Estimating covariance and precision matrices along subspaces

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Abstract

We study the accuracy of estimating the covariance and the precision matrix of a $D$-variate sub-Gaussian distribution along a prescribed subspace or direction using the finite sample covariance with $N \geq D$ samples. Our results show that the estimation accuracy depends almost exclusively only on the components of the distribution that correspond to desired subspaces or directions. This is relevant for problems where behavior of data along a lower-dimensional space is of specific interest, such as dimension reduction or structured regression problems. As a by-product of the analysis, we reduce the effect the matrix condition number has on the estimation of precision matrices. Two applications are presented: direction-sensitive eigenspace perturbation bounds, and estimation of the single-index model. For the latter, a new estimator, derived from the analysis, with strong theoretical guarantees and superior numerical performance is proposed.

Keywords: covariance matrix, precision matrix, finite sample bounds, dimension reduction, rate of convergence, ordinary least squares, single-index model

1 Introduction

Let $X \in \mathbb{R}^D$ be a centered random vector with the covariance matrix $\Sigma := \text{Cov}(X) = \mathbb{E}(X - \mathbb{E}X)(X - \mathbb{E}X)\top$. The covariance matrix encodes marginal correlations between pairs of variables, while its inverse, the precision matrix $\Sigma^\dagger$ encodes correlations between pairs of variables conditioned on the remaining variables. Estimating $\Sigma$ and $\Sigma^\dagger$ is a standard and long standing problem in multivariate statistics, with applications in a variety of mathematical and applied fields. Notable applications include any form of dimension reduction such as principal component analysis, nonlinear dimension reduction, manifold learning, but also problems ranging from classification, regression, and signal processing to econometrics, brain imaging and social networks.

We consider the problem of estimating the covariance and the precision matrix from $N \geq D$ independent copies $X_1, \ldots, X_N$ of $X$, through the sample covariance $\hat{\Sigma} := \frac{1}{N} \sum_{i=1}^{N} X_iX_i\top$, and the inverse thereof. The question is then to quantify the minimal number of samples $N$ which guarantees that for a desired accuracy $\varepsilon > 0$ and a confidence level $u > 0$ we have

$$\|\hat{\Sigma} - \Sigma\|_2 \leq \varepsilon S_{\Sigma}(X), \text{ respectively, } \|\hat{\Sigma}^\dagger - \Sigma^\dagger\|_2 \leq \varepsilon S_{\Sigma^\dagger}(X),$$

with probability at least $1 - \exp(-u)$. Constants $S_{\Sigma}(X)$ and $S_{\Sigma^\dagger}(X)$ in (1) describe the dependence of the error with respect to the distribution of $X$ and properties of $\Sigma$, respectively $\Sigma^\dagger$. This

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problem has received significant attention over the years, see Sections 1.1 and 1.2 for a detailed overview.

In practice however, we are often not directly interested in matrices $\Sigma$ or $\Sigma^\dagger$, but rather in how they act on specific vectors or matrices. Examples include the ordinary least squares estimator for regression problems, which computes $\Sigma^\dagger \text{Cov}(X,Y)$ for the dependent variable $Y$, or linear discriminant analysis, which considers the vector $\Sigma^\dagger (\mu_1 - \mu_0)$ that defines a hyperplane separating two classes, one with mean $\mu_0$, and the other with mean $\mu_1$. In these cases the object of interest is lower-dimensional, and more importantly, the behavior of $\Sigma$ or $\Sigma^\dagger$ along desired vectors or subspaces is often beneficial for the estimation, resulting in better performance.

In this work we consider these types of problems and provide corresponding error bounds. More specifically, we develop concentration bounds for matrices $A(\hat{\Sigma} - \Sigma)B^\top$ and $A(\hat{\Sigma}^\dagger - \Sigma^\dagger)B^\top$ for any pair of matrices $A$, $B$, and in cases of sub-Gaussian distributions (see Definition in Section 1.4), and separate bounds for bounded distributions. A particularly relevant case is when $A$ and $B$ are orthogonal projections corresponding to directions or subspaces of interest.

1.1 State of the art: covariance estimation and eigenspace perturbation

The most common bounds for estimating the covariance matrix from finitely many observations in the regime $N \geq D$ consider sub-Gaussian [34, 35] and bounded [31] random vectors. They state that with probability at least $1 - \exp(-u)$

$$\|\hat{\Sigma} - \Sigma\|_2 \leq \varepsilon \|X\|_{\psi^2}^2, \quad \text{provided } N > C\varepsilon^{-2}(D + u), (2)$$

$$\|\hat{\Sigma}^\dagger - \Sigma\|_2 \leq \varepsilon C_X^2, \quad \text{provided } N > C\varepsilon^{-2}(\log(D) + u), \|X\|_2 \leq C_X \text{ a.s.} (3)$$

Besides these two cases, researchers have over the years investigated the minimum moment-or tail conditions on $X$ such that bounds similar to (2) can be achieved. We refer to the papers [1, 29, 33, 34] that consider more general classes of distributions. The most general setting we are aware of is [29], that considers distributions which for universal $C, \eta > 0$ satisfy the tail condition

$$\mathbb{P}(\|PX\|_2^2 > t) \leq Ct^{-1-\eta}, \quad \text{for } t > C \text{ rank}(P),$$

for every orthogonal projection $P$. The class of distributions satisfying this condition includes log-concave random variables (e.g. uniform distributions on convex sets), and product distributions, where the marginals have uniformly bounded $4 + s$ moments for some $s > 0$.

In the regime $N < D$, covariance estimation from samples is in general not possible, since the sample covariance is rank deficient. Instead, structural assumptions, such as sparsity or low-rankness of $\Sigma$, are needed to reduce the effective complexity of the problem and allow consistent estimation. These assumptions can be leveraged by regularized estimation techniques, which include banding [6], thresholding [5,10], or penalized likelihood estimation [16]. See [10,12] for a more detailed review of existing methods.

1.2 State of the art: precision matrix estimation

Estimation of the precision matrix is relevant for many problems, ranging from simple tasks such as data transformations (e.g. standardizing $Z := \Sigma^{-1/2}X$), to applications that include linear discriminant analysis, graphical modeling, or complex data visualization. Furthermore, precision matrix encodes information about partial correlations of features of $X$. Namely, if $X$ follows a Gaussian (or paranormal) distribution, the $ij$-th entry of $\Sigma^\dagger$ is zero if the $i$-th and the $j$-th feature are conditionally independent.

The inverse $\hat{\Sigma}^\dagger$ of the sample covariance, constructed from $N$ independent copies of a mean zero random vector $X \in \mathbb{R}^D$, is a well-behaved estimator of $\Sigma^\dagger$ as $N \to \infty$ and $D$ is considered
fixed [2]. In such a case bounds for the precision matrix can be obtained by using general 
perturbation bounds for the Moore-Penrose inverse. One of the first such bounds [36] states that 
for $G \in \mathbb{R}^{d_1 \times d_2}$, and an additively perturbed matrix $H = G + \Delta$, we have

$$
\left\| H^\dagger - G^\dagger \right\| \leq \omega \max \left\{ \left\| G^\dagger \right\|_2^2, \left\| H^\dagger \right\|_2^2 \right\} \| \Delta \|, \quad \text{and} \\
\left\| H^\dagger - G^\dagger \right\| \leq \omega \left\| G^\dagger \right\|_2 \left\| H^\dagger \right\|_2 \| \Delta \|, \quad \text{if rank}(G) = \text{rank}(H),
$$

where $\| \cdot \|$ is any unitarily invariant norm, and $\omega$ is a small universal constant [24]. Recent 
studies [20,38] examine the influence of the perturbation in greater detail, implying the bound

$$
\left\| H^\dagger - G^\dagger \right\|_F \leq \min \left\{ \left\| H^\dagger \right\|_2 \left\| G^\dagger \right\|_F, \left\| G^\dagger \right\|_2 \left\| H^\dagger \right\|_2 \right\}, \quad \text{if rank}(G) = \text{rank}(H) = \min\{d_1, d_2\}.
$$

From the above perturbation bounds, it is easy to derive concentration bounds for the precision 
matrix. For example, assuming $X$ is sub-Gaussian and the number of independent data samples 
is sufficiently large with respect to $D$ and $\| \Sigma \|_2$, Weyl’s bound [37] implies $\lambda_i(\hat{\Sigma}) \geq \lambda_i(\Sigma) - 
\| \hat{\Sigma} - \Sigma \|_2 = \lambda_i(\Sigma) + O(N^{-1/2})$, and consequently $\| \hat{\Sigma} \|_2 = \| \Sigma \|_2 + O(N^{-1/2})$. Neglecting the 
higher order term, the perturbation bound (5) and the covariance bound for sub-Gaussian random 
 vectors (2) give

$$
\left\| \hat{\Sigma} - \Sigma \right\|_2 \lesssim \left\| \Sigma \right\|_2 \left\| \hat{\Sigma} - \Sigma \right\|_2 \lesssim \epsilon \left\| \Sigma \right\|^2_2 \| X \|^2_{\psi_2}.
$$

On the other hand, we are not aware of results that give bounds on directional estimates 
$\| A(\hat{\Sigma} - \Sigma)B \|_2$, neither in the case of general matrices, nor for covariance matrices.

The precision matrix cannot be estimated well by inverting the sample covariance matrix 
if $D$ grows with $N$, since $\hat{\Sigma}$ is not a consistent estimator of $\Sigma$, and thus the sample precision 
matrix can contain large errors. As for the covariance matrices, various families of structured 
precision matrices have been studied to mitigate these issues, motivated by applications in 
genomics, finance, and other fields. The dominant assumptions are sparsity or low-rankness, 
which are exploited through the use of regularized estimators. Algorithms for estimating $\Sigma^\dagger$ 
under regularization include computing $\Sigma^\dagger$ column by column through entry-wise Lasso [13,23], 
constrained $\ell_1$ minimization [8], adaptive $\ell_1$ minimization [9], $\ell_1$ regularized score matching [21], 
or ridge regressors [32]. See [10,12] for comprehensive overviews.

1.3 Overview and contributions

Let $X \in \mathbb{R}^D$ be a sub-Gaussian random vector with $\bar{X} := X - \mathbb{E}X$ and $\Sigma = \text{Cov}(X)$, and let 
$X_1, \ldots, X_N$ be independent copies of $X$. Define finite sample estimators of of $\mathbb{E}X$ and $\Sigma$ by 
$\bar{X}_N := N^{-1} \sum_{i=1}^N X_i$ and $\hat{\Sigma} := N^{-1} \sum_{i=1}^N (X_i - \mu X)(X_i - \mu X)^\top$.

In this paper we develop concentration bounds for $A(\Sigma - \hat{\Sigma})B^\top$ and $A(\Sigma^\dagger - \hat{\Sigma}^\dagger)B$, where 
$A \in \mathbb{R}^{d_1 \times D}$, $B \in \mathbb{R}^{d_2 \times D}$ are arbitrary matrices determining a direction, subspace, or generally an 
object, of interest. We can summarize our findings as follows.

(1) In Section 2 we show that with probability at least $1 - \exp(-u)$

$$
\left\| A(\Sigma - \hat{\Sigma})B^\top \right\|_2 \leq \epsilon \left\| A\bar{X} \right\|_{\psi_2} \left\| B\bar{X} \right\|_{\psi_2},
$$

provided $N > C(d_A + d_B + u)(\epsilon^{-1} \vee \epsilon^{-2})$ for some universal constant $C$, where $d_A = \text{rank}(A\Sigma)$ 
and $d_B = \text{rank}(B\Sigma)$. This result is similar to [34, Proposition 2.1] but replaces the sub-
Gaussian norm $\| \bar{X} \|_{\psi_2}$ by direction/subspace dependent quantities $\| A\bar{X} \|_{\psi_2}$ and $\| B\bar{X} \|_{\psi_2}$.
We only use \( p = 1 \) (sub-Exponential) and \( p = 2 \) (sub-Gaussian). If \( \Omega \) is a finite set, \( |\Omega| \) denotes its cardinality. If \( \Omega \) is an interval, \( |\Omega| \) denotes its length. Throughout the paper, \( C \) is a placeholder for a positive universal constant that may have a different value in each occurrence, even within the same line of text.
2 Covariance matrix estimation

In this section we present bounds for covariance and eigenspace estimation that are sensitive to the distribution of a given random vector in directions of interest. The following result is the fundamental tool of our analysis.

