** Let \( \Theta \) be the class of all symmetric matrices whose eigenvalues satisfy
\[
1 + \kappa x \geq \lambda_1 \geq \ldots \geq \lambda_d \geq 1 + x \quad \text{and} \quad \lambda_{d+1} = \ldots = \lambda_p = 1,
\]
where \( x \geq 0 \) and \( \kappa > 1 \). Then it holds
\[
\sup_{\Sigma \in \Theta} \mathbb{E}[\mathcal{E}_d^{PCA}] \leq \min \left( C \kappa \frac{(1 + \kappa x)d(p-d)}{nx}, d\kappa x, (p-d)\kappa x \right) + \kappa xe^{-\frac{n}{d\kappa x^2}},
\]
provided that \( d \leq cn \), where \( c, C > 0 \) are constants depending only on \( C_1 \).

Considering separately the cases \( x \leq c \) and \( x > c \), we see that the excess risk is always smaller than the oracle risk \( R(P_{\leq d}) = p - d \). To prove (2.16), it suffices to apply Theorem 2.6. Indeed, the claim follows from applying either Lemma 2.5 with \( \mu = 1 \) and the first inequality in Theorem 2.6 or Lemma 2.5 with \( \mu = 1 + \kappa x \) and the second inequality in Theorem 2.6 (depending on whether \( (1 + \kappa x)d \leq p - d \) or \( (1 + \kappa x)d > p - d \)).

In fact, since
\[
x\|P_{\leq d} - \hat{P}_{\leq d}\|_2^2 \leq 2\mathcal{E}_d^{PCA} \leq \kappa x\|P_{\leq d} - \hat{P}_{\leq d}\|_2^2,
\]
(2.16) is equivalent to a result by Cai, Ma, and Wu [8, Theorem 9]. Moreover, their minimax lower bound [8, Theorem 8] gives
\[
\inf_{P_{\leq d}} \sup_{\Sigma \in \Theta} \mathbb{E}[\mathcal{E}[\Sigma, P_{\leq d} - \hat{P}_{\leq d}]] \geq c \min \left( \frac{(1 + x)d(p-d)}{nx}, dx, (p-d)x \right),
\]
(2.17)
where the infimum is taken over all estimators \( \hat{P}_{\leq d} \) based on \( X_1, \ldots, X_n \) with values in \( P_d \) and \( c > 0 \) is a constant.
Oracle inequality. One interesting conclusion in the above typical situations is a nonasymptotic bound by the oracle risk, more precisely:

2.12. Corollary. In the cases (2.12), (2.13) and (2.15), there are constants \(c,C > 0\) (depending only on \(\kappa\) and \(\alpha\), respectively) such that the oracle inequality

\[
\mathbb{E}[R(\hat{P}_{\leq d})] \leq C \cdot R(P_{\leq d}),
\]

holds for all \(d \leq cn\).

2.5. Discussion. We review some connections and implications for related questions.

Subspace distance. Many results cover the Hilbert-Schmidt distance \(\|\hat{P}_{\leq d} - P_{\leq d}\|_2^2\), which has a geometric interpretation in terms of canonical angles \([23, 16, 19, 30, 8]\). It can be written as

\[
\|\hat{P}_{\leq d} - P_{\leq d}\|_2^2 = 2\sum_{j \leq d} \langle P_j, \hat{P}_{\leq d}\rangle = 2\sum_{k > d} \langle P_k, \hat{P}_{\leq d}\rangle
\]  

(2.18)

and also as \(\|\hat{P}_{\leq d} - P_{\leq d}\|_2^2 = 2\sum_{k > d} \langle P_k, \hat{P}_{\leq d}\rangle\). Comparing these representations to Lemma 2.5, we see that the excess risk and the Hilbert-Schmidt distance differ in the weighting of the projector angles. These weightings lead to different behaviour. On the one hand, estimation of \(P_{\leq d}\) becomes highly unstable in the Hilbert-Schmidt loss when the spectral gap \(\lambda_d - \lambda_{d+1}\) is small. In the extreme case \(\lambda_d = \lambda_{d+1}\) that loss depends on the choice of \((u_d, u_{d+1})\) and is thus not even uniquely defined. For the reconstruction error, however, a small spectral gap \(\lambda_d - \lambda_{d+1}\) means that contributions of \(\hat{P}_{\leq d}\) in direction of \(u_{d+1}\) have only small impact on the excess risk, as can be seen from Lemma 2.5.

Despite this difference, one can use our bounds for the excess risk to derive upper bounds for the Hilbert-Schmidt distance. For instance, applying (2.18), Lemma 2.5 with \(\mu = \lambda_{d+1}\) and using \(\langle P_k, \hat{P}_{\leq d}\rangle \geq 0\), we obtain

\[
\|\hat{P}_{\leq d} - P_{\leq d}\|_2^2 \leq \frac{2\varepsilon_{d\text{PCA}}(\lambda_{d+1})}{\lambda_d - \lambda_{d+1}} \leq \frac{2\varepsilon_{d\text{PCA}}}{\lambda_d - \lambda_{d+1}},
\]  

(2.19)

which is a first inequality relating the Hilbert-Schmidt distance with the excess risk. This means that all excess risk bounds a fortiori imply bounds on the Hilbert-Schmidt distance up to a spectral gap factor. For instance, in our setting, (2.19) implies most versions of the Davis-Kahan \(\sin \Theta\) theorem, e.g. those in Yu, Wang and Samworth \([31]\), by using the basic inequality \(|\Delta, P_{\leq d} - \hat{P}_{\leq d}| \geq \varepsilon_{d\text{PCA}}^2\) in (2.5) and bounding the scalar product by a Cauchy-Schwarz or operator norm inequality. Note that a more sophisticated version of (2.19) can be found in Proposition B.2 in Appendix B.
Asymptotic versus non-asymptotic. For the Hilbert-Schmidt distance it is known that for $\mathcal{H} = \mathbb{R}^p$ and $X \sim N(0, \Sigma)$ with fixed $\Sigma$ in the case $\lambda_d > \lambda_{d+1}$

$$n\|\hat{P}_{\leq d} - P_{\leq d}\|_2 \overset{d}{\to} 2 \sum_{j \leq d, k > d} \frac{\lambda_j \lambda_k}{(\lambda_j - \lambda_k)^2} g_{jk}^2$$

(2.20)

holds as $n \to \infty$, where $(g_{jk})_{j \leq d < k}$ is an array of independent standard Gaussian random variables, see e.g. Dauxois, Pousse and Romain [10] and also Koltchinskii and Lounici [17, 16]. The projector calculus developed in Section 3.1 allows to obtain readily the analogue of the asymptotic result (2.20) for the excess risk $\mathcal{E}_d^{PCA}$ without any spectral gap condition. More precisely, we prove in Appendix A:

2.13. Proposition. Let $\mathcal{H} = \mathbb{R}^p$ and $X \sim N(0, \Sigma)$ with $\Sigma$ fixed. As $n \to \infty$ we have for the excess risk $\mathcal{E}_{d,n}^{PCA} = \mathcal{E}_d^{PCA}$

$$n\mathcal{E}_{d,n}^{PCA} \overset{d}{\to} \sum_{j \leq d, k > d} \frac{\lambda_j \lambda_k}{\lambda_j - \lambda_k} g_{jk},$$

where $(g_{jk})_{j \leq d < k}$ are independent standard Gaussian random variables.

We see that the excess risk $\mathcal{E}_d^{PCA}$ converges with $n^{-1}$-rate also in the case $\lambda_d = \lambda_{d+1}$. Remark, however, that the convergence cannot be uniform in the parameter $\Sigma$ in view of the discontinuity of the right-hand side in $(\lambda_j)$. In certain examples, including the spiked covariance model and exponential decay of eigenvalues, the eigenvalue expression in Theorem 2.9 (with $r = s = d$) coincides up to a constant with the asymptotic limit in Proposition 2.13. Sometimes the eigenvalue expression differs, e.g. for polynomial decay in Theorem 2.9 it equals to $Cd^{3-\alpha} \log d$, while the asymptotic limit in Proposition 2.13 is equal to $Cd^2$. These asymptotic leading terms can be obtained by first or higher order expansions using perturbation theory for linear operators. This requires stronger eigenvalue conditions (including $\lambda_d > \lambda_{d+1}$), see Appendix B, where we state upper bounds for the excess risk and the Hilbert-Schmidt distance, using linear expansions of $\hat{P}_{>d}$. In contrast, our main results in Section 2.3 also apply to the case of small or vanishing spectral gaps.

Eigenvalue concentration. We obtain deviation inequalities for empirical eigenvalues which are of independent interest. Concentration inequalities for eigenvalues using tools from measure concentration are widespread, see e.g. [21] [23] [22] [1] [7] [4]. The main difference to our deviation inequalities is that we take into account the local eigenvalue structure. For instance, from Theorem 3.7 and 3.10 we get the following corollary:
2.14. **Corollary.** Grant Assumption 2.1. Then there is a constant $c > 0$ such that for all $y > 0$ satisfying
\[
\frac{1}{n(y + 1)} \sum_{k > d} \frac{\lambda_k}{\lambda_d - \lambda_k + y\lambda_d} \leq 1/(2C_3^2)
\]
we have
\[
P\left(\frac{\hat{\lambda}_d - \lambda_d}{\lambda_d} > y\right) \leq e^{1-cn(y^2)}.
\]
Moreover, for all $y > 0$ satisfying
\[
\frac{1}{n(y + 1)} \sum_{j < d} \frac{\lambda_j}{\lambda_j - \lambda_d + y\lambda_d} \leq 1/(2C_3^2)
\]
we have
\[
P\left(\frac{\hat{\lambda}_d - \lambda_d}{\lambda_d} < -y\right) \leq e^{1-cn(y^2)}.
\]

If $\lambda_d$ is a simple eigenvalue, then Corollary 2.14 can be seen as a non-asymptotic version of the classical central limit theorem $\sqrt{n} (\hat{\lambda}_d/\lambda_d - 1) \to N(0, 2)$ which holds for $X$ Gaussian, compare Anderson [2, Theorem 13.5.1] and Dauxois, Pousse and Romain [10, Proposition 8]. Moreover, the conditions imposed are related to $\mathbb{E}[\hat{\lambda}_d]$ by the following asymptotic expansion (see e.g. [25, Equation (2.22)])
\[
\mathbb{E}[\hat{\lambda}_d/\lambda_d] - 1 = \frac{1}{n} \sum_{k \neq d} \frac{\lambda_k}{\lambda_d - \lambda_k} + \ldots.
\]

The relative conditions in Corollary 2.14 can be compared to the following global one. Suppose, for instance, we are interested in the one-sided separation event $\{\hat{\lambda}_d - \lambda_d \geq -(\lambda_d - \lambda_{d+1})/2\}$. This corresponds to choosing $y = (\lambda_d - \lambda_{d+1})/(2\lambda_d) \leq 1$ in which case the second condition in Corollary 2.14 holds if
\[
\frac{\lambda_d}{\lambda_d - \lambda_{d+1}} \sum_{j < d} \frac{\lambda_j}{n(\lambda_j - \lambda_{d+1})} \leq 1/(8C_3^2),
\]
which is (up to a constant) Condition (2.11) with $s = d$. On the other hand, we have $\{\hat{\lambda}_d - \lambda_d \geq -(\lambda_d - \lambda_{d+1})/2\} \subseteq \{\lVert \Delta \rVert_\infty \leq (\lambda_d - \lambda_{d+1})/2\}$ and by (3.19) below the latter global event occurs with high probability if
\[
\frac{\lambda_1 \text{tr}(\Sigma)}{n(\lambda_d - \lambda_{d+1})^2} \leq 1/(4C_3^2),
\]
i.e. if $\|\Sigma\|_\infty \sqrt{\text{tr}(\Sigma)/n} \leq (\lambda_d - \lambda_{d+1})/(2C_3)$ with effective rank $r(\Sigma) = \text{tr}(\Sigma)/\|\Sigma\|_\infty$. The latter effective rank condition is underlying the analysis in [16, 19, 15, 14]. Much of our mathematical difficulties come from showing that this global condition can be replaced by the relative eigenvalue condition in (2.21).
3. **Main Tools**

3.1. **Projector-based calculus.** In this section, we present two formulas which form the basis of our analysis of the excess risk. We begin with an expansion of the quantities $\langle P_j, \hat{P}_d \rangle$ and $\langle P_k, \hat{P}_d \rangle$, which appeared in Lemma 2.5.