Lemma 2. Let $X \in \mathbb{R}^D$ be sub-Gaussian. Fix $u > 0$ and $\varepsilon > 0$, and let $A \in \mathbb{R}^{d_1 \times D}$, $B \in \mathbb{R}^{d_2 \times D}$. Provided $N > C(\text{rank}(A\Sigma) + \text{rank}(B\Sigma) + u)(\varepsilon^{-1} \vee \varepsilon^{-2})$, with probability at least $1 - \exp(-u)$ we have
\[
\|A(\hat{\Sigma} - \Sigma)B^\top\|_2 \leq \varepsilon \left\|A\hat{X}\right\|_{\psi_2} \left\|B\hat{X}\right\|_{\psi_2}.
\] (10)

Remark 3. An analogous result holds for bounded random variables by using matrix Bernstein inequality as in [31]. In that case $\|\cdot\|_{\psi_2}$ can be replaced by a bound for the Euclidean norm $\|\cdot\|_2$, and the dimensionality appears only logarithmically in the requirement on $N$. We will return to this point at the end of Section 3.

The proof of Lemma 2 follows along the lines of traditional concentration results [34, Proposition 2.1], but it requires a careful tracking of the behavior of the random vector $X$ with respect to changes along the directions induced by matrices $A$ and $B$. As (10) suggests, the payoff is that the error rate scales only with components of $X$ along those directions. Applying Lemma 2 we can now easily reconstruct known error rates in case of low-rank distributions in a high-dimensional ambient spaces.

Corollary 4. Let $X \in \mathbb{R}^D$ be sub-Gaussian. Then, provided $N > C(\text{rank}(\Sigma) + u)(\varepsilon^{-1} \vee \varepsilon^{-2})$, with probability at least $1 - \exp(-u)$ we have
\[
\left\|\hat{\Sigma} - \Sigma\right\|_2 \leq \varepsilon \left\|\hat{X}\right\|_{\psi_2}^2.
\] (11)

Lemma 2 also has an immediate effect on the estimation of eigenvectors and eigenspaces. Denote by $P_{i,l}(\Sigma) := \sum_{k=1}^l u_k(\Sigma)u_k(\Sigma)^\top$ the orthoprojector onto the space spanned by $i$-th to $l$-th eigenvectors of $\Sigma$, and let $P_{i,l}(\hat{\Sigma})$ be the corresponding finite sample version. Moreover, denote $Q_{i,l}(\Sigma) := \text{Id} - P_{i,l}(\Sigma)$, and $\text{dist}(I_1; I_2) := \inf_{t \in I_1, t' \in I_2} |t - t'|$ for $I_1, I_2 \subset \mathbb{R}$.

Proposition 5. Let $X \in \mathbb{R}^D$ be sub-Gaussian, and fix $u > 0$, $\varepsilon > 0$. Let $i \leq l \in \mathbb{N}$, and define
\[
\delta_{il} = \text{dist}([\lambda_i(\Sigma), \lambda_l(\Sigma)]; [\infty, \lambda_{l-1}(\hat{\Sigma})] \cup [\lambda_{l+1}(\Sigma), -\infty]), \quad \text{with } \lambda_0(\hat{\Sigma}) := \infty, \lambda_{D+1}(\hat{\Sigma}) = -\infty.
\]
Provided $N > C(\text{rank}(\Sigma) + u)(\varepsilon^{-1} \vee \varepsilon^{-2})$, with probability at least $1 - \exp(-u)$ we have
\[
\left\|Q_{i,l}(\Sigma)P_{i,l}(\Sigma)\right\|_2 \leq \varepsilon \left\|P_{i,l}(\Sigma)\hat{X}\right\|_{\psi_2} \left\|\hat{X}\right\|_{\psi_2} \frac{\delta_{il}}{\delta_{il}}.
\] (12)

Proof. Davis-Kahan Theorem in [4, Theorem 7.3.2] gives
\[
\left\|Q_{i,l}(\Sigma)P_{i,l}(\Sigma)\right\|_2 \leq \frac{\pi}{2} \left\|Q_{i,l}(\hat{\Sigma})(\Sigma - \hat{\Sigma})P_{i,l}(\Sigma)\right\|_2 \leq \frac{\pi}{2} \left\|\Sigma - \hat{\Sigma}\right\|_2 \frac{\delta_{il}}{\delta_{il}}.
\]

The claim now follows by applying Lemma 2 with $A = \text{Id}$ and $B = P_{i,l}(\Sigma)$.

Typical bounds for eigenspace perturbations $\|Q_{i,l}(\Sigma)P_{i,l}(\Sigma)\|_2$ take the specific eigenspace into account only through the denominator, whereas the numerator relies on squared terms of the form $\|X\|_{\psi_2}^2$ in the sub-Gaussian case, or $\|X\|_2^2$ in the bounded case. Expression (12) is thus beneficial if $\|P_{i,l}(\Sigma)\hat{X}\|_{\psi_2}$ is smaller than $\|\hat{X}\|_{\psi_2}$ to get a sharper error bound.
In order to ensure $\delta_\ell > 0$, the covariance matrix $\Sigma$ must have a population eigengap, that is, $\delta_\ell := |\lambda_{i+1}(\Sigma) - \lambda_i(\Sigma)| \wedge |\lambda_i(\Sigma) - \lambda_{i-1}(\Sigma)| > 0$, and sufficiently many samples are required in order to stabilize $\delta_\ell$ around $\delta_*$. The latter is typically achieved by first using Weyl’s bound [37], giving $|\lambda_j(\Sigma) - \lambda_i(\Sigma)| \leq ||\Sigma - \Sigma||_2$ for all $j \in [D]$, and then applying a concentration bound for $||\Sigma - \Sigma||_2$. A consequence however is that Proposition 5 is only informative if we have sufficiently samples with respect to $\delta_\ell$ and $||X||_{\psi_2}$.

Recently, [39] provided a useful alternative by showing

\[\left\|Q_{i,i}(\Sigma)P_{i,i}(\Sigma)\right\|_F \leq C \frac{(D^{1/2}||\Sigma - \Sigma||_2 \wedge ||\Sigma - \Sigma||_F)}{\delta_*^\eta}.\]  \hspace{1cm} (13)

Compared to (12), the remarkable fact about (13) is that the denominator $\delta_*^\eta$ is the population eigengap, and is therefore independent of $\hat{\Sigma}$. Thus, with (13) we do not have to stabilize the sample eigengap, and the eigenspace perturbation bound (13) can be used for arbitrary $N \geq 1$.

A natural question to ask is whether Proposition 5 holds if $\delta_\ell$ is replaced with $\delta_*$. The following example strongly suggests this is not the case.

**Example 1.** Assume that Proposition 5 holds with $\delta_\ell$ in place of $\delta_*$. Let $X \sim \mathcal{N}(0, \Sigma)$, where $\Sigma = \sum_{i=1}^{D-1}u_i u_i^\top + \eta^2 u_D u_D^\top$, for $\eta < 1$. Notice that in this case $||\tilde{X}||_{\psi_2} \leq C$, and $||u_D X||_{\psi_2} \leq C\eta$ by Lemma 15. For any $N \geq 1$ by choosing $\varepsilon = 1 \lor C(D + u)N^{-1}$ we get

\[\left\|Q_{D,D}(\Sigma)P_{D,D}(\Sigma)\right\|_2 \leq \left(1 \lor C(D + u)N^{-1}\right) \frac{C\eta ||\tilde{X}||_{\psi_2}}{1 - \eta^2} \leq C(D + u) \frac{\eta}{1 - \eta^2}.\]

In particular, the bound suggests that in the limit $\eta \to 0$ we would have a very small estimation error, and that the accuracy improves with $\eta$, by using only one data sample, i.e., by estimating $P_{D,D}(\Sigma)$ the eigendecomposition of a rank one matrix $XX^\top$.

## 3 Precision matrix estimation

In this section we investigate directional estimates of the precision matrix $\Sigma^\dagger$ through the empirical precision matrix $\hat{\Sigma}^\dagger$, analogously to results in Section 2. To begin, we introduce a directional condition number for sub-Gaussian random vectors.

**Definition 6.** For $A \in \mathbb{R}^{d \times D}$ and a sub-Gaussian random vector $X \in \mathbb{R}^D$ we define $\kappa(A, X) := ||A\Sigma^\dagger X||_{\psi_2}^2 ||A\hat{X}||_{\psi_2}^2$. 

To interpret this quantity, note first that $\text{Cov}(A\Sigma^\dagger \tilde{X}) = A\Sigma^\dagger A^\top$ and $\text{Cov}(A\hat{X}) = A\Sigma A^\top$. Provided the squared sub-Gaussian norm is a proxy for the variance of the random vector, that is

\[||A\Sigma^\dagger \tilde{X}||_{\psi_2}^2 \approx ||A\Sigma^\dagger A^\top||_2, \quad \text{and} \quad ||A\hat{X}||_{\psi_2}^2 \approx ||A\Sigma A^\top||_2,\]  \hspace{1cm} (14)

as is the case for $X \sim \mathcal{N}(0, \Sigma)$, we can now read $\kappa(A, X)$ as a variant of the matrix condition number, $\kappa(A, \Sigma) := ||A\Sigma A^\top||_2 ||A\Sigma^\dagger A^\top||_2$. Moreover, for arbitrary sub-Gaussian random vectors the two quantities satisfy $\kappa(A, X) \geq C\kappa(A, \Sigma)$, as shown in Lemma 15.

The rationale for using $\kappa(A, X)$ instead of $\kappa(A, \Sigma)$ is of technical nature and is due to the fact that $\kappa(A, X)$ naturally crops up in the sub-Gaussian framework when using concentration inequalities. Namely, if instead of $||A\hat{X}||_{\psi_2}$, Lemma 2 depended on $||\text{Cov}(AX)||_2$, then $\kappa(A, \Sigma)$ would indeed be a natural choice.

We now present the main results of this section in two settings: arbitrary sub-Gaussian $X$, and sub-Gaussian $X$ that satisfy

\[\mathbb{P}\left(\text{Im}(\hat{\Sigma}) = \text{Im}(\Sigma)\right) > 1 - \exp(-u), \quad \text{whenever } N > C(\text{rank}(\Sigma) + u),\]  \hspace{1cm} (15)
which allows stronger bounds. We note that (15) is not a restrictive condition. For example, if the measure of $X$ is absolutely continuous with respect to the Lebesgue measure on $\text{Im}(\Sigma)$ we have $\text{Im}(\hat{\Sigma}) = \text{Im}(\Sigma)$ almost surely whenever $N \geq \text{rank}(\Sigma)$.

**Theorem 7.** Fix $u > 0$, and $\varepsilon > 0$, let $A \in \mathbb{R}^{d \times D}$, $B \in \mathbb{R}^{d^2 \times D}$, and assume (15) holds. Provided $N > C(\text{rank}(\Sigma) + u) \left( \kappa(\text{Id}, X) \vee \varepsilon^{-2} \right)$, with probability at least $1 - \exp(-u)$ we have

$$
\left\| A \left( \hat{\Sigma}^\dagger - \Sigma^\dagger \right) B^\top \right\|_2 \leq \varepsilon \left\| A\Sigma^\dagger \hat{X} \right\|_{\psi_2} \left\| B\Sigma^\dagger \hat{X} \right\|_{\psi_2}.
$$

(16)

If (15) is not satisfied then (16) holds whenever $N > C(\text{rank}(\Sigma) + u) \left( \kappa(\text{Id}, X)^2 \vee \varepsilon^{-2} \right)$.