3.1. **Lemma.** For $j \leq d$ we have

$$\langle P_j, \hat{P}_d \rangle = \sum_{k>d} \frac{\|P_j \Delta \hat{P}_k\|^2}{(\lambda_j - \hat{\lambda}_k)^2}$$

and for $k > d$ we have

$$\langle P_k, \hat{P}_d \rangle = \sum_{j \leq d} \frac{\|P_k \Delta \hat{P}_j\|^2}{(\hat{\lambda}_j - \lambda_k)^2}$$

Both identities hold provided that all denominators are non-zero.

**Proof.** The main ingredient is the formula

$$P_j \hat{P}_k = \frac{1}{\lambda_j - \lambda_k} P_j \Delta \hat{P}_k,$$

which follows from inserting the representation

$$\Delta = \Sigma - \hat{\Sigma} = \sum_{l \geq 1} \lambda_l P_l - \sum_{l \geq 1} \hat{\lambda}_l \hat{P}_l$$

into the right-hand side. Indeed,

$$P_j \Delta \hat{P}_k = \sum_{l \geq 1} \lambda_l P_j P_l \hat{P}_k - \sum_{l \geq 1} \hat{\lambda}_l P_j \hat{P}_l \hat{P}_k = (\lambda_j - \hat{\lambda}_k) P_j \hat{P}_k.$$ 

The identity $\langle P_j, \hat{P}_d \rangle = \|P_j \hat{P}_d\|_2^2$ combined with (3.1) gives

$$\langle P_j, \hat{P}_d \rangle = \frac{\|P_j \Delta \hat{P}_d\|_2^2}{(\lambda_j - \hat{\lambda}_k)^2}.$$ 

Summation over $k$ gives the first claim. The second claim follows similarly by switching $j$ and $k$ and summation over $j$. \qed

Identity (3.1) can be seen as a building block to derive expansions for empirical spectral projectors. Indeed, using (3.1), we get

$$P_j \hat{P}_d = \sum_{k>d} \frac{P_j \Delta \hat{P}_k}{\lambda_j - \hat{\lambda}_k}$$

(3.2)

(and a similar formula for $P_k \hat{P}_d$) and thus

$$\hat{P}_d - P_d = P_{\leq d} \hat{P}_d - P_d \hat{P}_{\leq d} = \sum_{j \leq d} \sum_{k>d} \left( \frac{P_j \Delta \hat{P}_k}{\lambda_j - \hat{\lambda}_k} + \frac{P_k \Delta \hat{P}_j}{\hat{\lambda}_j - \lambda_k} \right).$$
Thus we have

\[ \sum_{k \leq d} P_{p_{\leq d}} = \sum_{k \leq d} \sum_{l \leq d} \frac{P_{j} \Delta P_{k} \Delta \hat{P}_{l}}{(\lambda_j - \lambda_k)(\lambda_l - \lambda_t)} + \sum_{k \leq d} \sum_{l > d} \frac{P_{j} \Delta P_{k} \Delta \hat{P}_{l}}{(\lambda_j - \lambda_k)(\lambda_l - \lambda_t)} \]

and for \( k > d \) we have

\[ \sum_{k > d} P_{p_{\leq d}} = \sum_{j \leq d} \frac{P_{j} \Delta P_{k} \Delta \hat{P}_{l}}{(\lambda_k - \lambda_j)(\lambda_l - \lambda_j)} + \sum_{j \leq d} \sum_{l > d} \frac{P_{j} \Delta P_{k} \Delta \hat{P}_{l}}{(\lambda_k - \lambda_j)(\lambda_l - \lambda_j)} \]

Both identities hold provided that all denominators are non-zero.

Note that compared to (3.2), where only spectral gaps between \( j \) and \( k > d \) appear, the first formula in Lemma 3.2 includes all spectral gaps between \( k > d \) and \( l \leq d \), even if we consider \( P_{j} \hat{P}_{d} \).

Proof. We only prove the first identity, since the second one follows by the same line of arguments. First using (3.2) and the identities \( I = P_{\leq d} + P_{> d} = \hat{P}_{\leq d} + \hat{P}_{> d} \), we get

\[ P_{j} \hat{P}_{d} = \sum_{l > d} \sum_{l \leq d} \frac{P_{j} \Delta P_{l}}{(\lambda_j - \lambda_l)(\lambda_l - \lambda_t)} + \sum_{l > d} \sum_{l \leq d} \frac{P_{j} \Delta P_{l}}{(\lambda_j - \lambda_l)(\lambda_l - \lambda_t)} \]

and

\[ \sum_{k > d} P_{j} \Delta P_{k} = \sum_{k > d} \sum_{l \leq d} \frac{P_{j} \Delta P_{k}}{(\lambda_j - \lambda_k)(\lambda_l - \lambda_t)} + \sum_{k > d} \sum_{l \leq d} \frac{P_{j} \Delta P_{k}}{(\lambda_j - \lambda_k)(\lambda_l - \lambda_t)} \]

Thus

\[ P_{j} \hat{P}_{d} = \sum_{k > d} \sum_{l \leq d} \frac{P_{j} \Delta P_{k}}{(\lambda_j - \lambda_k)(\lambda_l - \lambda_t)} + \sum_{l > d} \sum_{l \leq d} \frac{P_{j} \Delta P_{l}}{(\lambda_j - \lambda_l)(\lambda_l - \lambda_t)} = \sum_{k > d} \sum_{l \leq d} \frac{P_{j} \Delta P_{k} \Delta \hat{P}_{l}}{(\lambda_j - \lambda_k)(\lambda_l - \lambda_t)} \]

Using (3.1), we get

\[ \sum_{l > d} \sum_{l \leq d} \frac{P_{j} \Delta P_{l} \Delta \hat{P}_{l}}{(\lambda_j - \lambda_l)(\lambda_l - \lambda_t)} = \sum_{k \leq d} \sum_{l > d} \frac{P_{j} \Delta P_{k} \Delta \hat{P}_{l}}{(\lambda_j - \lambda_k)(\lambda_l - \lambda_t)} \]
and
\[ - \sum_{k>d} P_j \Delta P_k \hat{P}_{\leq d} \frac{\lambda_j - \lambda_k}{\lambda_j - \lambda_k} = \sum_{k>d} \sum_{l\leq d} \frac{P_j \Delta P_k \Delta \hat{P}_l}{(\lambda_j - \lambda_k)(\hat{\lambda}_l - \lambda_k)}. \]

Moreover, again using (3.1), the term in brackets in (3.3) is equal to
\[ \sum_{l>d} P_j \Delta \hat{P}_{>d} - \sum_{k>d} \frac{P_j \Delta P_k \hat{P}_{>d}}{\lambda_j - \lambda_k} \]
\[ = \sum_{k>d} \sum_{l>d} \frac{P_j \Delta P_k \hat{P}_l}{(\lambda_j - \lambda_k)(\hat{\lambda}_l - \lambda_k)} \]
\[ = - \sum_{k>d} \sum_{l>d} \frac{\lambda_k - \hat{\lambda}_l}{(\lambda_j - \lambda_k)(\hat{\lambda}_l - \lambda_k)} P_j \Delta P_k \hat{P}_l \]
\[ = - \sum_{k>d} \sum_{l>d} \frac{1}{(\lambda_j - \lambda_k)(\hat{\lambda}_l - \lambda_k)} P_j \Delta P_k \Delta \hat{P}_l, \]

and the claim follows. \( \square \)

3.2. Deterministic error decomposition. In this section, we prove deterministic upper bounds for the excess risk which form the basis of our new upper bounds in Section 2.3. For \( \mathcal{E}^{PCA}_d(\mu) \) we split the sum into indices \( j \leq r \), where we expect the spectral gaps \( \lambda_j - \lambda_{d+1} \) to be large, meaning that we can insert the expansions of Lemma 3.1, and \( r < j \leq d \), where wrong projections do not incur a large error because \( \lambda_j - \mu \) is small. The terms of the first sum can then be controlled by a recursion argument.

3.3. Proposition. For \( \mu \in [\lambda_{d+1}, \lambda_d] \) and \( r = 0, \ldots, d \), we have
\[ \mathcal{E}^{PCA}_{\leq d}(\mu) \leq 4 \sum_{j \leq r} (\lambda_j - \mu) \frac{\|P_j \Delta \hat{P}_{>d}\|_2^2}{(\lambda_j - \lambda_{d+1})^2} + d \lambda(r+p-d) \sum_{j=r+1} (\lambda_j - \mu) \]
\[ + \sum_{j \leq r}(\lambda_j - \mu) \mathbb{1}(\hat{\lambda}_{d+1} - \lambda_{d+1} > (\lambda_j - \lambda_{d+1})/2). \] (3.4)

Furthermore, for \( s = r, \ldots, d \) and the weighted projector
\[ S_{\leq s} = S_{\leq s}(\mu) = \sum_{j \leq s} \frac{1}{\sqrt{\lambda_j - \mu}} P_j \]
(assuming \( \lambda_s > \mu \)) we obtain
\[ \mathcal{E}^{PCA}_{\leq d}(\mu) \leq 16 \sum_{j \leq r} (\lambda_j - \mu) \frac{\|P_j \Delta \hat{P}_{>s}\|_2^2}{(\lambda_j - \lambda_{d+1})^2} + 2 d \lambda(r+p-d) \sum_{j=r+1} (\lambda_j - \mu) \]
\[ + 2 \sum_{j \leq r}(\lambda_j - \mu) \mathbb{1}(\hat{\lambda}_{d+1} - \lambda_{d+1} > (\lambda_j - \lambda_{d+1})/2) \]
\[ + 8 \sum_{j \leq r} (\lambda_j - \mu) \frac{\|P_j \Delta\|^2}{(\lambda_j - \lambda_{d+1})^2} 1(\|S_{\leq s} \Delta S_{\leq s}\|_\infty > 1/16). \]  

(3.6)

3.4. Remark. The constants are chosen for simplicity. For each \( \varepsilon > 0 \), the constant 16 in (3.6) can be replaced by \( 1 + \varepsilon \) provided that the constants 1/2 and 1/16 in the definition of the events are replaced by smaller constants depending on \( \varepsilon \).