**Proof sketch for Theorem 7.** Provided $\text{Im}(\hat{\Sigma}) = \text{Im}(\Sigma)$, using [36, Theorem 2.1] we have

$$
\hat{\Sigma}^\dagger - \Sigma^\dagger = -\hat{\Sigma}^\dagger \Delta \Sigma^\dagger = -\Sigma^\dagger \Delta \hat{\Sigma}^\dagger = -\Sigma^\dagger \Delta \Sigma^\dagger - \Sigma^\dagger \Delta (\hat{\Sigma}^\dagger - \Sigma^\dagger),
$$

(17)

for $\Delta := \hat{\Sigma} - \Sigma$. Multiplying by $\hat{A} \in \mathbb{R}^{d_1 \times D}$ and $\hat{B}^\top \in \mathbb{R}^{D \times d_2}$ from left and right, respectively, and rearranging the terms we get

$$
\hat{A}(\text{Id} + \Sigma^\dagger \Delta)(\hat{\Sigma}^\dagger - \Sigma^\dagger)\hat{B}^\top = -\hat{A} \Sigma^\dagger \Delta \Sigma^\dagger \hat{B}^\top.
$$

For a sufficiently large $N$ we have $\left\| \Sigma^\dagger \Delta \right\|_2 < 1$, by Lemma 2. Thus, we can express $(\text{Id} + \Sigma^\dagger \Delta)^{-1}$ by a Neumann series. Choosing $\hat{A} = A(\text{Id} + \Sigma^\dagger \Delta)^{-1}$ and $\hat{B} = B$ gives

$$
A(\hat{\Sigma}^\dagger - \Sigma^\dagger)B^\top = -A(\text{Id} + \Sigma^\dagger \Delta)^{-1} \Sigma^\dagger \Delta \Sigma^\dagger B^\top = -A \Sigma^\dagger \Delta \Sigma^\dagger B^\top - A \Sigma^\dagger \Delta \sum_{k=0}^{\infty} (-\Sigma^\dagger \Delta) \Sigma^\dagger \Delta \Sigma^\dagger B^\top.
$$

The spectral norm of the first term on the right hand side is bounded by $\varepsilon \left\| A\Sigma^\dagger \hat{X} \right\|_{\psi_2} \left\| B\Sigma^\dagger \hat{X} \right\|_{\psi_2}$, by Lemma 2. On the other hand, the second term is of higher order and can be treated similarly.

Let us comment on the implications of Theorem 7. First, similar to Lemma 2, the error estimates in (16) depend only on the components of $X$ induced by $A$ and $B$. Following (14), this is an improvement over non-directional bounds whenever the eigenvalues of $A\Sigma^\dagger A^\top$ and $B\Sigma^\dagger B^\top$ are small compared to those of $\Sigma^\dagger$.

Second, if we consider the regime where $\varepsilon^{-2} > \kappa(\text{Id}, X)$, the estimation rate in (16) is similar to the covariance estimation rate in Lemma 2. That is, assume we are trying to estimate $\Sigma^\dagger$ through the covariance matrix of the random vector $Z = \Sigma^\dagger X$ by using iid. copies $Z_i := \Sigma^\dagger X_i$. In that case Lemma 2 gives precisely the bound (16). This should come as a bit surprising, since it states that estimating the precision matrix through the inverse of the sample covariance has the same theoretical guarantees as if we had access to a random vector $Z$ whose covariance is exactly $\Sigma^\dagger$. To further stress this point, we now compare Theorem 7 for $A = B = \text{Id}$ with the bound

$$
\left\| \hat{\Sigma} - \Sigma \right\|_2 \leq \varepsilon \kappa(\text{Id}, \Sigma) \left\| \Sigma^\dagger \right\|_2 = \varepsilon \left\| \Sigma^\dagger \right\|_2 \left\| \Sigma \right\|_2,
$$

(18)

that was derived in Section 1.2 using general perturbation bounds for the matrix inverse.

**Corollary 8.** Provided (15) holds and $N > C(\text{rank}(\Sigma) + u) \left( \kappa(\text{Id}, X) \vee \varepsilon^{-2} \right)$, we have with probability at least $1 - \exp(-u)$

$$
\left\| \hat{\Sigma}^\dagger - \Sigma^\dagger \right\|_2 \leq \varepsilon \left\| \Sigma^\dagger \hat{X} \right\|_{\psi_2}.
$$

(19)

If (15) is not satisfied, we require $N > C(\text{rank}(\Sigma) + u) \left( \kappa(\text{Id}, X)^2 \vee \varepsilon^{-2} \right)$ instead.
Assuming the squared sub-Gaussian norm is a good proxy for the variance, i.e., if \((14)\) holds, the right hand side in \((19)\) is approximately \(\varepsilon \|\Sigma^T\|_2\). Compared to \((18)\), this shows that using a general perturbation bound overestimates the influence of the condition number \(\kappa(\mathbf{I}, \Sigma)\) on precision matrix estimation. The discrepancy between these two results suggests that the finite sample covariance estimator is a specific type of a perturbation that admits a form of regularization when estimating the inverse.

Our last result in this section further improves the dependency on the condition number \(\kappa(\mathbf{I}, X)\) whenever \(A\) and \(B\) correspond to an orthogonal decomposition of the identity.

**Theorem 9.** Fix \(u > 0\), and \(\varepsilon > 0\) and assume \((15)\) holds. Let \(\mathbf{I} = P + Q\) be an orthogonal decomposition of the identity. Provided \(N > C(\text{rank}(\Sigma) + u) (\kappa(P, X) \vee \kappa(Q, X) \vee \varepsilon^{-2})\) we have with probability at least \(1 - \exp(-u)\)

\[
\left\| P \left( \hat{\Sigma}^\dagger - \Sigma^\dagger \right) P \right\|_2 \leq \varepsilon \left\| P \Sigma^\dagger \tilde{X} \right\|_{\psi_2}^2, \text{ and } \left\| Q \left( \hat{\Sigma}^\dagger - \Sigma^\dagger \right) P \right\|_2 \leq \varepsilon \left\| P \Sigma^\dagger \tilde{X} \right\|_{\psi_2} \left\| Q \Sigma^\dagger \tilde{X} \right\|_{\psi_2}. \tag{20}
\]

**Proof sketch for Theorem 9.** Using again \((17)\), and first multiplying by \(P\) from both sides, and then by \(Q\) from the left and \(P\) from the right, we get from \(\mathbf{I} = P + Q\),

\[
P(\hat{\Sigma}^\dagger - \Sigma^\dagger) = -P \Sigma^\dagger \Delta \Sigma^\dagger P - P \Sigma^\dagger \Delta P(\hat{\Sigma}^\dagger - \Sigma^\dagger) P - P \Sigma^\dagger \Delta Q(\hat{\Sigma}^\dagger - \Sigma^\dagger) P,
\]
\[
Q(\hat{\Sigma}^\dagger - \Sigma^\dagger) = -Q \Sigma^\dagger \Delta \Sigma^\dagger P - Q \Sigma^\dagger \Delta P(\hat{\Sigma}^\dagger - \Sigma^\dagger) P - Q \Sigma^\dagger \Delta Q(\hat{\Sigma}^\dagger - \Sigma^\dagger) P.
\]

This is a two-by-two, matrix-valued linear system for the two unknowns, \(P(\hat{\Sigma}^\dagger - \Sigma^\dagger) P\) and \(Q(\hat{\Sigma}^\dagger - \Sigma^\dagger) P\). Its analytic solution is derived by block matrix inversion. Namely, the second component satisfies

\[
Q(\hat{\Sigma}^\dagger - \Sigma^\dagger) P = - \sum_{k=0}^{\infty} (-H)^k Q \Sigma^\dagger \Delta P \sum_{k=0}^{\infty} (-P \Sigma^\dagger \Delta P)^k P \Sigma^\dagger \Delta \Sigma^\dagger P + \sum_{k=0}^{\infty} (-H)^k Q \Sigma^\dagger \Delta \Sigma^\dagger P, \tag{21}
\]

where \(H := Q \Sigma^\dagger \Delta Q + Q \Sigma^\dagger \Delta P \sum_{k=0}^{\infty} (-P \Sigma^\dagger \Delta P)^k P \Sigma^\dagger \Delta Q\).

To complete the proof we can now apply Lemma 2, first to ensure \(\|H\|_2 < 1\), and then to ensure \(\|P \Sigma^\dagger \Delta P\|_2 < 1\), so that a Neumann series argument can be applied. Balancing the contributions of the two summands in \((21)\), yields the desired bound. \(\square\)

**Numerical validation.** To validate the results in this section we sample the orthoprojector \(P\) uniformly at random with \(\dim(\text{Im}(P)) = 3\), and consider \(X \sim \mathcal{N}(0, \Sigma)\), for two types of covariance matrices \(\Sigma \in \mathbb{R}^{10 \times 10}\).

**Setting 1:** Set \(\Sigma = USU^T\), where \(U \in \mathbb{R}^{10 \times 10}\) is sampled uniformly at random from the space of orthonormal matrices, and \(S = \text{Diag}(1, 1, 1, 1, \nu, \nu, \nu, \nu)\). We consider \(\nu = 10^{-j+1}\) for \(j \in [10]\). Hence, the condition number \(\kappa(\mathbf{I}, \Sigma)\) ranges from 1 to 100.

**Setting 2:** Set \(\Sigma_{i,j} = \nu^{i-j}\), with \(\nu \in \{0.5, 0.55, \ldots, 0.9, 0.95\}\). This is a common model for distributions where entries of \(X\) correspond to values of a certain feature at different time stamps. It leads to correlated entries when the time stamps are close by, i.e., when \(|i-j|\) is small.

We repeat each experiment 100 times and report the averaged relative errors in Figure 1. Different lines of the same color correspond to different values of \(\nu\).

The estimation error shows the expected \(N^{-1/2}\) rate. Moreover, the directional errors show a clear and direct dependence on the directional spectral norm. On the other hand, since we
are sampling Gaussians, the squared sub-Gaussian norm is a proxy for the variance of the given random vector, and the results confirm that the error term in Theorem 9 scales with the corresponding (directional) sub-Gaussian norm. Lastly, although the condition number of $\Sigma$ depends on $\nu$, the specific value of $\nu$ does not affect how accurate $\hat{\Sigma}^\dagger$ is, as predicted by the theory.

**Bounded random vectors.** As mentioned in Remark 3, a stronger form of direction dependent covariance and precision matrix estimation bounds (and their consequences) hold for bounded random vectors. The proofs for the bounded case follow along similar lines as for the sub-Gaussian case, except for the use of a slightly different probabilistic argument. We now state only the results for the estimation of covariance and precision matrix, since the remaining bounds follow by analogy.

**Theorem 10.** Fix $u > 0$ and $\varepsilon > 0$, and let $A \in \mathbb{R}^{d_1 \times D}, B \in \mathbb{R}^{d_2 \times D}$. Let $X$ be a random vector with $\|AX\|_2 \leq C_A, \|BX\|_2 \leq C_B$ almost surely. Provided $N > C (\log(\text{rank}(A\Sigma) + \text{rank}(B\Sigma)) + u)\varepsilon^{-2}$, with probability at least $1 - \exp(-u)$ we have

$$\left\| A \left( \hat{\Sigma} - \Sigma \right) B^\top \right\|_2 \leq \varepsilon C_A C_B.$$

Assume (15), and that $\|A\Sigma^\dagger X\|_2 \leq C_A^\dagger, \|B\Sigma^\dagger X\|_2 \leq C_B^\dagger, \|X\|_2 \|\Sigma^\dagger X\|_2 \leq \kappa(X)$ holds almost surely. Provided $N > C (\log(\text{rank}(\Sigma)) + u) (\kappa(X) \vee \varepsilon^{-1})^2$, with probability at least $1 - \exp(-u)$ we have

$$\left\| A \left( \hat{\Sigma}^\dagger - \Sigma^\dagger \right) B^\top \right\|_2 \leq \varepsilon C_A^\dagger C_B^\dagger.$$

**4 Application to single index model estimation**

In this section we use the results of Sections 2 and 3 to establish sharp concentration bounds for estimating the index vector in the single index model. Directional terms in the resulting bound provide an insight into how to further improve the performance of the estimator by splitting up the data, conditioning and averaging. The second half of the section is thus devoted to describing this strategy, proving the error estimates, and providing numerical evidence that show and examine the claimed performance gains.
4.1 Ordinary least squares for the single index model

Single index model (SIM) is a popular semi-parametric regression model that poses the relationship between the features \( X \in \mathbb{R}^D \) and responses \( Y \in \mathbb{R} \) as \( \mathbb{E}[Y|X] = f(a^T X) \), where \( f \) is an unknown link function and \( a \in S^{D-1} \) is an unknown index vector. SIM was developed in the 80s and 90s [7,17] as an extension of generalized linear regression that does not specify the link function, and which could thus avoid errors incurred by model misspecification. Common applications are in econometrics [11, 22] and signal processing under sparsity assumptions on the index vector [27,28]. It has been shown, e.g. in [14], that (in certain scenarios) the minimax estimation rate of SIM equals that of nonparametric univariate regression, in which case sample efficient estimation is possible.

Methods for estimating the SIM from finite data set \( \{(X_i,Y_i) : i \in [N] \} \) often first construct an approximate index vector \( \hat{a} \), and then use nonparametric regression on \( \{(a^T X_i,Y_i) : i \in [N] \} \) to estimate the link function. With such an approach the generalization error of the resulting estimator depends largely on the error incurred by estimating the index vector, due to which the construction of \( \hat{a} \) becomes the critical point. An efficient approach, which first appeared in [7,19], and later in modified forms in [3,15], is to start by solving the ordinary least squares problem

\[
(\hat{c}, \hat{b}) = \arg\min_{c \in \mathbb{R}, \ b \in \mathbb{R}^D} \sum_{i=1}^N \left( Y_i - c - b^T (X_i - \hat{\mu}_X) \right)^2, \quad \text{where} \quad \hat{\mu}_X = \frac{1}{N} \sum_{i=1}^N X_i. \tag{24}
\]

and then set \( \hat{a} = \hat{b}/\|\hat{b}\|_2 \). It was recently shown [3] that \( \sqrt{N}(\hat{a} - a) \) is asymptotically normal with mean zero provided \( X \) has an elliptical distribution. Thus, \( \hat{a} \) is an unbiased estimator of the index vector \( a \), converging at an \( N^{-1/2} \) rate. Moreover, the minimal \( \|\cdot\|_2 \)-norm solution of (24) admits an exact solution

\[
\hat{c} = \hat{\mu}_Y, \quad \hat{b} = \Sigma^\dagger \hat{r}, \quad \text{where} \quad \hat{\mu}_Y := \frac{1}{N} \sum_{i=1}^N Y_i, \quad \text{and} \quad \hat{r} := \frac{1}{N} \sum_{i=1}^N (X_i - \hat{\mu}_X)(Y_i - \hat{\mu}_Y). \tag{25}
\]

Using the results of the previous two sections we can now show a direction dependent concentration bound for the population vector \( b := \Sigma^\dagger \text{Cov}(X,Y) \).

**Lemma 11.** Let \( X \in \mathbb{R}^D \) and \( Y \in \mathbb{R} \) be sub-Gaussian, and fix \( u > 0, \varepsilon > 0 \). Let \( P = \|b\|_2^{-2} bb^\top \), \( Q := \text{id} - P \), and \( \kappa_{PQ} = \kappa(P,X) \lor \kappa(Q,X) \). Provided (15) holds and \( N > C(\text{rank}(\Sigma) + u)(\kappa_{PQ} \lor \varepsilon^{-2}) \), we have with probability at least 1 \(-\exp(-u)\)

\[
\|P (b - \hat{b})\|_2 \leq \varepsilon \|\hat{Y}\|_{\psi_2} \|P \Sigma^\dagger \hat{X}\|_{\psi_2} \sqrt{\kappa_{PQ}}, \tag{26}
\]

\[
\|Q (b - \hat{b})\|_2 \leq \varepsilon \|\hat{Y}\|_{\psi_2} \|Q \Sigma^\dagger \hat{X}\|_{\psi_2} \sqrt{\kappa_{PQ}}. \tag{27}
\]

If (15) is not satisfied, the same results hold if \( N > C(\text{rank}(\Sigma) + u)(\kappa(\text{id},X)^2 \lor \varepsilon^{-2}) \).

The result can also be used to obtain a concentration bound for the normalized vector \( \hat{a} = \hat{b}/\|\hat{b}\|_2 \).

**Corollary 12.** Assume the setting of Lemma 11, \( b \neq 0 \), and set \( a = b/\|b\|_2 \). Provided (15) holds, for \( \hat{a} = \hat{b}/\|\hat{b}\|_2 \) we get with probability at least 1 \(-\exp(-u)\)

\[
\|\hat{a} - a\|_2 \leq \varepsilon \|\hat{Y}\|_{\psi_2} \|Q \Sigma^\dagger \hat{X}\|_{\psi_2} \sqrt{\kappa_{PQ}}. \tag{28}
\]

provided that \( N > C(\text{rank}(\Sigma) + u) \left( 1 + \|\hat{Y}\|_{\psi_2}^2 \|P \Sigma^\dagger \hat{X}\|_{\psi_2}^2 / \|b\|_2^2 \right) \kappa_{PQ} \lor \varepsilon^{-2} \). \tag{29}

If (15) is not satisfied, the same result holds after replacing \( \kappa_{PQ} \) in (29) with \( \kappa(\text{id},X)^2 \).
Corollary 12 confirms the expected $N^{-1/2}$ rate of the estimator $\hat{a}$. Furthermore, (28) and (29) reveal the influence of directional terms on the error. To make this influence more precise we now focus on SIMs with a strictly monotonic link function, where $X \sim \mathcal{N}(0, \Sigma)$ and $a$ is an eigenvector of $\Sigma$.

**Corollary 13.** Fix $u > 0$, $\varepsilon > 0$, and let $a \in S^{D-1}$, $P := aa^\top$, $Q := \text{Id} - P$, and $X \sim \mathcal{N}(0, \Sigma)$ with $\Sigma a = \sigma_P^2 a$. Let $Y = f(a^\top X) + \zeta$, for some $f \in \mathcal{C}^1$ with $L^{-1} \leq \sup_t f'(t) \leq L$, and assume the noise satisfies $\mathbb{E}[\zeta^2|a^\top X] = 0$, $\|\zeta\|_{\mathbb{V}_2} = \sigma_\zeta < \infty$. Provided $N > \text{CL}^4(\text{rank}(\Sigma) + u)(1 + \sigma_\zeta^2\sigma_P^{-2})(\kappa(Q, X) \vee \varepsilon^2)$, we have with probability at least $1 - \exp(-u)$

$$\|\hat{a} - a\|_2 \leq \varepsilon L^2 (\sigma_P + \sigma_\zeta) \sqrt{\|Q\Sigma^\top Q\|_2 \kappa(Q, X)}. \quad (30)$$

**Proof.** By the assumptions and the law of total expectation we have

$$\text{Cov}(a^\top X, \zeta) = \mathbb{E}[a^\top X \zeta] = \mathbb{E}[a^\top X \mathbb{E}[\zeta|a^\top X]] = 0,$$

Therefore, Stein’s Lemma [30] implies

$$\|b\|_2 = \frac{\text{Cov}(a^\top X, Y)}{\text{Var}(a^\top X)} = \frac{\text{Cov}(a^\top X, f(a^\top X))}{\text{Var}(a^\top X)} = \frac{\text{Var}(a^\top X) \mathbb{E}[f(a^\top X)]}{\text{Var}(a^\top X)} \geq L^{-1}.$$

To bound $\|\hat{Y}\|_{\mathbb{V}_2}$ we now first apply [35, Theorem 5.2.2] to the transformed variable $Z = \sigma_P^{-1}a^\top X$, which satisfies $Z \sim \mathcal{N}(0, 1)$, to get $\|f(a^\top X) - \mathbb{E}[f(a^\top X)]\|_{\mathbb{V}_2} \leq \text{CL}\sigma_P$. Therefore

$$\|\hat{Y}\|_{\mathbb{V}_2} \leq \|f(a^\top X) - \mathbb{E}[f(a^\top X)] + \zeta\|_{\mathbb{V}_2} \leq \|f(a^\top X) - \mathbb{E}[f(a^\top X)]\|_{\mathbb{V}_2} + \|\zeta\|_{\mathbb{V}_2} \leq \text{CL}\sigma_P + \sigma_\zeta.$$

Using $\kappa(P, X) \leq C$, and plugging in the bounds on $\|\hat{Y}\|_{\mathbb{V}_2}$, $\|b\|_2$, and $\|P\Sigma^\top \hat{X}\|_{\mathbb{V}_2} = \frac{C}{\sigma_P}$ and $\|Q\Sigma^\top \hat{X}\|_{\mathbb{V}_2} = C\sqrt{\|Q\Sigma^\top Q\|_2}$ (which by (14) holds for some universal constants $C > 0$), the claim follows. \(\square\)

Corollary 13 shows that in case of monotonic SIMs the variance in the direction of the index vector, $\sigma_P^2 = \text{Var}(a^\top X)$, influences the index estimation differently than the spectrum of $Q\Sigma^\top Q$. Namely, as long as $\sigma_P^2 \gg \sigma_\zeta^2$, a smaller $\sigma_P$ has a provably beneficial effect on index vector estimation, whereas small nonzero eigenvalues of $\Sigma$ corresponding to eigenvectors in $\text{Im}(Q)$ could worsen the accuracy. We will use this observation in the next section as a guiding principle for developing a modified estimator. We also note that the normality of $X$ is only a technical condition (needed for the use of Stein’s Lemma), and is not crucial for the observation.

### 4.2 Averaged conditional least squares for the single index model

Following the preceding discussion, we study an alternative estimation procedure. We first split the data into subsets, each of which has reduced variance in the direction of the index vector. Then, we compute and average out the estimators from each subset. Since we have no a priori

| $J = 1$ | $J = 2$ | $J = 3$ | $J = 4$ | $J = 5$ |
|--------|--------|--------|--------|--------|
| ![Subset 1](image1.png) | ![Subset 2](image2.png) | ![Subset 3](image3.png) | ![Subset 4](image4.png) | ![Subset 5](image5.png) |

**Figure 2:** $(X, Y)$ sampled according to $X \sim \text{Uni}(\{X : \|X\|_2 \leq 1\})$, $Y = f(a^\top X) + \zeta$ where $\text{span}(a)$ is the horizontal line, and $\zeta \sim \mathcal{N}(0, 0.01 \text{Var}(f(a^\top X)))$. The data is partitioned according to a dyadic level set partition in into $J$ intervals, and the color indicates the labeling.
knowledge about the index vector, constructing such a partition seems challenging. However, in the case of a monotonic link function the partitioning is induced by a decomposition of \( \text{Im}(Y) \) into equisized intervals, see Figure 2. In the following we assume \( Y \in [0,1) \) almost surely, for notational simplicity, and propose the following procedure.

Denote by \( \mathcal{R}_{J,\ell} := \left[ \frac{\ell - 1}{J}, \frac{\ell}{J} \right) \) a dyadic decomposition of \([0,1)\) into \( J \) intervals. Furthermore, define so-called level sets \( \mathcal{S}_{J,\ell} = \{(X_i, Y_i) : Y_i \in \mathcal{R}_{J,\ell}\} \), which induce a partition of the data set into \( J \) subsets based on the respective response. Then estimate \( a \) according to the following algorithm.

**Step 1** Solve (25) on each subset \( \mathcal{S}_{J,\ell} \), by computing \( \hat{c}_{J,\ell} \in \mathbb{R} \) and \( \hat{b}_{J,\ell} \in \mathbb{R}^D \).

**Step 2** Denote the empirical density \( \hat{\rho}_{J,\ell} := |\mathcal{S}_{J,\ell}|/N \), set the thresholding parameter \( \alpha > 0 \), and compute the averaged outer product matrix

\[
\hat{M}_J = \sum_{\ell=1}^J \mathbb{1}_{[\alpha J^{-1},1]}(\hat{\rho}_{J,\ell})\hat{\rho}_{J,\ell}\hat{b}_{J,\ell}\hat{b}_{J,\ell}^\top.
\]

**Step 3** Use the eigenvector corresponding to the largest eigenvalue of \( M_J \), denoted as \( u_1(\hat{M}_J) \), as an approximation of the index vector \( a \).