Proof. Using \( \langle P_j, \hat{P}_{>d} \rangle \leq 1 \) and \( \sum_{j=r+1}^d \langle P_j, \hat{P}_{>d} \rangle \leq p - d \), we obtain

\[ \mathcal{E}_{\leq d}^{\text{PCA}}(\mu) = \sum_{j \leq d} (\lambda_j - \mu) \langle P_j, \hat{P}_{>d} \rangle \]
\[ \leq \sum_{j \leq r} (\lambda_j - \mu) \langle P_j, \hat{P}_{>d} \rangle + \sum_{j=r+1}^d (\lambda_j - \mu). \]  

(3.7)

By Lemma 3.1 we have

\[ \langle P_j, \hat{P}_{>d} \rangle = \sum_{k>d} \frac{\|P_j \Delta \hat{P}_k\|^2}{(\lambda_j - \lambda_k)^2}. \]

Moreover, on the event

\[ \{\hat{\lambda}_{d+1} - \lambda_{d+1} \leq (\lambda_j - \lambda_{d+1})/2\} = \{\lambda_j - \hat{\lambda}_{d+1} \geq (\lambda_j - \lambda_{d+1})/2\} \]

we can bound

\[ \langle P_j, \hat{P}_{>d} \rangle \leq \sum_{k>d} 4 \frac{\|P_j \Delta \hat{P}_k\|^2}{(\lambda_j - \lambda_{d+1})^2} = 4 \frac{\|P_j \Delta \hat{P}_{>d}\|^2}{(\lambda_j - \lambda_{d+1})^2}. \]  

(3.8)

By (3.8) and \( \langle P_j, \hat{P}_{>d} \rangle \leq 1 \), we conclude

\[ \langle P_j, \hat{P}_{>d} \rangle \leq 4 \frac{\|P_j \Delta \hat{P}_{>d}\|^2}{(\lambda_j - \lambda_{d+1})^2} + 1(\hat{\lambda}_{d+1} - \lambda_{d+1} > (\lambda_j - \lambda_{d+1})/2). \]  

(3.9)

Inserting (3.9) into (3.7), we obtain the first claim (3.4). The second claim follows from an additional recursion argument. First, we introduce the operator

\[ R_{\leq s} = R_{\leq s}(\mu) = \sum_{j \leq s} \sqrt{\lambda_j - \mu} P_j, \]  

(3.10)

which satisfies the identities

\[ S_{\leq s} R_{\leq s} = P_{\leq s} \]

and

\[ \sum_{j \leq s} (\lambda_j - \mu) \langle P_j, \hat{P}_{>d} \rangle = \sum_{j \leq s} (\lambda_j - \mu) \|P_j \hat{P}_{>d}\|^2 = \|R_{\leq s} \hat{P}_{>d}\|^2. \]  

(3.11)

Then we have

\[ \sum_{j \leq r} (\lambda_j - \mu) \|P_j \Delta \hat{P}_{>d}\|^2 \]
\[
\leq 2 \sum_{j \leq r}(\lambda_j - \mu)\frac{\|P_j \Delta \hat{P}_{>d}\|_2^2}{(\lambda_j - \lambda_{d+1})^2} + 2 \sum_{j \leq r}(\lambda_j - \mu)\frac{\|P_j \Delta \hat{P}_{\leq s}\|_2^2}{(\lambda_j - \lambda_{d+1})^2}
\]
\[
\leq 2 \sum_{j \leq r}(\lambda_j - \mu)\frac{\|P_j \Delta \hat{P}_{>s}\|_2^2}{(\lambda_j - \lambda_{d+1})^2} + 2 \sum_{j \leq r}\|P_j \Delta \hat{P}_{\leq s}\|_2^2
\]
\[
= 2 \sum_{j \leq r}(\lambda_j - \mu)\frac{\|P_j \Delta \hat{P}_{>s}\|_2^2}{(\lambda_j - \lambda_{d+1})^2} + 2 \|S_{\leq r} \Delta \hat{P}_{\leq d}\|_2^2. \tag{3.12}
\]

On the event \(\{\|S_{\leq s} \Delta S_{\leq s}\|_\infty \leq 1/16\}\), the last term is bounded via
\[
2\|S_{\leq r} \Delta \hat{P}_{<s} \hat{P}_{>d}\|_2^2 = 2\|S_{\leq r} \Delta S_{<s} R_{<s} \hat{P}_{>d}\|_2^2
\]
\[
\leq 2\|S_{\leq r} \Delta S_{<s}\|_\infty^2 \|R_{<s} \hat{P}_{>d}\|_2^2
\]
\[
\leq 2\|S_{<s} \Delta S_{<s}\|_\infty^2 \|R_{<s} \hat{P}_{>d}\|_2^2 \leq \|R_{<s} \hat{P}_{>d}\|_2^2 / 8,
\]

where we also used that \(r \leq s\). Consequently, on \(\{\|S_{\leq s} \Delta S_{\leq s}\|_\infty \leq 1/16\}\), we get
\[
\sum_{j \leq r}(\lambda_j - \mu)\frac{\|P_j \Delta \hat{P}_{>d}\|_2^2}{(\lambda_j - \lambda_{d+1})^2}
\]
\[
\leq 2 \sum_{j \leq r}(\lambda_j - \mu)\frac{\|P_j \Delta \hat{P}_{>s}\|_2^2}{(\lambda_j - \lambda_{d+1})^2} + \frac{1}{8} \sum_{j \leq s}(\lambda_j - \mu)\langle P_j, \hat{P}_{>d} \rangle. \tag{3.13}
\]

Using also that \(\|P_j \Delta \hat{P}_{>d}\|_2^2 \leq \|P_j \Delta \|_2^2\), we conclude that
\[
4 \sum_{j \leq r}(\lambda_j - \mu)\frac{\|P_j \Delta \hat{P}_{>d}\|_2^2}{(\lambda_j - \lambda_{d+1})^2}
\]
\[
\leq 8 \sum_{j \leq r}(\lambda_j - \mu)\frac{\|P_j \Delta \hat{P}_{>s}\|_2^2}{(\lambda_j - \lambda_{d+1})^2} + \frac{1}{2} \varepsilon^{\text{PCA}}_{d}(\mu)
\]
\[
+ 4 \sum_{j \leq r}(\lambda_j - \mu)\frac{\|P_j \Delta \|_2^2}{(\lambda_j - \lambda_{d+1})^2} 1(\|S_{\leq s} \Delta S_{\leq s}\|_\infty > 1/16).
\]

Plugging this into (3.12), we obtain the second claim. \(\square\)

Similarly, we can upper-bound the second risk part \(\varepsilon^{\text{PCA}}_{d}(\mu)\). The only difference in the proof is that an additional argument deals with the sum over all sufficiently large \(k\).

3.5. Proposition. For \(\mu \in [\lambda_{d+1}, \lambda_d]\) and \(l = d + 1, \ldots, p + 1\), we have
\[
\varepsilon^{\text{PCA}}_{d}(\mu) \leq 4 \sum_{k \geq l}(\mu - \lambda_k)\frac{\|P_k \Delta \hat{P}_{\leq d}\|_2^2}{(\lambda_d - \lambda_k)^2} + \sum_{k = (d+1) \lor (l-d)}^{l-1}(\mu - \lambda_k)
\]
\[
+ \sum_{k \geq l; \lambda_k \geq \lambda_d/2}(\mu - \lambda_k)1(\lambda_d - \lambda_d < -(\lambda_d - \lambda_k)/2)
\]
\[ + d(\mu - \lambda_p) \mathbb{1}(\hat{\lambda}_d - \lambda_d < -\lambda_d/4). \] (3.14)

Note that for \( p = \infty \) the convention of Theorem 2.6 is still in force.

**Proof.** Using \( \langle P_k, \hat{P}_{\leq d} \rangle \leq 1 \) and \( \sum_{d < k < l} \langle P_k, \hat{P}_{\leq d} \rangle \leq d \), we obtain

\[
\mathcal{E}_{d}^{PCA}(\mu) = \sum_{k > d} (\mu - \lambda_k) \langle P_k, \hat{P}_{\leq d} \rangle \leq \sum_{k \geq l} (\mu - \lambda_k) \langle P_k, \hat{P}_{\leq d} \rangle + \sum_{k = (d+1) \lor (l-d)}^{l-1} (\mu - \lambda_k).
\] (3.15)

Proceeding as in the proof of Proposition 3.3, on the event \( \{ \hat{\lambda}_d - \lambda_d \geq - (\lambda_d - \lambda_k)/2 \} = \{ \hat{\lambda}_d - \lambda_k \geq (\lambda_d - \lambda_k)/2 \} \), we have

\[
\langle P_k, \hat{P}_{\leq d} \rangle \leq 4 \frac{\| P_k \Delta \hat{P}_{\leq d} \|_2^2}{(\lambda_d - \lambda_k)^2}.
\] (3.16)

Using \( \langle P_k, \hat{P}_{\leq d} \rangle \leq 1 \), we get

\[
\langle P_k, \hat{P}_{\leq d} \rangle \leq 4 \frac{\| P_k \Delta \hat{P}_{\leq d} \|_2^2}{(\lambda_d - \lambda_k)^2} + \mathbb{1}(\hat{\lambda}_d - \lambda_d < -(\lambda_d - \lambda_k)/2).
\] (3.17)

For \( k \geq l \) such that \( \lambda_k < \lambda_d/2 \), we have

\[
\{ \hat{\lambda}_d - \lambda_d < -(\lambda_d - \lambda_k)/2 \} \subseteq \{ \hat{\lambda}_d - \lambda_d < -\lambda_d/4 \}.
\]

Hence, by (3.16) and the bound

\[
\sum_{k \geq l: \lambda_k < \lambda_d/2} (\mu - \lambda_k) \langle P_k, \hat{P}_{\leq d} \rangle \leq d(\mu - \lambda_p),
\]

we have

\[
\sum_{k \geq l: \lambda_k < \lambda_d/2} (\mu - \lambda_k) \langle P_k, \hat{P}_{\leq d} \rangle \leq 4 \sum_{k \geq l: \lambda_k < \lambda_d/2} (\mu - \lambda_k) \frac{\| P_k \Delta \hat{P}_{\leq d} \|_2^2}{(\lambda_d - \lambda_k)^2} + d(\mu - \lambda_p) \mathbb{1}(\hat{\lambda}_d - \lambda_d < -\lambda_d/4).
\] (3.18)

Inserting (3.17) (for \( k \geq l \) such that \( \lambda_k \geq \lambda_d/2 \)) and (3.18) into (3.15), the claim follows. \( \square \)

### 3.3. Concentration inequalities.

In order to make the deterministic upper bounds of the previous section useful, one has to show that the events in the remainder terms occur with small probability. We establish concentration inequalities for the weighted sample covariance operators as well as deviation inequalities for the empirical eigenvalues \( \hat{\lambda}_d \) and \( \hat{\lambda}_{d+1} \), based on
the concentration inequality [17, Corollary 2] for sample covariance operators which we use in the form
\[ P(\|\Delta\|_\infty > C_3 \lambda_1 x) \leq e^{-n(x^2 - x^2)}, \]  
whenever
\[ \text{tr}(\Sigma) \leq n\lambda_1 (x^2 - x^2), \]
where \( C_3 > 1 \) is a constant which depends only on \( C_1 \). First, consider the weighted projector \( S_{\leq s} \) from (3.5) for \( \mu \in [0, \lambda_s) \). Then, as in (2.9), \( X' = S_{\leq s}X \) satisfies Assumption 2.1 with the same constant \( C_1 \) as \( X \) and has covariance operator
\[ \Sigma' = S_{\leq s} \Sigma S_{\leq s} = \sum_{j \leq s} \frac{\lambda_j}{\lambda_j - \mu} P_j. \]
The eigenvalues of \( \Sigma' \) (in decreasing order) are \( \lambda'_j = \lambda_{s+1-j} / (\lambda_{s+1-j} - \mu) \), noting that the order is reversed by the weighting. Using the sample covariance \( \hat{\Sigma}' = S_{\leq s} \hat{\Sigma} S_{\leq s} \) and choosing \( x = 1/(16C_3\lambda_1^2) \), which is smaller than 1, the concentration inequality (3.19) applied to \( \Delta' = \Sigma' - \hat{\Sigma}' \) yields:

3.6. Lemma. **Grant Assumption 2.1.** If \( \mu \in [0, \lambda_s) \) and if
\[ \frac{\lambda_s}{\lambda_s - \mu} \sum_{j \leq s} \frac{\lambda_j}{\lambda_j - \mu} \leq n/(256C_3^2) \]
holds with the constant \( C_3 \) from (3.19), then
\[ P(\|S_{\leq s} \Delta S_{\leq s}\|_\infty > 1/16) \leq \exp \left( - \frac{n(\lambda_s - \mu)^2}{256C_3^2 \lambda_s^2} \right). \]

Next, we will state deviation inequalities for the empirical eigenvalues \( \hat{\lambda}_d \) and \( \hat{\lambda}_{d+1} \), namely right-deviation inequalities for \( \hat{\lambda}_{d+1} \) and left-deviation inequalities for \( \hat{\lambda}_d \).