The parameter \( \alpha \) is used to ensure numerical stability by suppressing the contributions of sparsely populated subsets. In other words, we only keep those level sets whose empirical mass behaves as if \( Y \) were uniformly distributed over \( \text{Im}(Y) \) (which can in some problems be achieved through a suitable transformation of the responses). The parameter \( J \) on the other hand defines the number of sets we use in the partition of the given data set, and dictates the trade-off between the magnitude of \( \text{Var}(a^\top X|Y \in \mathcal{R}_{J,\ell}) \) and the number of samples \( |\mathcal{S}_{J,\ell}| \) in a given level set.

We now conduct a theoretical analysis of this approach under the following assumptions:

(A1) \( b_{J,\ell} := \text{Cov}(X|Y \in \mathcal{R}_{J,\ell}) \text{Cov}(X,Y|Y \in \mathcal{R}_{J,\ell}) \in \text{span}\{a\} \) for all \( \ell \in [J] \).

(A2) Condition (15) holds for all conditional distributions induced by \( Y \in \mathcal{R}_{J,\ell} \).

Note that assumptions (A1) and (A2) are not particularly restrictive. For example, it can be shown that (A1) holds if \( X \) is elliptically symmetric, which is a standard assumption when using the ordinary least squares functional (25), and if the function noise \( Y = E[Y|X] \) is independent of \((\text{Id} - aa^\top)X \) given \( a^\top X \). On the other hand (A2) is satisfied \( e.g. \) if conditional measures of \( X|Y \in \mathcal{R}_{J,\ell} \) are absolutely continuous with respect to the Lebesgue measure on \( \text{Im}(\text{Cov}(X,Y|Y \in \mathcal{R}_{J,\ell})) \) for all \( \ell \in [J] \).

**Theorem 14.** Assume (A1), (A2), \( Y \in [0,1) \) almost surely, and that \( X \) is sub-Gaussian. Let \( J > 0, \alpha > 0, u > 0, \varepsilon > 0 \) and assume we are given \( N \) iid. copies of \((X,Y)\). Denote \( \text{P} := aa^\top, Q := \text{Id} - \text{P}, \Sigma_{J,\ell} := \text{Cov}(X|Y \in \mathcal{R}_{J,\ell}) \) and

\[
\kappa_{J,\ell} := \kappa(P, X|Y \in \mathcal{R}_{J,\ell}) \vee \kappa(Q, X|Y \in \mathcal{R}_{J,\ell}), \quad \text{and} \quad \kappa_J := \max_{\ell \in I_J} \kappa_{J,\ell},
\]

where \( I_J \) contains the active level sets, i.e. \( I_J := \{\ell \in [J] : \hat{\rho}_{J,\ell} \geq \alpha J^{-1}\} \). Provided

\[
\frac{N}{J(1 + \log(J))} > \alpha^{-1} C(\text{rank}(\Sigma) + u)(\kappa_J \vee \varepsilon^{-2}),
\]

there exists a sign \( s \in \{-1, 1\} \) so that with probability at least \( 1 - \exp(-u) \)

\[
\|su_1(\hat{M}_J) - a\|_2 \leq \frac{\varepsilon}{\sqrt{J}} \left( \frac{\sum_{\ell \in I_J} \hat{\rho}_{J,\ell} \kappa_{J,\ell} \|Q\Sigma_{J,\ell}^\top \tilde{X}|Y \in \mathcal{R}_{J,\ell}\|_2^2}{\lambda_1(\hat{M}_J)} \right)^{1/2}.
\]
There are several ways to read Theorem 14. First, for a fixed parameter $J$, we can consider the asymptotic setting $N \to \infty$, and select $\varepsilon^{-2} > \kappa_J$. Rewriting (33) then gives $N^{-1/2}$ consistency. In other words, we have the same error rate as with the standard estimator (25).

Second, we can also try and improve the rate beyond $N^{-1/2}$ by selecting $J$ as a function that grows with $N$, so long as Step 1 can be conducted. Namely, expressing $J$ through the requirement on $N$ in (32), and plugging into (33), implies that an $\log(N)N^{-1}$ rate is achievable with the choice $J \asymp N/\log(N)$ as long as the remaining terms are balanced. As we will now discuss, the latter does not hold in the limit $N \to \infty$, that is, once the number of points (and thus the number of level sets $J$), is large enough. In short, this due to the effects the splitting of data has on the distribution of $X|Y \in \mathcal{R}_{f,t}$ in presence of noise, which is observed through the behavior of $\lambda_1(\hat{M}_J)$ with respect to $J$.

**Numerical setup and parameter choice.** We sample $X \sim \mathcal{N}(0, I_d)$, with $D = 10$, and let $a = (1, 0, \ldots, 0) \top$ (the specific choice of $a$ is irrelevant for the results due to the rotational
invariance of $X$). Responses are generated by $Y = f(a^\top X) + \zeta$, where $\zeta \sim \mathcal{N}(0, \sigma^2 \text{Var}(f(a^\top X)))$. We set $\alpha = 0.05$ and additionally exclude subsets with $|\mathcal{S}_{J,\ell}| < 2D$, for the sake of numerical stability. Our goal is to compare estimation of the index vector using the standard approach (25), with the strategy proposed in this section.

For the latter, the critical step of the approach is the selection of $J$ with respect to $N$ and other parameters. The main issue of why $J$ cannot always grow with $N$ at a sufficiently high rate is to do with the behavior of ordinary least squares solutions $b_{J,\ell}$. Recall first that $\|b_{J,\ell}\|_2 = \text{Cov}(a^\top X, Y|Y \in \mathcal{R}_{J,\ell})/\text{Var}(a^\top X|Y \in \mathcal{R}_{J,\ell})$. By (28) and (29), the precision of estimating the index vector would degrade if $\|b_{J,\ell}\|_2$ decays with $J$. Thus, the issue arises if $\text{Cov}(a^\top X, Y|Y \in \mathcal{R}_{J,\ell})$ starts rapidly decreasing as $J$ increases beyond a certain threshold, whereas at the same time $\text{Var}(a^\top X|Y \in \mathcal{R}_{J,\ell})$ stays roughly constant.

If the link function $f$ is monotonic, this happens when $|\mathcal{R}_{J,\ell}| = J^{-1}$ approaches the noise level $\sigma_\zeta$, due to the fact that increasing $J$ further will not decrease $\text{Var}(a^\top X|Y \in \mathcal{R}_{J,\ell})$, which is dominated by noise level, but it will decrease $\text{Cov}(a^\top X, Y|Y \in \mathcal{R}_{J,\ell})$, since we decrease the variability in $Y$. If the link is not monotonic, the same phenomenon usually occurs earlier, but instead depends on the non-monotonicity.

The consequence of the decay of $\|b_{J,\ell}\|_2$ is that $\lambda_1(\hat{M}_J)$, also start rapidly decreasing, which in terms of (33) degrades the error rate. Therefore, we instead pursue a pragmatic strategy for the selection of $J$. Inserting the relationship between $\varepsilon$, $J$ and $N$ from (32) we see that the error is minimized when maximizing $J\lambda_1(\hat{M}_J)$. We thus propose to adaptively choose $J$ according to

$$J^* := \max\{J = \lceil(1.5)^k\rceil \mid k \in \mathbb{N}_0 : J\lambda_1(\hat{M}_J) > J'\lambda_1(\hat{M}_{J'}) \text{ for all } J' \text{ such that } J' < J\},$$

where we choose an exponential grid in $\mathbb{N}$ in order to decrease the computational demands.

**Numerical experiments.** Figure 3 shows the errors $\|\hat{a} - a\|_2$ and the corresponding optimized choices $J^*$, of the number of level sets $J$, for different link functions $f$. Solid lines correspond to the estimator (25), the dashed lines to $u_{\lambda_1}(\hat{M}_{J^*})$, and different colors represent different noise levels $\sigma_\zeta$. In Figures 3b - 3d we see that the strategy presented in this section performs substantially better for monotonic link function. On the other hand, in Figures 3a, 3e and 3f the two approaches achieve similar performance. In case of 3a this is because (25) is indeed optimal, according to the Gauss-Markov Theorem, whereas link functions in 3e, 3f, are not monotonic. In the latter case, the plots of $J^*$ confirm that $\lambda_1(\hat{M}_J)$ decays rapidly as a function of $J$, leaving $J^*$ essentially constant as a function of $N$.

Let us examine the results for monotonic functions in more detail. The plots for $J^*$ in Figures 3b - 3d show that the number of level sets $J^*$ indeed grows as a function of $N$, and it does so up to a level dictated by the noise $\sigma_\zeta$. This shows that $\lambda_1(\hat{M}_J)$ does not decay rapidly over a reasonably large range of $N$ values, i.e. until $J^{-1} \approx \sigma_\zeta$. A consequence of this approach is an $N^{-1}$ estimation rate for the index vector, provided the noise level is not dominant compared to $J^{-1}$. Specifically, in the noise-free case this holds asymptotically as $N \to \infty$. On the other hand, in the case of corrupted $Y$'s we have a sharp transition from an $N^{-1}$ rate into the usual $N^{-1/2}$ rate. The number of points $N$ at which this transition occurs depends inversely on the level of noise.

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5 Appendix

5.1 Additional technical results

Lemma 15 (Some properties of the sub-Gaussian norm). Let \( X, Z \) be two sub-Gaussian random vectors in \( \mathbb{R}^D \), let \( \Sigma = \text{Cov}(X) \), and \( A \in \mathbb{R}^{D \times D} \). Then we have

1. \( \|X - \mathbb{E}X\|_{\psi_2} \leq C\|X\|_{\psi_2} \) (holds also for sub-Exponential random variables),
2. \( \|A\mathbb{E}X\|_{\psi_2} \leq \|A\|_2\|P_{\text{Im}(A^\top)}\tilde{X}\|_{\psi_2} \),
3. \( \|\Sigma A^\top\|_2 \leq C\|A\tilde{X}\|_{\psi_2} \),
4. \( \kappa(A, X) \geq C\kappa(A, \Sigma) \geq C \) if \( A\Sigma \neq 0 \),
5. \( X^\top Z \) is sub-Exponential with \( \|\tilde{X}^\top \tilde{Z} - \mathbb{E}[\tilde{X}^\top \tilde{Z}]\|_{\psi_1} \leq C\|\tilde{X}\|_{\psi_2}\|\tilde{Z}\|_{\psi_2} \).

Proof. Property (1) is shown in [35, Lemma 2.6.8] for sub-Gaussian random variables, for an absolute constant \( C \). Applying the definition of the sub-Gaussian norm (9) the claim follows, since \( v^\top X \) is a sub-Gaussian random variable for every \( v \in \mathbb{S}^{D-1} \). The same line of arguments holds for sub-Exponential vectors as well.

For (2) we compute for arbitrary \( v \in \mathbb{S}^{D-1} \) and \( A^\top v \in \text{Im}(A^\top) \)

\[
\left\|v^\top A\tilde{X}\right\|_{\psi_2} = \left\|A^\top v\right\|_2 \left\| \left( A^\top v / \left\|A^\top v\right\|_2 \right)^\top \tilde{X} \right\|_{\psi_2} \leq \left\|A\right\|_2 \sup_{u \in \text{Im}(A^\top)} \left\| u^\top \tilde{X} \right\|_{\psi_2} \leq \left\|A\right\|_2 \left\|P_{\text{Im}(A^\top)}\tilde{X}\right\|_{\psi_2}.
\]

For (3) we first note that [35, Proposition 2.5.2] implies \( \text{Var}(u) \leq C\|\tilde{u}\|_{\psi_2}^2 \) for any sub-Gaussian \( u \), where \( \tilde{u} = u - \mathbb{E}u \) and \( C > 0 \) is an absolute constant. Thus, for every \( v \in \mathbb{S}^{D-1} \)

\[
v^\top \text{Cov}(AX) v = \text{Var}(v^\top AX) \leq C\left\|v^\top A\tilde{X}\right\|_{\psi_2}^2.
\]

Taking the supremum over \( v \in \mathbb{S}^{D-1} \), the result follows since \( \text{Cov}(AX) \) is positive semidefinite.

Property (4) is an immediate consequence of (3) for \( X \) and \( \Sigma^\top X \), and since \( \kappa(A, \Sigma) \geq 1 \).

Property (5) follows from the centering property (1) and [35, Lemma 2.7.6]. \( \square \)

Lemma 16. Let \( A \in \mathbb{R}^{D \times D} \) be positive semidefinite, and \( B_1 \in \mathbb{R}^{d_1 \times D} \), \( B_2 \in \mathbb{R}^{d_2 \times D} \). For \( u \in \mathbb{R}^{d_1} \), \( v \in \mathbb{R}^{d_2} \) we have \( u^\top B_1 A^\top B_2^\top v \leq \sqrt{u^\top B_1 A^\top B_1^\top u} \sqrt{v^\top B_2 A^\top B_2^\top v} \). Moreover, \( \|B_1 A B_2\|_2 \leq \|B_1^\top A^\top B_2^\top\|_2 \|B_2 A B_2^\top\|_2 \).

Proof. Applying the Cauchy-Schwartz inequality we have

\[
u^\top B_1 A B_2^\top v = \left\langle A^{1/2} B_1^\top u, A^{1/2} B_2^\top v \right\rangle \leq \left\|A^{1/2} B_1^\top u\right\|_2 \left\|A^{1/2} B_2^\top v\right\|_2.
\]

By the same line of argument we have \( \left\|A^{1/2} B_1^\top u\right\|_2^2 = u^\top B_1 A B_1^\top u \) and \( \left\|A^{1/2} B_2^\top v\right\|_2^2 = v^\top B_2 A B_2^\top v \), giving the first statement. Considering now \( \|u\|_2 = \|v\|_2 = 1 \), we have

\[
\sup_{\|u\|_2=1, \|v\|_2=1} u^\top B_1 A B_2^\top v \leq \sqrt{\sup_{\|u\|_2=1} u^\top B_1 A B_1^\top u} \sqrt{\sup_{\|v\|_2=1} v^\top B_2 A B_2^\top v}.
\]

(36)

Notice that since \( A \) is positive semidefinite, then \( B_1 A B_1^\top \) and \( B_2 A B_2^\top \) are positive semidefinite. Therefore,

\[
\sup_{\|u\|_2=1} u^\top B_1 A B_1^\top u = \sup_{\|u\|_2=1} \left\| (B_1 A B_1^\top)^{1/2} u \right\|_2^2 = \left\| B_1 A B_1^\top \right\|_2,
\]

and an analogous expression holds for the other term. Identifying the quadratic form on the left hand side in (36) as the operator norm of \( B_1 A B_2 \), the conclusion follows. \( \square \)
The following is a standard concentration bound for sub-Gaussian and sub-Exponential random vectors around their mean.

**Lemma 17.** Fix $u > 0$, $\varepsilon > 0$, and let $\{X_i : i \in [N]\}$ be independent copies of a centred random vector $X \in \mathbb{R}^D$, and denote the sample mean $\hat{\mu} := \frac{1}{N} \sum_{i=1}^{N} X_i$. We then have

1. If $\|X\|_{\psi_2} < \infty$ and $N > C(D + u)\varepsilon^{-2}$, we have $\|\hat{\mu}\|_{2} \leq \varepsilon \|X\|_{\psi_2}$ with probability at least $1 - \exp(-u)$.

2. If $\|X\|_{\psi_1} < \infty$ and $N > C(D + u)(\varepsilon^{-1} \lor \varepsilon^{-2})$, we have $\|\hat{\mu}\|_{2} \leq \varepsilon \|X\|_{\psi_1}$ with probability at least $1 - \exp(-u)$.

**Proof.** The argument for the two bounds follows along analogous lines. Let $\delta < 1/4$, and $\mathcal{N}$ be a $\delta$-net of $S^{D-1}$. We first use [35, Exercise 4.4.3] to rewrite

$$\|\hat{\mu}\|_{2} = \sup_{v \in S^{D-1}} \|v^\top \hat{\mu}\| = \sup_{v \in S^{D-1}} \sum_{i=1}^{N} v^\top X_i \leq 2 \sup_{v \in \mathcal{N}} \sum_{i=1}^{N} v^\top X_i.$$ 

Considering fixed $v \in \mathcal{N}$, $N^{-1} \sum_{i=1}^{N} v^\top X_i$ is a sum of either sub-Gaussian, or sub-Exponential random variables, with norm given by $\|v^\top X_i\|_{\psi_1} \leq \|X\|_{\psi_1}$, or $\|v^\top X_i\|_{\psi_2} \leq \|X\|_{\psi_2}$. Therefore, Hoeffding’s inequality [35, Theorem 2.6.2], in the sub-Gaussian case, or Bernstein’s inequality [35, Theorem 2.8.1], in the sub-Exponential case, provide concentration bounds for the sums. The result follows by combining the concentration bounds with the union bound over $v \in \mathcal{N}$, where the number of events is bounded by $|\mathcal{N}| \leq 12^D$ [35, Corollary 4.2.13].

### 5.2 Proofs for Section 2

**Proof of Lemma 2.** Let $\tilde{X} = X - \mathbb{E}X$, and define $d_A = \text{rank}(A\Sigma)$, $d_B = \text{rank}(B\Sigma)$. Let $U_A \in \mathbb{R}^{d_A \times D}$ and $U_B \in \mathbb{R}^{d_B \times D}$ be matrices whose rows contain the orthonormal basis for $\text{Im}(A\Sigma)$ and $\text{Im}(B\Sigma)$, respectively. Since $\Sigma$ and $\hat{\Sigma}$ are symmetric, and $\text{Im}(\hat{\Sigma}) \subset \text{Im}(\Sigma)$, we have $\hat{\Sigma} - \Sigma = P_\Sigma(\hat{\Sigma} - \Sigma)P_\Sigma$, where $P_\Sigma$ is the orthogonal projection onto $\text{Im}(\Sigma)$. We thus have

$$\left\|A(\hat{\Sigma} - \Sigma)^{B\top}\right\|_{2} = \left\|A(\hat{\Sigma} - \Sigma)B_\Sigma^\top\right\|_{2},$$

for $A_\Sigma = U_AAP_\Sigma \in \mathbb{R}^{d_A \times D}$ and $B_\Sigma = U_BBP_\Sigma \in \mathbb{R}^{d_B \times D}$. Denote now $\hat{\Sigma} = N^{-1} \sum_{i=1}^{N} \hat{X}_i\hat{X}_i^\top$. Notice that $\hat{\Sigma}$, compared to the empirical covariance $\hat{\Sigma}$, uses the true, instead of the empirical mean of $\tilde{X}$. We then have

$$\left\|A_\Sigma(\hat{\Sigma} - \Sigma)B_\Sigma^\top\right\|_{2} \leq \left\|A_\Sigma(\hat{\Sigma} - \Sigma)B_\Sigma^\top\right\|_{2} + \left\|\frac{1}{N} \sum_{i=1}^{N} A_\Sigma \hat{X}_i\right\|_{2} + \left\|\frac{1}{N} \sum_{i=1}^{N} B_\Sigma \hat{X}_i\right\|_{2}.$$ 

Using the concentration inequality for sub-Gaussian random variables, i.e., Lemma 17, the second term is always of higher order, and the resulting error can be absorbed into the first term. Thus, in the following we focus on $\|A_\Sigma(\hat{\Sigma} - \Sigma)B_\Sigma^\top\|_{2}$.

We closely follow the proof of [34, Proposition 2.1]. Let $\delta < 1/4$, and by $\mathcal{N}$, $\mathcal{M}$ denote $\delta$-nets of spheres $S^{d_A}$ and $S^{d_B}$. From [35, Exercise 4.4.3], and using $(1 - 2\delta)^{-1} \leq 2$, we get

$$\left\|A_\Sigma(\hat{\Sigma} - \Sigma)B_\Sigma^\top\right\|_{2} \leq 2 \sup_{x \in \mathcal{N}} \left\langle A_\Sigma(\hat{\Sigma} - \Sigma)B_\Sigma^\top x, y \right\rangle \leq 2 \sup_{x \in \mathcal{N}} \left\langle (\hat{\Sigma} - \Sigma)B_\Sigma^\top x, A_\Sigma y \right\rangle. \quad (37)$$

Consider now any pair $(x, y) \in \mathcal{N} \times \mathcal{M}$, and write

$$\left\langle (\hat{\Sigma}B_\Sigma^\top x, A_\Sigma y) = \frac{1}{N} \sum_{i=1}^{N} \left\langle \hat{X}_i(\hat{X}_i^\top B_\Sigma x), A_\Sigma y \right\rangle = \frac{1}{N} \sum_{i=1}^{N} \left\langle A_\Sigma \hat{X}_i, y \right\rangle \left\langle B_\Sigma \hat{X}_i, x \right\rangle. \right.$$
Since \( \langle A_\Sigma \tilde{X}_i, y \rangle \) and \( (B_\Sigma \tilde{X}_i, x) \) are sub-Gaussian, their product is sub-Exponential, and from [35, Lemma 2.7.7] we have
\[
\| \langle A_\Sigma \tilde{X}_i, y \rangle \langle B_\Sigma \tilde{X}_i, x \rangle \|_{\psi_1} \leq \left\| \langle A_\Sigma \tilde{X}_i, y \rangle \right\|_{\psi_2} \left\| \langle B_\Sigma \tilde{X}_i, x \rangle \right\|_{\psi_2} \leq \| A_\Sigma \tilde{X} \|_{\psi_2} \| B_\Sigma \tilde{X} \|_{\psi_2}.
\]
Since \( E[\Sigma] = \Sigma \), by Lemma 17 we have for \( \varepsilon > 0 \) and whenever \( N > C(1 + u)(\varepsilon^{-1} \vee \varepsilon^{-2}) \)
\[
P \left( \left| \langle \Sigma B_\Sigma^T x, A_\Sigma^T y \rangle - \langle \Sigma B_\Sigma^T x, A_\Sigma^T y \rangle \right| \geq \varepsilon \| A_\Sigma \tilde{X} \|_{\psi_2} \| B_\Sigma \tilde{X} \|_{\psi_2} \right) \leq \exp(-u).
\]
The size of the nets can be bounded as \( |N| \leq \| E \| \leq \| \Sigma \| \), see [35, Corollary 4.2.13]. Thus, considering all pair \( (x, y) \in N \times M \) and using the union bound we get
\[
P \left( \sup_{x \in N, y \in M} \left| \langle \Sigma B_\Sigma^T x, A_\Sigma^T y \rangle - \langle \Sigma B_\Sigma^T x, A_\Sigma^T y \rangle \right| \geq \varepsilon \| A_\Sigma \tilde{X} \|_{\psi_2} \| B_\Sigma \tilde{X} \|_{\psi_2} \right) \leq |N| \| M \| \exp(-u - \delta(d_A + d_B) \log(12)) \]
\[
\leq \exp((-d_A + d_B) \varepsilon^{-1} \vee \varepsilon^{-2}),
\]
whenever \( N > C(d_A + d_B + u)(\varepsilon^{-1} \vee \varepsilon^{-2}) \), where we adjust the confidence level \( u \) to compensate for the union bound. Using the \( \delta \)-net approximation bound (37) we thus get
\[
P \left( \left\| A_\Sigma (\tilde{\Sigma} - \Sigma) B_\Sigma^T \right\|_2 \geq \varepsilon \| A_\Sigma \tilde{X} \|_{\psi_2} \| B_\Sigma \tilde{X} \|_{\psi_2} \right) \]
\[
\leq P \left( \sup_{x \in N, y \in M} \left| \langle \Sigma B_\Sigma^T x, A_\Sigma^T y \rangle - \langle \Sigma B_\Sigma^T x, A_\Sigma^T y \rangle \right| \geq \varepsilon \frac{\| A_\Sigma \tilde{X} \|_{\psi_2} \| B_\Sigma \tilde{X} \|_{\psi_2}}{2} \right).
\]
The result now follows since \( \| A_\Sigma \tilde{X} \|_{\psi_2} = \| A \tilde{X} \|_{\psi_2} \) and \( \| B_\Sigma \tilde{X} \|_{\psi_2} = \| B \tilde{X} \|_{\psi_2} \).