3.7. Theorem. **Grant Assumption 2.1.** For all \( x > 0 \) satisfying
\[ \max \left( \frac{C_3 \lambda_{d+1}}{x}, 1 \right) \sum_{k > d} \frac{\lambda_k}{\lambda_{d+1} - \lambda_k + x} \leq n/C_3, \]  
we have
\[ P(\hat{\lambda}_{d+1} - \lambda_{d+1} > x) \leq \exp \left( - n \min \left( \frac{x^2}{C_3^2 \lambda_{d+1}^2}, \frac{x}{C_3 \lambda_{d+1}} \right) \right), \]
where \( C_3 \) is the constant in (3.19).

Proof. First, we apply the min-max characterisation of eigenvalues and obtain \( \lambda_{d+1} \leq \lambda_1(P_{>d} \Sigma P_{>d}) \). This gives
\[ P(\hat{\lambda}_{d+1} - \lambda_{d+1} > x) \leq P(\lambda_1(P_{>d} \Sigma P_{>d}) - \lambda_1(P_{>d} \Sigma P_{>d}) > x). \]  
We now use the following lemma, proven later.
Lemma. Let $S$ and $T$ be self-adjoint, positive compact operators on $H$ and $y > \lambda_1(S)$. Then:

$$\lambda_1(T) > y \iff \lambda_1((y - S)^{-1/2}(T - S)(y - S)^{-1/2}) > 1.$$ 

Applying this lemma to $S = P_d \Sigma P_d$, $T = P_d \hat{\Sigma} P_d$, and $y = \lambda_1(S) + x = \lambda_{d+1} + x$, we get

$$\mathbb{P}(\lambda_1(P_d \hat{\Sigma} P_d) - \lambda_1(P_d \Sigma P_d) > x) \leq \mathbb{P}(\|T_d \Delta T_d\|_\infty > 1) \quad (3.22)$$

with

$$T_d = \sum_{k > d} \frac{1}{\sqrt{\lambda_{d+1} - \lambda_k + x}} P_k.$$

Thus, as in (2.9), we consider $X' = T_d X$, satisfying Assumption 2.1 with the same constant $C_1$, and obtain the covariance operator

$$\Sigma' = T_d \Sigma T_d = \sum_{k > d} \frac{\lambda_k}{\lambda_{d+1} - \lambda_k + x} P_k.$$

Hence choosing

$$x' = \frac{1}{C_3 \lambda_1} = \frac{x}{C_3 \lambda_{d+1}},$$

the concentration inequality (3.19), applied to $\Delta' = T_d \Delta T_d$ and $x'$, gives

$$\mathbb{P}(\|T_d \Delta T_d\|_\infty > 1) \leq \exp\left(-n \min\left(\frac{x^2}{C_3 \lambda_{d+1}^2}, \frac{x}{C_3 \lambda_{d+1}}\right)\right) \quad (3.23)$$

in view of Condition (3.20). Combining (3.21)-(3.23), the claim follows.

It remains to prove Lemma 3.8. We have

$$\lambda_1((y - S)^{-1/2}(T - S)(y - S)^{-1/2}) \leq 1$$

if and only if (for a linear operator $L : \mathcal{H} \to \mathcal{H}$, we write $L \geq 0$ if $L$ is positive, i.e. if $\langle Lx, x \rangle \geq 0$ for all $x \in \mathcal{H}$)

$$(y - S)^{-1/2}(y - T)(y - S)^{-1/2} = I - (y - S)^{-1/2}(T - S)(y - S)^{-1/2} \geq 0.$$ 

Since $(y - S)^{-1/2}$ is self-adjoint and strictly positive, this is the case if and only if $y - T \geq 0$, that is $\lambda_1(T) \leq y$. A logical negation yields the assertion of the lemma. 

In view of the error decompositions (3.4) and (3.6), we want to apply Theorem 3.7 with $x = (\lambda_j - \lambda_{d+1})/2$, $j \leq d$. For this, we need the condition

$$\max \left(\frac{2C_3 \lambda_{d+1}}{\lambda_j - \lambda_{d+1}}, 1\right) \sum_{k > d} \frac{\lambda_k}{\lambda_j - \lambda_k} \leq n/(2C_3).$$

Simplifying the maximum yields:
3.9. Corollary. Grant Assumption 2.1 and let \( j \leq d \). Suppose that
\[
\frac{\lambda_j}{\lambda_j - \lambda_{d+1}} \sum_{k > d} \frac{\lambda_k}{\lambda_j - \lambda_k} \leq \frac{n}{(4C_3^2)}. \tag{3.24}
\]
Then
\[
\mathbb{P}\left( \hat{\lambda}_{d+1} - \lambda_{d+1} > \frac{\lambda_j}{2} - \lambda_{d+1} \right) \leq \exp\left( - \frac{n(\lambda_j - \lambda_{d+1})^2}{4C_3^2\lambda_j^2} \right). \tag{3.25}
\]

The corresponding left-deviation result for \( \hat{\lambda}_d \) is as follows.

3.10. Theorem. Grant Assumption 2.1. For all \( x > 0 \) satisfying
\[
\max \left( \frac{C_3\lambda_d}{x}, 1 \right) \sum_{j \leq d} \frac{\lambda_j}{\lambda_j - \lambda_d + x} \leq \frac{n}{C_3}, \tag{3.26}
\]
we have
\[
\mathbb{P}(\hat{\lambda}_d - \lambda_d < -x) \leq \exp\left( - n \min \left( \frac{x^2}{C_3^2\lambda_d^2}, \frac{x}{C_3\lambda_d} \right) \right),
\]
where \( C_3 \) is the constant in (3.19).

Proof. First, we apply the max-min characterisation of eigenvalues and obtain \( \lambda_d \geq \lambda_d(P_{\leq d}\Sigma P_{\leq d}) \). This gives
\[
\mathbb{P}(\hat{\lambda}_d - \lambda_d < -x) \leq \mathbb{P}(\lambda_d(P_{\leq d}\tilde{\Sigma}P_{\leq d}) - \lambda_d(P_{\leq d}\Sigma P_{\leq d}) < -x). \tag{3.27}
\]

Similar to Lemma 3.8, we have for self-adjoint, positive operators \( S, T \) on \( V_d = \text{span}(u_1, \ldots, u_d) \) and \( y < \lambda_d(S) \)
\[
\lambda_1((S - y)^{-1/2}(S - T)(S - y)^{-1/2}) \leq 1
\]
if and only if (for the operator partial ordering)
\[
(S - y)^{-1/2}(T - y)(S - y)^{-1/2} = I - (S - y)^{-1/2}(S - T)(S - y)^{-1/2} \geq 0.
\]
This is the case if and only if \( T - y \geq 0 \), that is \( \lambda_d(T) \geq y \).

Applying the negation of this equivalence to \( S = P_{\leq d}\Sigma P_{\leq d}, T = P_{\leq d}\tilde{\Sigma}P_{\leq d}, \) and \( y = \lambda_d(S) - x = \lambda_d - x \), we get
\[
\mathbb{P}(\lambda_d(P_{\leq d}\tilde{\Sigma}P_{\leq d}) - \lambda_d(P_{\leq d}\Sigma P_{\leq d}) < -x) \leq \mathbb{P}(\|T_{\leq d}\Delta T_{\leq d}\|_\infty > 1) \tag{3.28}
\]
with
\[
T_{\leq d} = \sum_{j \leq d} \frac{1}{\sqrt{\lambda_j - \lambda_d + x}} P_j.
\]
We consider \( X' = T_{\leq d}X \), satisfying Assumption 2.1 with the same constant \( C_1 \), and obtain the covariance operator
\[
\Sigma' = T_{\leq d}\Sigma T_{\leq d} = \sum_{j \leq d} \frac{\lambda_j}{\lambda_j - \lambda_d + x} P_j.
\]
Hence, noting that \( \lambda \mapsto \lambda/(\lambda - \lambda_d + x) \) is decreasing for \( \lambda \geq \lambda_d \), we choose
\[
x' = \frac{1}{C_3\lambda_1} = \frac{x}{C_3\lambda_d}.
\]
Then (3.19), applied to \( \Delta' = T_{\leq d} \Delta T_{\leq d} \) and \( x' \), gives
\[
\mathbb{P}(\|T_{\leq d} \Delta T_{\leq d}\|_\infty > 1) \leq \exp\left(-n \min\left(\frac{x^2}{C_3^2\lambda_1^2}, \frac{x}{C_3\lambda_d}\right)\right)
\]
in view of Condition (3.26). We conclude by (3.27)-(3.29). \( \square \)

In particular, choosing \( x = (\lambda_d - \lambda_k)/2 \), we get:

3.11. **Corollary.** Grant Assumption 2.1 and let \( k > d \). Suppose that
\[
\frac{\lambda_d}{\lambda_d - \lambda_k} \sum_{j \leq d} \frac{\lambda_j}{\lambda_j - \lambda_k} \leq n/(4C_3^2).
\]
Then
\[
\mathbb{P}(\hat{\lambda}_d - \lambda_d < -(\lambda_d - \lambda_k)/2) \leq 2 \exp\left(-\frac{n(\lambda_d - \lambda_k)^2}{4C_3^2\lambda_d^2}\right).
\]

4. **Proofs**

4.1. **Proof of Lemma 2.5** Inserting the spectral representation of \( \Sigma \), the excess risk can be written as
\[
\mathcal{E}_d^{PC} = \langle \Sigma, P_{\leq d} - \hat{P}_{\leq d} \rangle = \sum_{j \geq 1} \lambda_j \langle P_j, P_{\leq d} - \hat{P}_{\leq d} \rangle.
\]
By \( P_{\leq d} - \hat{P}_{\leq d} = \hat{P}_{>d} - P_{>d} \) we obtain
\[
\mathcal{E}_d^{PC} = \sum_{j \leq d} \lambda_j \langle P_j, \hat{P}_{>d} - P_{>d} \rangle - \sum_{k > d} \lambda_k \langle P_k, \hat{P}_{\leq d} - P_{\leq d} \rangle
\]
\[
= \sum_{j \leq d} \lambda_j \langle P_j, \hat{P}_{>d} \rangle - \sum_{k > d} \lambda_k \langle P_k, \hat{P}_{\leq d} \rangle.
\]
Moreover, the identity
\[
\langle P_{\leq d}, \hat{P}_{>d} \rangle = \langle P_{\leq d}, \hat{P}_{>d} - P_{>d} \rangle = -\langle P_{>d}, P_{\leq d} - \hat{P}_{\leq d} \rangle = \langle P_{>d}, \hat{P}_{\leq d} \rangle
\]
implies \( \sum_{j \leq d} \mu(P_j, \hat{P}_{>d}) = \sum_{k > d} \mu(P_k, \hat{P}_{\leq d}) \) and the claim follows. \( \square \)

4.2. **Proof of Theorem 2.6** Taking expectation in (3.4) and plugging in the bound \( n\mathbb{E}[\|P_j \Delta \hat{P}_{>d}\|_2^2] \leq n\mathbb{E}[\|P_j \Delta\|_2^2] \leq 2C_2\lambda_j \text{tr} \Sigma \) (with \( C_2 \) from (2.4)), we get
\[
\mathbb{E}[\mathcal{E}_d^{PC}^{\mu}(\mu)] \leq 8C_2 \sum_{j \leq r} (\lambda_j - \mu) \frac{\lambda_j \text{tr} \Sigma}{n(\lambda_j - \lambda_{d+1})^2} + \mathbb{E}_{j=r+1}^{d}(\lambda_j - \mu) \mathbb{P}(\hat{\lambda}_{d+1} - \lambda_{d+1} > (\lambda_j - \lambda_{d+1})/2).
\]
Hence, the first claim follows from the following lemma.
4.1. **Lemma.** Let \( j \leq d \). Then
\[
8C_2 \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2} + \mathbb{P}(\hat{\lambda}_{d+1} - \lambda_{d+1} > (\lambda_j - \lambda_{d+1})/2) \\
\leq (8C_2 + 4C_3^2) \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2}.
\]

**Proof of Lemma 4.1.** If
\[
\frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2} \leq 1/(4C_3^3),
\]
then Condition (3.24) is satisfied and we can apply (3.25). Thus, in this case, the left-hand side can be bounded by
\[
8C_2 \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2} + \exp \left( - \frac{n(\lambda_j - \lambda_{d+1})^2}{4C_3^3 \lambda_j^2} \right).
\]

Using the inequality \( x \exp(-x) \leq 1/e \leq 1/2 \), \( x \geq 0 \), this is bounded by
\[
(8C_2 + 2C_3^2) \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2}.
\]

On the other hand, if (4.1) is not satisfied, then the left-hand side can be bounded by
\[
8C_2 \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2} + 1 \leq (8C_2 + 4C_3^2) \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2}.
\]

Hence, we get the claim in both cases. \( \square \)

It remains to prove the second inequality. Taking expectation in (3.14) and plugging in the bound \( n\mathbb{E}[\|P_k \Delta \hat{P}_{<d}\|^2] \leq n\mathbb{E}[\|P_k \Delta \|^2] \leq 2C_2 \lambda_k \text{tr}(\Sigma) \), we get
\[
\mathbb{E} [S_{\geq d}^{PCA}(\mu)] \leq 8C_2 \sum_{k \geq l} (\mu - \lambda_k) \frac{\lambda_k \text{tr}(\Sigma)}{n(\lambda_d - \lambda_k)^2} + \sum_{k = (d+1) \lor (l-1)}^{l-1} \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2}
\]
\[
+ \sum_{k \geq l : \lambda_k > \lambda_d/2} (\mu - \lambda_k) \mathbb{P}(\hat{\lambda}_d - \lambda_d < -(\lambda_d - \lambda_k)/2)
\]
\[
+ d(\mu - \lambda_p) \mathbb{P}(\hat{\lambda}_d - \lambda_d < -\lambda_d/4).
\]

Consider the last term. Since \( d \leq n/(16C_3^2) \), Condition (3.26) is satisfied with \( x = \lambda_d/4 \) and we obtain
\[
\mathbb{P}(\hat{\lambda}_d - \lambda_d < -\lambda_d/4) \leq e^{-\frac{n}{16C_3^2}}.
\]

Using this and the bounds \( x \exp(-x) \leq (2/e) \exp(-x/2) \leq \exp(-x/2) \), \( x \geq 0 \), and \( d \leq n/(16C_3^2) \), we see that
\[
d \mathbb{P}(\hat{\lambda}_d - \lambda_d < -\lambda_d/4) \leq de^{-\frac{n}{16C_3^2}} \leq e^{-\frac{n}{32C_3^2}}.
\]
This gives the desired bound for the last term. Now, the second inequality of the theorem follows from the lemma below.

4.2. **Lemma.** Let \( k > d \) be such that \( \lambda_k \geq \lambda_d/2 \). Then

\[
8C_2 \frac{\lambda_k \operatorname{tr}(\Sigma)}{n(\lambda_d - \lambda_k)^2} + \mathbb{P}(\hat{\lambda}_d - \lambda_d < -(\lambda_d - \lambda_k)/2) \\
\leq (8C_2 + 8C_2^3) \frac{\lambda_k \operatorname{tr}(\Sigma)}{n(\lambda_d - \lambda_k)^2}.
\]

**Proof of Lemma 4.2.** If

\[
\frac{\lambda_d \operatorname{tr}(\Sigma)}{n(\lambda_d - \lambda_k)^2} \leq 1/(4C_2^3),
\]

then Condition (3.30) is satisfied and we can apply (3.31). Thus, in this case, the left-hand side can be bounded by

\[
8C_2 \frac{\lambda_k \operatorname{tr}(\Sigma)}{n(\lambda_d - \lambda_k)^2} + \exp\left(\frac{-n(\lambda_d - \lambda_k)^2}{4C_2^3 \lambda_d^2}\right).
\]

Using the inequality \( x \exp(-x) \leq 1/e \leq 1/2, \ x \geq 0 \), this is bounded by

\[
8C_2 \frac{\lambda_k \operatorname{tr}(\Sigma)}{n(\lambda_d - \lambda_k)^2} + \frac{2C_2^3 \lambda_d^2}{n(\lambda_d - \lambda_k)^2} \leq (8C_2 + 4C_2^3) \frac{\lambda_k \operatorname{tr}(\Sigma)}{n(\lambda_d - \lambda_k)^2},
\]

where we applied the bound \( \lambda_d/2 \leq \lambda_k \) in the second inequality. On the other hand, if (4.2) is not satisfied, then the left-hand side can be bounded by

\[
8C_2 \frac{\lambda_k \operatorname{tr}(\Sigma)}{n(\lambda_d - \lambda_k)^2} + 1 \leq (8C_2 + 8C_2^3) \frac{\lambda_k \operatorname{tr}(\Sigma)}{n(\lambda_d - \lambda_k)^2},
\]

where we again applied the bound \( \lambda_d/2 \leq \lambda_k \). Hence, we get the claim in both cases. \( \square \)

4.3. **Proof of Corollary 2.8.** In Corollary 2.7, only summands with \( \lambda_j > \lambda_{d+1} \) and \( \lambda_k < \lambda_l \), respectively, appear. Neglecting the minimum with \( \lambda_j - \lambda_{d+1} \) (resp. \( \lambda_d - \lambda_k \)) in each summand, the local bound follows.

For the global bound use the inequality \( \min(a/x, x) \leq \sqrt{a} \) for \( a, x \geq 0 \) to obtain from Corollary 2.7

\[
\mathbb{E}[\mathcal{E}_{\leq d}^{\text{PCA}}(\mu)] \leq \sum_{j \leq d} \sqrt{C\lambda_j \operatorname{tr}(\Sigma)}.
\]

Considering \( \mathcal{E}_{>d}^{\text{PCA}}(\mu) \), the value \( l \) in Theorem 2.6 has to be chosen carefully. For \( a > 0 \) let \( d < l = l(a) \leq p + 1 \) be the index such that \( \lambda_d - \lambda_k \geq a \) for \( k \geq l \) and \( \lambda_d - \lambda_k < a \) for \( d < k < l \). Then the second inequality of Theorem 2.6 with \( \mu \leq \lambda_d \) implies the upper bound

\[
\sum_{k > d} \frac{C\lambda_k \operatorname{tr}(\Sigma)}{na} + da + \lambda_d e^{-\frac{n}{4C_2}},
\]
Minimizing over $a > 0$ and incorporating the remainder in the summand for $j = d$ gives the global bound in (2.10).

4.4. **Proof of Theorem 2.9.** Theorem 2.9 follows from taking expectation in (3.6) with $\mu = \lambda_{d+1}$. We begin with two preliminary lemmas. Proceeding as in the proof of Lemma 4.1, we have:

4.3. **Lemma.** Let $j \leq s \leq d$. Then

$$16C_2 \frac{\lambda_j \text{tr}_s(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2} + 2\mathbb{P}(\hat{\lambda}_d - \lambda_d > (\lambda_j - \lambda_{d+1})/2)$$

$$\leq (16C_2 + 8C^2_3) \frac{\lambda_j \text{tr}_s(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2}.$$

(4.3)

**Proof.** If

$$\frac{\lambda_j \text{tr}_s(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2} \leq 1/(4C^2_3),$$

(4.4)

then the Condition (3.24) is satisfied and the left-hand side of (4.3) can be bounded by

$$16C_2 \frac{\lambda_j \text{tr}_s(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2} + 2 \exp\left(-n \min\left(\frac{(\lambda_j - \lambda_{d+1})^2}{4C^2_3\lambda^2_{d+1}}, \frac{\lambda_j - \lambda_{d+1}}{2}\right)\right)$$

$$\leq (16C_2 + 8C^2_3) \frac{\lambda_j \text{tr}_s(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2}.$$

where we used the bounds $x \exp(-x) \leq 1/e \leq 1/2$ and $x^2 \exp(-x) \leq 4/e^2 \leq 1$. On the other hand, if (4.4) is not satisfied, then (4.3) can be bounded by

$$16C_2 \frac{\lambda_j \text{tr}_s(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2} + 2 \leq (16C_2 + 8C^2_3) \frac{\lambda_j \text{tr}_s(\Sigma)}{n(\lambda_j - \lambda_{d+1})^2}.$$

This completes the proof.

Since we will apply the Cauchy-Schwarz inequality to the remainder term, we will also need the following bound on the $L^2$-norm.

4.4. **Lemma.** For all $r \leq d$, we have

$$\left(\mathbb{E}\left[\left(\sum_{j \leq r} \frac{\|P_j \Delta\|_2^2}{\lambda_j - \lambda_{d+1}}\right)^2\right]\right)^{1/2} \leq C \sum_{j \leq r} \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})}.$$

**Proof.** By the Minkovski inequality, the left-hand side is bounded by

$$\sum_{j \leq r} \frac{\mathbb{E}\left[\|P_j \Delta\|_2^2\right]}{\lambda_j - \lambda_{d+1}}^{1/2}.$$

(4.5)

By Assumption 2.1 there is a constant $C$ depending only on $C_1$ such that

$$\left(\mathbb{E}\left[\|P_j \Delta P_k\|_2^2\right]\right)^{1/2} \leq C \frac{\lambda_j \lambda_k}{n}.$$
Thus, by the Minkovski inequality,
\[
\left( \mathbb{E} \left[ \|P_j \Delta\|_2^4 \right] \right)^{1/2} \leq C \frac{\lambda_j \text{tr}(\Sigma)}{n}.
\]
Plugging this into (4.5), the claim follows. \qed

Now let us finish the proof of Theorem 2.9. Taking expectation in (3.6) and using Lemma 4.3, we obtain
\[
\mathbb{E} [\mathcal{E}_{\leq d}^{PCA}(\mu)] \leq (16C_2 + 8C_3^2) \sum_{j \leq r} \frac{\lambda_j \text{tr}_{>s}(\Sigma)}{n(\lambda_j - \lambda_{d+1})} + 2 \sum_{r < j \leq d} (\lambda_j - \lambda_{d+1})
\]
\[
+ 8 \mathbb{E} \left[ \sum_{j \leq r} \frac{\|P_j \Delta\|_2^2}{\lambda_j - \lambda_{d+1}} 1(\|S_{\leq s} \Delta S_{\leq s}\|_\infty > 1/16) \right].
\]

If Condition (2.11) holds, then Corollary 3.6 (with \( \mu = \lambda_{d+1} \)) gives
\[
\mathbb{P} (\|S_{\leq s} \Delta S_{\leq s}\|_\infty > 1/16) \leq \exp \left( - \frac{n(\lambda_s - \lambda_{d+1})^2}{256C_3^2 \lambda_s^2} \right). \tag{4.6}
\]
Thus the claim follows from applying the Cauchy-Schwarz inequality, Lemma 4.4, and (4.6) to the remainder term. \qed

4.5. Proof of Corollary 2.10. By assumption, we have \( \frac{\lambda_j - \lambda_{d+1}}{\lambda_j - \lambda_p} \geq c_1 \) for all \( j \leq d \). Thus, Lemma 2.5 applied with \( \mu = \lambda_p \) yields
\[
\mathcal{E}_{d}^{PCA} \leq \sum_{j \leq d} (\lambda_j - \lambda_p) \langle P_j, \hat{P}_{>d} \rangle
\]
\[
\leq c_1^{-1} \sum_{j \leq d} (\lambda_j - \lambda_{d+1}) \langle P_j, \hat{P}_{>d} \rangle = c_1^{-1} \mathcal{E}_{d}^{PCA}(\lambda_{d+1}). \tag{4.7}
\]
The local bound now follows from Theorem 2.9 applied with \( r = s = d \). In order to prove the global bound, we begin with the following lemma.