5.3 Proofs for Section 3

Lemma 18. Fix a confidence level \( u > 0 \). Whenever \( N > C(\text{rank}(\Sigma) + u) \kappa(\text{Id}, X)^2 \), we have \( \text{Im}(\Sigma) = \text{Im}(\Sigma) \) with probability \( 1 - \exp(-u) \).

Proof. Since \( \text{Im}(\Sigma) \) is the minimal dimensional vector space in which \( \tilde{X} \) is contained almost surely, it follows that \( \text{Im}(\tilde{\Sigma}) \subseteq \text{Im}(\Sigma) \) almost surely. Thus, it suffices to show that \( \text{rank}(\tilde{\Sigma}) = \text{rank}(\Sigma) =: d \). Let \( U = [u_1(\Sigma) \ldots u_d(\Sigma)] \in \mathbb{R}^{d \times d} \) whose rows form the eigenbasis for \( \text{Im}(\Sigma) \). Using Lemma 2 with \( \varepsilon = 1/\| \Sigma \|_2 \| U \tilde{X} \|_{\psi_2}^2 \), with probability \( 1 - \exp(-u) \) we have
\[
\left\| U^T (\tilde{\Sigma} - \Sigma) U \right\|_2 < \frac{1}{2} \| \Sigma \|_2^{-1}, \text{ if } N > C(d + u) \left( \| U \tilde{X} \|_{\psi_2}^2 \| \Sigma \|_2 \right) \vee \| U \tilde{X} \|_{\psi_2}^4 \| \Sigma \|_2^2. \tag{38}
\]
Conditioned on this event we get for any unit norm \( v \in \text{Im}(\Sigma) \)
\[
v^T \tilde{\Sigma} v = v^T \Sigma v + v^T (\tilde{\Sigma} - \Sigma) v \geq \lambda_d(\Sigma) - \frac{1}{2} \lambda_d(\Sigma) = \frac{1}{2} \lambda_d(\Sigma) > 0,
\]
which implies \( \text{rank}(\tilde{\Sigma}) = d \). It remains to simplify the condition on \( N \) in (38). Since \( U \) is a basis for \( \text{Im}(\Sigma) \), we have \( \| U \tilde{X} \|_{\psi_2} = \| \tilde{X} \|_{\psi_2} \). Moreover, since \( \text{Cov}(\Sigma^T X) = \Sigma^T \text{Cov}(X) \Sigma = \Sigma^T \), we always have \( \| \Sigma \|_2 \leq C \| \Sigma^T \tilde{X} \|_{\psi_2} \) according to Lemma 15. Therefore, \( \| U \tilde{X} \|_{\psi_2}^2 \| \Sigma \|_2 \leq C \kappa(\text{Id}, X) \), and the claim follows.
\textbf{Proof of Theorem 7.} We can condition on $\text{Im}(\hat{\Sigma}) = \text{Im}(\Sigma)$ since this holds with probability $1 - \exp(-u)$ either by assumption (15) or by Lemma 18 and the corresponding requirement on $N$, as assumed in the statement. Let now $\Delta = \hat{\Sigma} - \Sigma$ and use [36] to obtain the identity

\[\hat{\Sigma}^\dagger - \Sigma^\dagger = (\hat{\Sigma}^\dagger - \Sigma^\dagger)^\top = -\Sigma^\dagger \Delta \hat{\Sigma}^\dagger = -\Sigma^\dagger \Delta \Sigma^\dagger - \Sigma^\dagger \Delta (\hat{\Sigma}^\dagger - \Sigma^\dagger). \quad (39)\]

Multiplying from left with $\tilde{A}$ and from right with $\tilde{B}^\top$, for $\tilde{A} \in \mathbb{R}^{d_1 \times D}$, $\tilde{B} \in \mathbb{R}^{d_2 \times D}$, and rearranging the terms, gives

\[\tilde{A} \left( \text{Id} + \Sigma^\dagger \Delta \right) \left( \hat{\Sigma}^\dagger - \Sigma^\dagger \right) \tilde{B}^\top = -\tilde{A} \Sigma^\dagger \Delta \Sigma^\dagger \tilde{B}^\top. \]

Now, $\text{Id} + \Sigma^\dagger \Delta$ is invertible whenever $\|\Sigma^\dagger \Delta\|_2 < 1$. Thus, setting $\tilde{A} = A \left( \text{Id} + \Sigma^\dagger \Delta \right)^{-1}$ and $\tilde{B} = B$ we get

\[A \left( \hat{\Sigma}^\dagger - \Sigma^\dagger \right) B^\top = -A \left( \text{Id} + \Sigma^\dagger \Delta \right)^{-1} \Sigma^\dagger \Delta \Sigma^\dagger B^\top \]

\[= -A \Sigma^\dagger \Delta \Sigma^\dagger B^\top - A \Sigma^\dagger \sum_{k=0}^{\infty} (-\Sigma^\dagger \Delta)^k \Sigma^\dagger \Delta \Sigma^\dagger B^\top, \quad (40)\]

where we used the Neumann series form of the inverse. We can now use Lemma 2 to bound the spectral norms of individual terms in (40). With probability $1 - 4 \exp(-u)$ we have

\[\left\| A \Sigma^\dagger \Delta \Sigma^\dagger B^\top \right\|_2 \leq \frac{\varepsilon}{2} \left\| A \Sigma^\dagger \tilde{X} \right\|_{\psi_2} \left\| B \Sigma^\dagger \tilde{X} \right\|_{\psi_2}, \quad \left\| \Sigma^\dagger \Delta \Sigma^\dagger B^\top \right\|_2 \leq \frac{\varepsilon}{2} \left\| B \Sigma^\dagger \tilde{X} \right\|_{\psi_2} \left\| \Sigma^\dagger \tilde{X} \right\|_{\psi_2}, \quad \text{for } \varepsilon > 0 \]

and

\[\left\| A \Sigma^\dagger \Delta \right\|_2 \leq \frac{1}{2} \left\| \Sigma^\dagger \tilde{X} \right\|_{\psi_2}, \quad \left\| \Sigma^\dagger \right\|_2 \leq \frac{1}{2}, \quad \text{taking } \varepsilon = \frac{1}{2\sqrt{\kappa(\text{Id}, X)}}, \quad (41)\]

whenever $N > 4C(\text{rank}(\Sigma) + u)(\kappa(\text{Id}, X) \vee \varepsilon^{-2})$. The last inequality also ensures invertibility of $\Sigma^\dagger \Delta$, and thus conditioned on it we can use (40). Using (41) and the submultiplicity of the spectral norm we have

\[\left\| A \left( \hat{\Sigma}^\dagger - \Sigma^\dagger \right) B^\top \right\|_2 \leq \left\| A \Sigma^\dagger \Delta \Sigma^\dagger B^\top \right\|_2 + \left\| A \Sigma^\dagger \Delta \right\|_2 \sum_{k=0}^{\infty} (-\Sigma^\dagger \Delta)^k \left\| \Sigma^\dagger \Delta \Sigma^\dagger B^\top \right\|_2 \]

\[\leq \varepsilon \left\| A \Sigma^\dagger \tilde{X} \right\|_{\psi_2} \left\| B \Sigma^\dagger \tilde{X} \right\|_{\psi_2}. \]

The result follows by adjusting the probability $1 - 5 \exp(-u)$ to $1 - \exp(-u)$ by modifying the constant $C$ in the requirement on $N$. \qed

\textbf{Proof of Theorem 9.} We can condition on $\text{Im}(\hat{\Sigma}) = \text{Im}(\Sigma)$ since it holds with probability $1 - \exp(-u)$ either by assumption (15), or by Lemma 18 due to the assumption on $N$. Using (39) for $P, Q \in \mathbb{R}^{D \times D}$

\[P(\hat{\Sigma}^\dagger - \Sigma^\dagger) = -P \Sigma^\dagger \Delta \Sigma^\dagger P - P \Sigma^\dagger \Delta P(\hat{\Sigma}^\dagger - \Sigma^\dagger)P - P \Sigma^\dagger Q(\hat{\Sigma}^\dagger - \Sigma^\dagger)P, \quad (42)\]

\[Q(\hat{\Sigma}^\dagger - \Sigma^\dagger) = -Q \Sigma^\dagger \Delta \Sigma^\dagger P - Q \Sigma^\dagger \Delta P(\hat{\Sigma}^\dagger - \Sigma^\dagger)P - Q \Sigma^\dagger Q(\hat{\Sigma}^\dagger - \Sigma^\dagger)P. \quad (43)\]

This defines a system of matrix equations with two unknowns, which we write as $SU = R$ where

\[U = \begin{bmatrix} P(\hat{\Sigma}^\dagger - \Sigma^\dagger) \\ Q(\hat{\Sigma}^\dagger - \Sigma^\dagger) \end{bmatrix} \in \mathbb{R}^{2D \times D}, \quad R = \begin{bmatrix} -P \Sigma^\dagger \Delta \Sigma^\dagger P \\ -Q \Sigma^\dagger \Delta \Sigma^\dagger P \end{bmatrix} \in \mathbb{R}^{2D \times D}, \]

\[S = \begin{bmatrix} \text{Id}_D + P \Sigma^\dagger \Delta P & P \Sigma^\dagger Q \\ Q \Sigma^\dagger \Delta P & \text{Id}_D + Q \Sigma^\dagger Q \end{bmatrix} \]:

\[= \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \in \mathbb{R}^{2D \times 2D}.\]
Provided $S_{11}$ and $S_{22} - S_{21}S_{11}^{-1}S_{12}$ are invertible, the inverse of $S$ is precisely

$$S^{-1} = \begin{bmatrix}
S_{11}^{-1} + S_{11}^{-1}S_{12}(S_{22} - S_{21}S_{11}^{-1}S_{12})^{-1}S_{21}S_{11}^{-1} & -S_{11}^{-1}S_{12}(S_{22} - S_{21}S_{11}^{-1}S_{12})^{-1} \\
-(S_{22} - S_{21}S_{11}^{-1}S_{12})^{-1}S_{21}S_{11}^{-1} & (S_{22} - S_{21}S_{11}^{-1}S_{12})^{-1}
\end{bmatrix}.$$  

In order to bound entries of the solution $U$ we can now compute and estimate the entries of inverse $S^{-1}$. First, whenever $\|P\Sigma^t\Delta P\|_2 < 1$, we have $S_{11}^{-1} = \sum_{k=0}^{\infty} (-P\Sigma^t\Delta P)^k$. Moreover

$$S_{22} - S_{21}S_{11}^{-1}S_{12} = Id + Q\Sigma^t\Delta Q + Q\Sigma^t\Delta P \sum_{k=0}^{\infty} (-P\Sigma^t\Delta P)^k P\Sigma^t\Delta Q =: Id + H$$

This is invertible whenever $\|H\|_2 < 1$. In this case $(S_{22} - S_{21}S_{11}^{-1}S_{12})^{-1} = \sum_{k=0}^{\infty} (-H)^k$, and

$$-(S_{22} - S_{21}S_{11}^{-1}S_{12})^{-1}S_{21}S_{11}^{-1} = -\sum_{k=0}^{\infty} (-H)^k Q\Sigma^t\Delta P \sum_{k=0}^{\infty} (-P\Sigma^t\Delta P)^k.$$

Plugging this back into the equation we have that the second component of the solution satisfies

$$Q(\tilde{\Sigma}^t - \Sigma^t)P = \sum_{k=0}^{\infty} (-H)^k Q\Sigma^t\Delta P \sum_{k=0}^{\infty} (-P\Sigma^t\Delta P)^k P\Sigma^t\Delta Q - \sum_{k=0}^{\infty} (-H)^k Q\Sigma^t\Delta^2 P.$$