4.5. Lemma. Let \( s \leq d \) be the largest number such that Condition (2.11) is satisfied (and \( s = 0 \) if such a number does not exist). Then we have
\[
\frac{\lambda_{s+1} - \lambda_{d+1}}{\lambda_{s+1}} \leq 256C_3^2 \sum_{j \leq s} \frac{\lambda_j}{n(\lambda_j - \lambda_{d+1})} + \frac{16\sqrt{2}C_3}{\sqrt{n}}, \tag{4.8}
\]
\[
\sum_{s < j \leq d} (\lambda_j - \lambda_{d+1}) \leq 256C_3^2 \sum_{j \leq s} \frac{\lambda_j \text{tr}_{>s}(\Sigma)}{n(\lambda_j - \lambda_{d+1})} + \sum_{s < j \leq d} \frac{16\sqrt{2}C_3\lambda_j}{\sqrt{n}}. \tag{4.9}
\]

Proof. We start with (4.8). If Condition (2.11) does not hold for \( s + 1 \), then we have
\[
\frac{\lambda_{s+1} - \lambda_{d+1}}{\lambda_{s+1}} \leq 256C_3^2 \sum_{j \leq s+1} \frac{\lambda_j}{n(\lambda_j - \lambda_{d+1})},
\]
Multiplying both sides by \((\lambda_{s+1} - \lambda_{d+1})/\lambda_{s+1}\), we obtain
\[
\left(\frac{\lambda_{s+1} - \lambda_{d+1}}{\lambda_{s+1}}\right)^2 < \left(\frac{\lambda_{s+1} - \lambda_{d+1}}{\lambda_{s+1}}\right) 256C_3^2 \sum_{j \leq s} \frac{\lambda_j}{n(\lambda_j - \lambda_{d+1})} + \frac{256C_3^2}{n}.
\]
Using that for \(x, a, b \geq 0\) the inequality \(x^2 \leq ax + b\) implies \(x^2 \leq a^2 + 2b\), which in turn implies \(x \leq a + \sqrt{2b}\), we obtain (4.8). For (4.9) note that (4.8) yields
\[
\frac{\lambda_k - \lambda_{d+1}}{\lambda_k} \leq \frac{\lambda_{s+1} - \lambda_{d+1}}{\lambda_{s+1}} < 256C_3^2 \sum_{j \leq s} \frac{\lambda_j}{n(\lambda_j - \lambda_{d+1})} + \frac{16\sqrt{2}C_3}{\sqrt{n}}
\]
for all \(s < k \leq d\). Thus
\[
\sum_{s<k \leq d} (\lambda_k - \lambda_{d+1}) \leq 256C_3^2 \sum_{s<k \leq d} \sum_{j \leq s} \frac{\lambda_j \lambda_k}{n(\lambda_j - \lambda_{d+1})} + \sum_{s<k \leq d} \frac{16\sqrt{2}C_3 \lambda_k}{\sqrt{n}}
\]
\[
\leq 256C_3^2 \sum_{j \leq s} \frac{\lambda_j \text{tr}_{>s}(\Sigma)}{n(\lambda_j - \lambda_{d+1})} + \sum_{s<k \leq d} \frac{16\sqrt{2}C_3 \lambda_k}{\sqrt{n}}.
\]
This completes the proof.

Now let us finish the proof of of the global bound. Set
\[
A = \text{tr}_{>s}(\Sigma) + \text{tr}(\Sigma) \exp \left(-\frac{nC_3^2(\lambda_s - \lambda_p)^2}{256C_3^2\lambda_d^2}\right)
\]
and let \(j_0 \leq d\) be the unique number such that
\[
\frac{\lambda_j A}{n(\lambda_j - \lambda_{d+1})^2} \leq 1 \iff j \leq j_0
\]
(and \(j_0 = 0\) if such a number does not exist) If \(s \leq j_0\), then Theorem 2.9 with \(r = s\) and (4.9) give
\[
\mathbb{E} \left[\mathcal{E}^{PCA}_{\leq d}(\lambda_{d+1})\right] \leq C \sum_{j \leq s} \frac{\lambda_j A}{n(\lambda_j - \lambda_{d+1})} + 2 \sum_{s<j \leq d} (\lambda_j - \lambda_{d+1})
\]
\[
\leq (C + 512C_3^2) \sum_{j \leq s} \frac{\lambda_j A}{n(\lambda_j - \lambda_{d+1})} + \sum_{s<j \leq d} \frac{32\sqrt{2}C_3 \lambda_j}{\sqrt{n}}.
\]
From \(s \leq j_0\) we infer
\[
\frac{\lambda_j A}{n(\lambda_j - \lambda_{d+1})^2} \leq 1
\]
for all \(j \leq s\). Using this and for \(a, x \geq 0\) the implication \(a/x^2 \leq 1 \Rightarrow a/x \leq \sqrt{a}\), we find
\[
\mathbb{E} \left[\mathcal{E}^{PCA}_{\leq d}(\lambda_{d+1})\right] \leq (C + 512C_3^2) \sum_{j \leq s} \sqrt{\frac{\lambda_j A}{n}} + \sum_{s<j \leq d} \frac{32\sqrt{2}C_3 \lambda_j}{\sqrt{n}}. \quad (4.11)
\]
On the other hand, if \( s > j_0 \), then applying Theorem 2.9 with \( r = j_0 \) yields

\[
\mathbb{E} \left[ \mathcal{E}_{d}^{\text{PCA}}(\lambda_{d+1}) \right] \leq C \sum_{j \leq j_0} \frac{\lambda_j A}{n(\lambda_j - \lambda_{d+1})} + 2 \sum_{j_0 < j \leq d} (\lambda_j - \lambda_{d+1})
\]

\[
\leq C \sum_{j \leq d} \sqrt{\frac{\lambda_j A}{n}}
\]

(4.12)

with \( C > 2 \). Plugging the definition of \( A \) into (4.11) and (4.12), the claim follows from (4.7) and the inequality \( \sqrt{x + y} \leq \sqrt{x} + \sqrt{y}, \; x, y \geq 0 \). \( \square \)

4.6. Proof of Corollary 2.11. Similarly as in (4.7), we have

\[
\mathcal{E}_{d}^{\text{PCA}} \leq \sum_{j \leq d} \lambda_j \langle P_j, \hat{P}_d \rangle \leq \frac{\lambda_s}{\lambda_s - \lambda_{d+1}} \sum_{j \leq s} (\lambda_j - \lambda_{d+1}) \langle P_j, \hat{P}_d \rangle + \text{tr}_{>s}(\Sigma).
\]

(4.13)

By (3.9) and (3.13) with \( \mu = \lambda_{d+1} \) and \( r = s \), we have

\[
\sum_{j \leq s} (\lambda_j - \lambda_{d+1}) \langle P_j, \hat{P}_d \rangle \leq 16 \sum_{j \leq s} \frac{\|P_j \Delta \|_2^2}{\lambda_j - \lambda_{d+1}}
\]

\[
+ 2 \sum_{j \leq s} (\lambda_j - \lambda_{d+1}) \mathbb{1} (\hat{\lambda}_{d+1} - \lambda_{d+1} > (\lambda_j - \lambda_{d+1})/2)
\]

\[
+ 8 \sum_{j \leq s} \frac{\|P_j \Delta \|_2^2}{\lambda_j - \lambda_{d+1}} \mathbb{1} (\|S_{\leq s} \Delta S_{\leq s}\|_{\infty} > 1/16).
\]

As shown in the proof of Theorem 2.9, the inequality

\[
\mathbb{E} \left[ \sum_{j \leq s} (\lambda_j - \lambda_{d+1}) \langle P_j, \hat{P}_d \rangle \right] \leq C \sum_{j \leq s} \frac{\lambda_j \text{tr}_{>s}(\Sigma)}{n(\lambda_j - \lambda_{d+1})} + R
\]

holds with remainder term \( R \) given in Theorem 2.9 with \( r = s \). Thus

\[
\mathbb{E} [\mathcal{E}_{d}^{\text{PCA}}] \leq C \frac{\lambda_s}{\lambda_s - \lambda_{d+1}} \sum_{j \leq s} \frac{\lambda_j \text{tr}_{>s}(\Sigma)}{n(\lambda_j - \lambda_{d+1})} + \text{tr}_{>s}(\Sigma)
\]

\[
+ C \frac{\lambda_s}{\lambda_s - \lambda_{d+1}} \sum_{j \leq s} \frac{\lambda_j \text{tr}(\Sigma)}{n(\lambda_j - \lambda_{d+1})} \exp \left( - \frac{n(\lambda_s - \lambda_{d+1})^2}{256C_3^2 \lambda_s^2} \right)
\]

\[
\leq C \text{tr}_{>s}(\Sigma) + C \text{tr}(\Sigma) \exp \left( - \frac{n(\lambda_s - \lambda_{d+1})^2}{256C_3^2 \lambda_s^2} \right),
\]

where we have used Condition 2.11 in the last inequality. \( \square \)
Appendix A. Proof of Proposition 2.13

We begin by recalling the following asymptotic result from multivariate analysis. By [10, Proposition 5], we have
\[
\sqrt{n} \Delta = \sqrt{n} \Delta_n \xrightarrow{d} L = \sum_{j=1}^{p} \sum_{k=1}^{p} \sqrt{\lambda_j \lambda_k} \xi_{jk} (u_j \otimes u_k), \quad (A.1)
\]
where the upper triangular coefficients \(\xi_{jk}, k \geq j\) are independent and centered Gaussian random variables, with variance 1 for \(k > j\) and variance 2 for \(k = j\). The lower triangular coefficients \(\xi_{jk}, k < j\) are determined by \(\xi_{jk} = \xi_{kj}\).

For \(l = 1, \ldots, p\), let \(I_l = \{j : \lambda_j = \lambda_l\}\),
\[Q_l = \sum_{j \in I_l} P_j, \quad \text{and} \quad \hat{Q}_l = \sum_{j \in I_l} \hat{P}_j.\]

For \(l \geq 1\), we have
\[Q_l L Q_l = \lambda_l \sum_{j, k \in I_l} \xi_{jk} (u_j \otimes u_k)\]
and the random matrix
\[M_l = (\xi_{jk})_{j, k \in I_l}\]
is a GOE matrix. It is well known (see e.g. [28]) that the eigenvalues of \(M_l\) (in decreasing order) have a joint density with respect to the Lebesgue measure on \(\mathbb{R}_{\geq 0}^{m_l}\), where \(m_l = |I_l|\), and that the matrix of the corresponding eigenvectors is distributed according to the Haar measure on the orthogonal group \(O(m_l)\). It is easy to see that \(M_l\) and \(Q_l L Q_l\) have the same non-zero eigenvalues and that a matrix of eigenvectors of \(M_l\) gives the coefficients of a basis of eigenvectors of \(Q_l L Q_l\) with respect to the basis \((u_j)_{j \in I_l}\).

In particular, with probability 1, \(Q_l L Q_l\) has rank \(m_l\) and all \(m_l\) non-zero eigenvalues are distinct. Let \((P_{j}^{\text{Haar}})_{j \in I_l}\) denote the corresponding spectral projectors (ordered such that the orthogonal projection onto the eigenvector corresponding to the largest non-zero eigenvalue appears first, and so forth). The following key observation is proved below.

**A.1. Lemma.** We have
\[(\sqrt{n} \Delta, \hat{P}_1, \ldots, \hat{P}_p) \xrightarrow{d} (L, P_{1}^{\text{Haar}}, \ldots, P_{p}^{\text{Haar}}).\]

Lemma A.1 implies Proposition 2.13. By Lemma 2.5 and Lemma 3.1, we have
\[
\mathcal{E}_{d,n}^{\text{PCA}} = \sum_{j < d, k > d : \lambda_j > \lambda_d} (\lambda_j - \lambda_d) \frac{\|P_j \Delta \hat{P}_k\|^2}{(\lambda_j - \lambda_k)^2} + \sum_{j < d, k > d : \lambda_k < \lambda_d} (\lambda_d - \lambda_k) \frac{\|P_k \Delta \hat{P}_j\|^2}{(\lambda_j - \lambda_k)^2}. \quad (A.2)
\]
Using Lemma A.1 (A.2), the fact that \( \hat{\lambda}_l \xrightarrow{a.s.} \lambda_l \) for all \( l \) (see [10, Proposition 2]), and the continuous mapping theorem, we thus conclude that

\[
\begin{align*}
\frac{P_jLP_k}{\lambda_j - \lambda_k} & \xrightarrow{d} \sum_{j \leq d, k > d} \frac{\|P_jLP_k\|_2^2}{\lambda_j - \lambda_k} \\
+ \sum_{j \leq d, k > d} (\lambda_j - \lambda_d) \frac{\|P_jLP^{Haar}_k\|_2^2}{(\lambda_j - \lambda_k)^2} \\
+ \sum_{j \leq d, k > d} (\lambda_d - \lambda_k) \frac{\|P_kLP^{Haar}_j\|_2^2}{(\lambda_j - \lambda_k)^2},
\end{align*}
\]

where we also used the identities \( \sum_{j \in I_l} P^{Haar}_j = Q_l = \sum_{j \in I_l} P_j \) in the first summand of the limit. Further, note that the tuple \( (P^{Haar}_j)_{j \in I_d} \) is independent of \( \{P_jLP_k : \lambda_j \neq \lambda_d \text{ or } \lambda_k \neq \lambda_d\} \). Hence, the random variables \( \|P_jLP_k\|_2^2/\lambda_j \lambda_k \), \( \|P_jLP^{Haar}_k\|_2^2/\lambda_j \lambda_k \), and \( \|P_kLP^{Haar}_j\|_2^2/\lambda_j \lambda_k \) appearing in the above sums are independent and chi-square distributed. This gives Proposition 2.13. It remains to prove Lemma A.1.

**Proof of Lemma A.1.** Let \( I \subseteq \{1, \ldots, p\} \) be a subset which contains for each \( l \geq 1 \) exactly one element of \( I_l \). Then we have

\[
(\sqrt{n} \Delta, (Q_l \sqrt{n} \Delta Q_l)_{l \in I}) \xrightarrow{d} (L, (Q_lLQ_l)_{l \in I}).
\]

In [10] Section 2.2.1, it is shown that for each \( l \in I \),

\[
\hat{Q}_l \sqrt{n}(\hat{\Sigma} - \lambda_l I)\hat{Q}_l - Q_l \sqrt{n} \Delta Q_l \xrightarrow{p} 0. \tag{A.3}
\]

By Slutsky’s lemma, we thus have

\[
(\sqrt{n} \Delta, (\hat{Q}_l \sqrt{n}(\hat{\Sigma} - \lambda_l I)\hat{Q}_l)_{l \in I}) \xrightarrow{d} (L, (Q_lLQ_l)_{l \in I}). \tag{A.4}
\]

We now apply the continuous mapping theorem. For \( l \in I \), let \( h_l \) be a mapping sending a symmetric \( p \times p \) matrix of rank \( m_l \) to the spectral projectors corresponding to the \( m_l \) non-zero eigenvalues (ordered such that the orthogonal projection onto the eigenvector corresponding to the largest non-zero eigenvalue appears first, and so forth). Note that this map is uniquely determined and continuous if restricted to the open subset of symmetric matrices of rank \( m_l \) having distinct non-zero eigenvalues. As already argued above, with probability 1, \( Q_lLQ_l \) has rank \( m_l \) and all \( m_l \) non-zero eigenvalues are distinct. Moreover, since \( X \) is Gaussian, the same is true for \( Q_l \sqrt{n}(\hat{\Sigma} - \lambda_l I)\hat{Q}_l \). Thus, the claim follows from [5] Theorem 2.7] applied to \( h = (I, (h_l)_{l \in I}) \). \( \square \)
In this complementary section, we show that linear expansions of $\hat{P}_{>d}$ and $\hat{P}_{\leq d}$ may lead to tight bounds for the excess risk as well as for the Hilbert-Schmidt distance if stronger eigenvalue conditions are satisfied (including $\lambda_d > \lambda_{d+1}$). In particular, these bounds lead up to a constant to the exact leading terms which appeared in the asymptotic results in (2.20) and Proposition 2.13. Note that it is possible to derive higher order expansions by similar, but more tedious considerations.

Proceeding as in Section 3.2, we get the following deterministic upper bound for the excess risk.

**B.1. Proposition.** We have

$$\mathcal{E}_{d}^{PCA} \leq 32 \sum_{j \leq d} \sum_{k > d} \frac{\|P_j \Delta P_k\|^2}{\lambda_j - \lambda_k} + 128 \sum_{j \leq d} \frac{1}{\lambda_j - \lambda_{d+1}} \left\| \sum_{k > d} \frac{P_j \Delta P_k \Delta P_{>d}}{\lambda_j - \lambda_k} \right\|^2 + 128 \sum_{k > d} \frac{1}{\lambda_d - \lambda_k} \left\| \sum_{j \leq d} \frac{P_k \Delta P_j \Delta P_{\leq d}}{\lambda_j - \lambda_k} \right\|^2 + R_1 + R_2,$$

where the remainder terms $R_1$ and $R_2$ are given in (B.4) and (B.5) below, respectively.

Similarly, we have the following result for the Hilbert-Schmidt distance.

**B.2. Proposition.** On the event $\{\hat{\lambda}_{d+1} - \lambda_{d+1} \leq (\lambda_d - \lambda_{d+1})/2\}$ we have

$$\|P_{\leq d} - \hat{P}_{\leq d}\|_2^2 \leq 4 \sum_{j \leq d} \sum_{k > d} \frac{\|P_j \Delta P_k\|^2}{(\lambda_j - \lambda_k)^2} + 64 \sum_{j \leq d} \frac{1}{(\lambda_j - \lambda_{d+1})^2} \left\| \sum_{k > d} \frac{P_j \Delta P_k \Delta P_{>d}}{\lambda_j - \lambda_k} \right\|^2 + 32 \|S_{\leq d} \Delta S_{\leq d}\|_\infty^2 \mathcal{E}_{d}^{PCA} + 32 \|S_{\leq d} \Delta S_{\leq d}\|_\infty^2 \mathcal{E}_{d}^{PCA},$$

with $S_{\leq d} = S_{\leq d}(\lambda_{d+1})$ from (3.5) and $\mathcal{E}_{d}^{PCA} = \mathcal{E}_{d}^{PCA}(\lambda_{d+1})$.

Similarly as in Section 2.3, we can take expectation in Propositions B.1 and B.2. Since this leads to lengthy remainder terms, we only discuss the case of the Hilbert-Schmidt distance. In fact, the third and the last term can be bounded by using the Cauchy-Schwarz inequality and the fact that bounds of the same order as presented in Theorems 2.6 and 2.9 can be derived for the $L^2$-norm of $\mathcal{E}_{d}^{PCA}$ (see also the comment after Theorem 2.6).
Moreover, by [17, Corollary 2], we have under Assumption 2.1
\[
\left( \mathbb{E} \left[ \| S_{\leq d} \Delta S_{\leq d} \|^4_{\infty} \right] \right)^{1/2} \leq C \max \left( \frac{\lambda_d}{\lambda_d - \lambda_{d+1}}, \left( \sum_{j \leq d} \frac{\lambda_j}{n(\lambda_j - \lambda_{d+1})} \right)^2 \right).
\]

Let us apply Proposition B.2 in the case where the eigenvalue have exponential or polynomial decay. First, under exponential decay (2.12), we obtain
\[
\mathbb{E}[\| P_{\leq d} - \hat{P}_{\leq d} \|^2] \leq C \frac{1}{n} + C \frac{d^2}{n} + Ce^{-n/C},
\]
provided that \( d \leq cn \), where \( c, C > 0 \) are constants depending only on \( C_1 \) and \( \alpha \). This result can be compared to the non-asymptotic results by Mas and Ruymgaart [23] and Koltchinskii and Lounici [16], who used perturbation theory for linear operators. [23, Theorem 5] says that
\[
\mathbb{E}[\| (P_{\leq d} - \hat{P}_{\leq d})u \|^2] \leq C \frac{d^2 \log^2 n}{n}
\]
for all \( d \geq 2 \), \( n \geq 2 \), and certain unit vectors \( u \). Moreover, applying [16, Lemma 2], we have
\[
\mathbb{E}[\| \hat{P}_{\leq d} - P_{\leq d} \|^2] \leq C \frac{1}{n} + C \frac{d e^{5\alpha d}}{n^2}.
\]
For the remainder term to be small, this requires \( n^2 \) to be much larger than \( e^{5\alpha d} \), which our analysis avoids.

Second, under polynomial decay (2.13), we obtain
\[
\mathbb{E}[\| P_{\leq d} - \hat{P}_{\leq d} \|^2] \leq C \frac{d^2 \log d}{n} + C \frac{d^5 \log^2 d}{n} + C \frac{d^7 \log^4 d}{n^3} + Ce^{-\frac{n}{c^2d}},
\]
provided that \( d^2 \log d \leq cn \), where \( c, C > 0 \) are constants depending only on \( C_1 \) and \( \alpha \). Compared to [23, Theorem 5], where the order \( (d^2 \log^2 n \log^2 d)/n \) is derived, this bound improves upon the \( \log^2 n \)-factor, but involves a remainder which might be harmful for \( d^3/n \) large, but \( d^2/n \) small. For this case higher order than linear expansions can extend the domain where the bound \( (d^2 \log d)/n \) holds. Our aim being to provide very general bounds and methodology, this derivation is not pursued here.

**Proof of Proposition B.1**. We start with \( \mathcal{E}^{PCA}_{\leq d} = \mathcal{E}^{PCA}_{\leq d}(\lambda_{d+1}). \) By (3.11), we have
\[
\mathcal{E}^{PCA}_{\leq d} = \sum_{j \leq d} (\lambda_j - \lambda_{d+1})\|P_j \hat{P}_{>d}\|^2_2 = \|R_{\leq d} \hat{P}_{>d}\|^2_2.
\]
with \( R_{\leq d} = R_{\leq d}(\lambda_{d+1}) \) from (3.10). In the proof of Lemma 3.2 we have also shown that
\[
P_j \hat{P}_{>d} = \sum_{k > d} \frac{P_j \Delta P_k \hat{P}_{>d}}{\lambda_j - \lambda_k} + \sum_{t > d} \frac{P_j \Delta P_{\leq d} \hat{P}_t}{\lambda_j - \lambda_t} - \sum_{k > d} \sum_{t > d} \frac{P_j \Delta P_k \Delta \hat{P}_t}{(\lambda_j - \lambda_t)(\lambda_j - \lambda_k)}.
\]
Inserting this into the second term in (B.1) and applying the triangle inequality twice, we obtain

\[
E_{PCA}^{d} \leq 4 \sum_{j \leq d} (\lambda_{j} - \lambda_{d+1}) \left\| \sum_{k > d} \frac{P_{j} \Delta P_{k}}{\lambda_{j} - \lambda_{k}} \right\|^{2} + 2 \sum_{j \leq d} (\lambda_{j} - \lambda_{d+1}) \left\| \sum_{l > d} \frac{P_{j} \Delta P_{l}}{\lambda_{j} - \lambda_{l}} \right\|^{2} + 4 \sum_{j \leq d} (\lambda_{j} - \lambda_{d+1}) \left\| \sum_{k > d} \sum_{l > d} \frac{P_{j} \Delta P_{k} \Delta P_{l}}{(\lambda_{j} - \lambda_{l}) (\lambda_{j} - \lambda_{k})} \right\|^{2}.
\]

Thus

\[
E_{PCA}^{d} \leq 4 \sum_{j \leq d} \sum_{k > d} \frac{(\lambda_{j} - \lambda_{d+1})}{(\lambda_{j} - \lambda_{k})^{2}} \| P_{j} \Delta P_{k} \|^{2} + 8 \sum_{j \leq d} \sum_{l > d} \frac{(\lambda_{j} - \lambda_{d+1})}{(\lambda_{j} - \lambda_{d+1})^{2}} \| P_{j} \Delta P_{l} \|^{2} + 16 \sum_{j \leq d} \sum_{l > d} \frac{(\lambda_{j} - \lambda_{d+1})}{(\lambda_{j} - \lambda_{l})^{2}} \left\| \sum_{k > d} \frac{P_{j} \Delta P_{k} \Delta P_{l}}{\lambda_{j} - \lambda_{k}} \right\|^{2} + \sum_{j \leq d} (\lambda_{j} - \lambda_{d+1}) (\hat{\lambda}_{d+1} - \lambda_{d+1} > (\lambda_{j} - \lambda_{d+1})/2).
\]

Using the operator \( S_{\leq d} = S_{\leq d}(\lambda_{d+1}) \) from (3.5), the second term on the right-hand side of (B.3) is equal to

\[
8 \| S_{\leq d} \Delta P_{\leq d} \hat{P}_{> d} \|^{2} = 8 \| S_{\leq d} \Delta S_{\leq d} S_{\leq d} R_{\leq d} \hat{P}_{> d} \|^{2}
\]

which can be bounded by

\[
\| R_{\leq d} \hat{P}_{> d} \|^{2} / 2 + 8 \| S_{\leq d} \Delta P_{\leq d} \|^{2} (\| S_{\leq d} \Delta S_{\leq d} \|_{\infty} > 1/16) = \mathcal{E}_{PCA}^{d} / 2 + 8 \| S_{\leq d} \Delta P_{\leq d} \|^{2} (\| S_{\leq d} \Delta S_{\leq d} \|_{\infty} > 1/16).
\]

Similarly, the third term on the right-hand side of (B.3) is bounded via

\[
16 \sum_{j \leq d} \sum_{l > d} \frac{1}{\lambda_{j} - \lambda_{d+1}} \left\| \sum_{k > d} \frac{P_{j} \Delta P_{k} \Delta P_{l}}{\lambda_{j} - \lambda_{k}} \right\|^{2}
\]

\[
= 16 \sum_{j \leq d} \frac{1}{\lambda_{j} - \lambda_{d+1}} \left\| \sum_{k > d} \frac{P_{j} \Delta P_{k} \Delta P_{> d}}{\lambda_{j} - \lambda_{k}} \right\|^{2}
\]

\[
\leq 32 \sum_{j \leq d} \frac{1}{\lambda_{j} - \lambda_{d+1}} \left\| \sum_{k > d} \frac{P_{j} \Delta P_{k} \Delta P_{> d}}{\lambda_{j} - \lambda_{k}} \right\|^{2}
\]
\[ + 32 \sum_{j \leq d} \frac{1}{\lambda_j - \lambda_{d+1}} \left\| \sum_{k > d} \frac{P_j \Delta P_k \Delta S_{\leq d} R_{\leq d} \hat{P}_{> d}}{\lambda_j - \lambda_k} \right\|_2^2 \]

and the last term can be bounded by
\[
\mathcal{E}_{\leq d}^{\text{PCA}} / 4 + 32 \sum_{j \leq d} \frac{1}{\lambda_j - \lambda_{d+1}} \left\| \sum_{k > d} \frac{P_j \Delta P_k \Delta P_{\leq d}}{\lambda_j - \lambda_k} \right\|_2^2 1_{\mathcal{E}_1}
\]

with
\[
\mathcal{E}_1 = \left\{ \sum_{j \leq d} \frac{1}{\lambda_j - \lambda_{d+1}} \left\| \sum_{k > d} \frac{P_j \Delta P_k \Delta S_{\leq d}}{\lambda_j - \lambda_k} \right\|_2 > 1/128 \right\}.
\]

Inserting these bounds into (B.3), we obtain
\[
\mathcal{E}_{\leq d}^{\text{PCA}} \leq 16 \sum_{j \leq d} \sum_{k > d} \left\| \frac{P_j \Delta P_k}{\lambda_j - \lambda_k} \right\|_2^2 + 128 \sum_{j \leq d} \frac{1}{\lambda_j - \lambda_{d+1}} \left\| \sum_{k > d} \frac{P_j \Delta P_k \Delta P_{\leq d}}{\lambda_j - \lambda_k} \right\|_2^2 + R_1,
\]

where
\[
R_1 = 4 \sum_{j \leq d} (\lambda_j - \lambda_{d+1}) 1 (\hat{\lambda}_{d+1} - \lambda_{d+1} > (\lambda_j - \lambda_{d+1})/2)
\]
\[
+ 32 \sum_{j \leq d} \left\| \frac{P_j \Delta P_{\leq d}}{\lambda_j - \lambda_{d+1}} \right\|_2^2 1 (\|S_{\leq d} \Delta S_{\leq d}\|_{\infty} > 1/16)
\]
\[
+ 128 \sum_{j \leq d} \frac{1}{\lambda_j - \lambda_{d+1}} \left\| \sum_{k > d} \frac{P_j \Delta P_k \Delta P_{\leq d}}{\lambda_j - \lambda_k} \right\|_2^2 1_{\mathcal{E}_1}.
\]

Similarly, we have
\[
\mathcal{E}_{> d}^{\text{PCA}}(\lambda_d)
\]
\[
\leq 16 \sum_{k > d} \sum_{j \leq d} \left\| \frac{P_k \Delta P_j}{\lambda_j - \lambda_k} \right\|_2^2 + 128 \sum_{k > d} \frac{1}{\lambda_d - \lambda_k} \left\| \sum_{j \leq d} \frac{P_k \Delta P_j \Delta P_{\leq d}}{\lambda_j - \lambda_k} \right\|_2^2 + R_2,
\]

where
\[
R_2 = 4 \sum_{k > d} (\lambda_d - \lambda_k) 1 (\hat{\lambda}_d - \lambda_d < -(\lambda_d - \lambda_k)/2)
\]
\[
+ 32 \sum_{k > d} \left\| \frac{P_k \Delta P_{\leq d}}{\lambda_d - \lambda_k} \right\|_2^2 1 (\|S_{> d} \Delta S_{> d}\|_{\infty} > 1/16)
\]
\[
+ 128 \sum_{k > d} \frac{1}{\lambda_d - \lambda_k} \left\| \sum_{j \leq d} \frac{P_k \Delta P_j \Delta P_{> d}}{\lambda_j - \lambda_k} \right\|_2^2 1_{\mathcal{E}_2}.
\]
with $S_{>d} = \sum_{k>d+1} (\lambda_d - \lambda_k)^{-1/2} P_k$ and

$$E_2 = \left\{ \sum_{k>d} \frac{1}{\lambda_d - \lambda_k} \left\| \sum_{j\leq d} \frac{P_k \Delta P_j \Delta S_{>d}}{\lambda_j - \lambda_k} \right\|_2^2 > 1/128 \right\}.$$

Combining these bounds with $E_{<d}^\text{PCA} \leq E_{<d}^\text{PCA} (\lambda_d) + E_{>d}^\text{PCA} (\lambda_{d+1})$, the claim follows.

**Proof of Proposition B.2.** By (2.19) and the formula $\langle P_j, \hat{P}_{>d} \rangle = \|P_j \hat{P}_{>d}\|_2^2$, we get

$$\|P_{<d} - \hat{P}_{<d}\|_2^2 = 2 \sum_{j\leq d} \|P_j \hat{P}_{>d}\|_2^2.$$

Inserting (B.2) into the last term and applying the triangle inequality twice, we obtain

$$\|P_{<d} - \hat{P}_{<d}\|_2^2 \leq 4 \sum_{j\leq d} \left\| \sum_{k>d} \frac{P_j \Delta P_k \hat{P}_{>d}}{\lambda_j - \lambda_k} \right\|_2^2 + 8 \sum_{j\leq d} \left\| \sum_{l>d} \frac{P_j \Delta P_{<d} \hat{P}_{l}}{\lambda_j - \lambda_l} \right\|_2^2$$

$$+ 8 \sum_{j\leq d} \left\| \sum_{k>d \ l>d} \frac{P_j \Delta P_k \Delta \hat{P}_l}{(\lambda_j - \hat{\lambda}_l)(\lambda_j - \lambda_k)} \right\|_2^2.$$

Thus, on the event $\{\lambda_{d+1} - \lambda_{d+1} \leq (\lambda_d - \lambda_{d+1})/2\}$ we have

$$\|P_{<d} - \hat{P}_{<d}\|_2^2 \leq 4 \sum_{j\leq d} \sum_{k>d} \frac{\|P_j \Delta P_k\|_2^2}{(\lambda_j - \lambda_k)^2} + 32 \sum_{j\leq d} \sum_{l>d} \frac{\|P_j \Delta P_{<d} \hat{P}_l\|_2^2}{(\lambda_j - \lambda_{d+1})^2}$$

$$+ 32 \sum_{j\leq d} \sum_{l>d} \frac{1}{(\lambda_j - \lambda_{d+1})^2} \left\| \sum_{k>d} \frac{P_j \Delta P_k \Delta \hat{P}_l}{\lambda_j - \lambda_k} \right\|_2^2. \tag{B.6}$$

The second term on the right-hand side is equal to

$$32\|S_{<d}^2 \Delta P_{<d} \hat{P}_{>d}\|_2^2 = 32\|S_{<d}^2 \Delta S_{<d} R_{<d} \hat{P}_{>d}\|_2^2$$

which is bounded by

$$32\|S_{<d}^2 \Delta S_{<d}\|_2^2 \|R_{<d} \hat{P}_{>d}\|_2^2.$$

Similarly, the third term is bounded via

$$32 \sum_{j\leq d} \sum_{l>d} \frac{1}{(\lambda_j - \lambda_{d+1})^2} \left\| \sum_{k>d} \frac{P_j \Delta P_k \Delta \hat{P}_l}{\lambda_j - \lambda_k} \right\|_2^2$$

$$= 32 \sum_{j\leq d} \frac{1}{(\lambda_j - \lambda_{d+1})^2} \left\| \sum_{k>d} \frac{P_j \Delta P_k \Delta \hat{P}_{>d}}{\lambda_j - \lambda_k} \right\|_2^2$$

$$\leq 64 \sum_{j\leq d} \frac{1}{(\lambda_j - \lambda_{d+1})^2} \left\| \sum_{k>d} \frac{P_j \Delta P_k \Delta \hat{P}_{>d}}{\lambda_j - \lambda_k} \right\|_2^2.$$
\[ + 64 \sum_{j \leq d} \frac{1}{(\lambda_j - \lambda_{d+1})^2} \left\| \sum_{k > d} \frac{P_j \Delta P_k \Delta S_{\leq d}}{\lambda_j - \lambda_k} \right\|_2^2 \frac{R_{\leq d} \hat{\Delta}_{>d}}{2}. \]

Inserting these bounds into (B.6) and using \( \| R_{\leq d} \hat{\Delta}_{>d} \|_2^2 = \mathcal{E}_{\leq d}^{\text{PCA}} \) from (B.1), the claim follows.

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