Bounding the above expression through submultiplicity of the norm we have

$$\|Q(\tilde{\Sigma}^t - \Sigma^t)P\|_2 \leq \frac{1}{1 - \|H\|_2} \|Q\Sigma^t\Delta P\|_2 \frac{1}{1 - \|P\Sigma^t\Delta P\|_2} \|P\Sigma^t\Delta^2 P\|_2 \frac{1}{1 - \|P\Sigma^t\Delta Q\|_2}.$$

It remains to bound each term and ensure $\|P\Sigma^t\Delta P\|_2 < 1$ and $\|H\|_2 < 1$. For the latter write

$$\|H\|_2 \leq \|Q\Sigma^t\Delta Q\|_2 + \frac{\|Q\Sigma^t\Delta P\|_2 \|P\Sigma^t\Delta Q\|_2}{1 - \|P\Sigma^t\Delta P\|_2}.$$

Applying Lemma 2 on each term, with different $\varepsilon$, gives with probability $1 - 4 \exp(u)$

$$\|Q\Sigma^t\Delta Q\|_2 < \frac{1}{5}, \text{ for } \varepsilon = \frac{1}{5\sqrt{\kappa(P, X)}}; \quad \|P\Sigma^t\Delta P\|_2 < \frac{1}{5}, \text{ for } \varepsilon = \frac{1}{5\sqrt{\kappa(P, X)}};$$

$$\|Q\Sigma^t\Delta P\|_2 < \frac{1}{\sqrt{5}} \|P\Sigma^t\Delta X\|_{\psi_2}, \text{ for } \varepsilon = \frac{1}{\sqrt{5\kappa(P, X)}};$$

$$\|P\Sigma^t\Delta Q\|_2 < \frac{1}{\sqrt{5}} \|Q\Sigma^t\Delta X\|_{\psi_2}, \text{ for } \varepsilon = \frac{1}{\sqrt{5\kappa(P, X)}}$$

whenever $N > C(\text{rank}(\Sigma) + u)(\kappa(P, X) \vee \kappa(Q, X))$, where we use $\text{rank}(CD) \leq \text{rank}(C) \vee \text{rank}(D)$ for arbitrary matrices $C, D$. Thus, $\|P\Sigma^t\Delta P\|_2 < 1/5$ and $\|H\|_2 < 1/2$. Using Lemma 2 for the second time, with probability $1 - 3 \exp(-u)$ we have that whenever $N > C(\text{rank}(\Sigma) + u)(\kappa(P, X) \vee \varepsilon^2)$

$$\|Q\Sigma^t\Delta \Sigma^t P\|_2 \leq \frac{\varepsilon}{4} \|Q\Sigma^t\Delta X\|_{\psi_2}, \quad \|Q\Sigma^t\Delta P\|_2 \leq \frac{\varepsilon}{2} \|Q\Sigma^t\Delta X\|_{\psi_2} \|P\Sigma^t\Delta X\|_{\psi_2},$$

$$\|P\Sigma^t\Delta \Sigma^t P\|_2 \leq \frac{1}{4} \|P\Sigma^t\Delta X\|_{\psi_2}, \quad \text{for } \varepsilon = \frac{1}{4\sqrt{\kappa(P, X)}}.$$
Using the union bound over (44), (45) and \( \text{Im}(\Sigma) = \text{Im}(\tilde{\Sigma}) \) we now have
\[
\left\| Q(\tilde{\Sigma}^\dagger - \Sigma^\dagger)P \right\|_2 \leq \varepsilon \left\| Q\Sigma^\dagger \tilde{X} \right\|_{\psi_2} \left\| P\Sigma^\dagger \tilde{X} \right\|_{\psi_2}.
\]
with probability \( 1 - 8\exp(-u) \), whenever \( N > C(\text{rank}(\Sigma) + u) (\kappa(Q, X) \lor \kappa(P, X) \lor \varepsilon^{-2}) \). Adjusting the constant \( C \), the same bound holds with probability \( 1 - \exp(-u) \) and the first bound in (20) is proven. Repeating the same steps of the argument for the first entry of the solution, \( Q(\tilde{\Sigma}^\dagger - \Sigma^\dagger)P \), yields the claim. \( \square \)

**Proof of Theorem 10.** For the covariance estimation bound denote \( \hat{\Sigma} = N^{-1} \sum_{i=1}^N \tilde{X}_i \tilde{X}_i^\top \), where \( \tilde{X}_i = X_i - E X \), and decompose the error, as in the proof of Lemma 2 into
\[
\left\| A(\hat{\Sigma} - \Sigma)B^\top \right\|_2 = \left\| A_\Sigma(\hat{\Sigma} - \Sigma)B_\Sigma^\top \right\|_2 \leq \left\| A_\Sigma \left( \hat{\Sigma} - \Sigma \right) B_\Sigma^\top \right\|_2 + \left\| 1/N \sum_{i=1}^N A_\Sigma \tilde{X}_i \right\|_2 \left\| 1/N \sum_{i=1}^N B_\Sigma \tilde{X}_i \right\|_2.
\]
The second term is again of higher order, with high probability, and can thus be disregarded. For the first term, denote \( S_i := 1/N A_\Sigma \tilde{X}_i \tilde{X}_i^\top B_\Sigma - 1/N A_\Sigma \Sigma B_\Sigma \) and \( S := \sum_{i=1}^N S_i \). Since \( E[\tilde{X}_i \tilde{X}_i^\top] = \Sigma \) we have \( E[S_i] = 0 \), and since \( \tilde{X}_i \) and \( \tilde{X}_j \) are independent for \( i \neq j \) we get \( E[S_i S_j^\top] = E[S_i]E[S_j^\top] = 0 \). Thus,
\[
E[SS^\top] = \sum_{i=1}^N E[S_i S_i^\top] + \sum_{i \neq j} E[S_i S_j^\top] = \sum_{i=1}^N E[S_i S_i^\top].
\]
Since \( \|S_i\| \leq N^{-1}C_A C_B \) holds almost surely, we have \( \|ESS^\top\| \leq N^{-1}C_A C_B \). An analogous argument gives the same bound for \( \|ESS^\top S\|_2 \). Applying now Theorem 6.1.1. from [31] yields the desired result.

On the other hand, the first steps for establishing the bound for precision matrices are exactly the same as in the proof of Theorem 7. The only differences are in the following lines of inequalities. Provided \( N > C(\log(\text{rank}(\Sigma)) + v)(\kappa(X)^2 \lor \varepsilon^{-2}) \), instead of (41) we have
\[
\left\| A_\Sigma \Sigma^\dagger \Delta \Sigma^\dagger B_\Sigma^\top \right\|_2 \leq \frac{\varepsilon}{2} \left\| A_\Sigma \Sigma^\dagger \tilde{X} \right\|_2 \left\| B_\Sigma \Sigma^\dagger \tilde{X} \right\|_2, \quad \left\| \Sigma^\dagger \Delta \Sigma^\dagger B_\Sigma^\top \right\|_2 \leq \frac{\varepsilon}{2} \left\| B_\Sigma \Sigma^\dagger \tilde{X} \right\|_2 \left\| \Sigma^\dagger \tilde{X} \right\|_2,
\]
and \( \left\| A_\Sigma \Sigma^\dagger \Delta \right\|_2 \leq \frac{1}{2} \left\| A_\Sigma \Sigma^\dagger \tilde{X} \right\|_2 \), and \( \left\| \Sigma^\dagger \Delta \right\|_2 \leq \frac{1}{2} \), taking \( \varepsilon = \frac{1}{2\kappa(X)} \).

Plugging this into the bound for \( \|A_\Sigma (\hat{\Sigma}^\dagger - \Sigma^\dagger)B_\Sigma^\top\|_2 \) the claim follows. \( \square \)

### 5.4 Proofs for Section 4

We first need a bound for \( r = \text{Cov}(X, Y) \), and a concentration around the finite sample estimate \( \hat{r} = N^{-1} \sum_{i=1}^N (X_i - \hat{\mu}_X)(Y_i - \hat{\mu}_Y) \).

**Lemma 19.** Let \( A \in \mathbb{R}^{k \times D} \). If \( X \in \mathbb{R}^D, Y \in \mathbb{R} \) are sub-Gaussian, we have \( \| Ar \|_2 \leq C \| A \tilde{X} \|_{\psi_2} E \tilde{Y} \|_{\psi_2} \). Moreover, fix \( u > 0, \varepsilon > 0 \). Provided \( N > C(k + u)(\varepsilon^{-1} \lor \varepsilon^{-2}) \), we have with probability at least \( 1 - \exp(-u) \)
\[
\| A(r - \hat{r}) \|_2 \leq \varepsilon \| A \tilde{X} \|_{\psi_2} \| \tilde{Y} \|_{\psi_2}.
\]

**Proof.** By Lemma 15 we have \( \text{Var}(v^\top A X) \leq C \| A \tilde{X} \|_{\psi_2}^2 \), \( \text{Var}(Y) \leq C \| \tilde{Y} \|_{\psi_2}^2 \), which implies
\[
\| Ar \|_2 = \| \text{Cov}(AX, Y) \|_2 = \sup_{v \in \mathbb{S}^{D-1}} v^\top \text{Cov}(AX, Y) = \sup_{v \in \mathbb{S}^{D-1}} \text{Var} \left( v^\top AX, Y \right)
\leq \sup_{v \in \mathbb{S}^{D-1}} \sqrt{\text{Var}(v^\top AX) \text{Var}(Y)} \leq C \| A \tilde{X} \|_{\psi_2} \| \tilde{Y} \|_{\psi_2}.
\] (46)
Define the random variable $Z_i := \tilde{X}_i\tilde{Y}_i - \text{Cov}(X, Y)$ with $\mathbb{E}Z_i = 0$. We can rewrite

$$A(r - \hat{r}) = \frac{1}{N}\sum_{i=1}^{N} AZ_i - \left( \frac{1}{N}\sum_{i=1}^{N} A\tilde{X}_i \right) \left( \frac{1}{N}\sum_{i=1}^{N} \tilde{Y}_i \right).$$

As in the proof of Lemma 2, by applying Lemma 17 it follows that the second term is of higher order. On the other hand, the first term is an empirical mean of a sub-exponential centered variable $AZ_i$,

$$\|AZ_i\|_{\psi_1} = \|A\tilde{X}_i\tilde{Y}_i - \text{Cov}(AX, Y)\|_{\psi_1} \leq C \|A\tilde{X}_i\tilde{Y}_i\|_{\psi_1} \leq C \|A\tilde{X}_i\|_{\psi_2} \|\tilde{Y}_i\|_{\psi_2},$$

where we use the centering property of the sub-exponential norm, and the bound for the sub-exponential norm by the product of sub-Gaussian norms (Lemma 15). Applying Lemma 17, it follows that if $N > C(k + u)(\varepsilon^{-1} \lor \varepsilon^{-2})$ we have with probability at least $1 - \exp(-u)$

$$\|A(r - \hat{r})\|_2 \leq \varepsilon \|A\tilde{X}\|_{\psi_2} \|\tilde{Y}\|_{\psi_2}.$$

\[\square\]

**Proof of Lemma 11.** Denote for short $\Delta_r := \hat{r} - r$. We begin with a bound for $\|P(\Sigma^t r - \tilde{\Sigma}^t r)\|_2$.

$$\|P(\Sigma^t r - \tilde{\Sigma}^t r)\|_2 \leq \|P(\Sigma^t - \tilde{\Sigma}^t) P r\|_2 + \|P(\Sigma^t - \tilde{\Sigma}^t) Q r\|_2 + \|P\tilde{\Sigma}^t P \Delta_r\|_2 + \|P\tilde{\Sigma}^t Q \Delta_r\|_2 \leq \|P(\Sigma^t - \tilde{\Sigma}^t) P\|_2 \|Pr\|_2 + \|P(\Sigma^t - \tilde{\Sigma}^t) Q\|_2 \|Qr\|_2 + \|P\tilde{\Sigma}^t P\|_2 \|\Delta_r\|_2 + \|P\tilde{\Sigma}^t Q\|_2 \|\Delta_r\|_2.$$ By Lemma 19 we have $\|Qr\|_2 \leq \|Q\tilde{X}\|_{\psi_2} \|\tilde{Y}\|_{\psi_2}$, $\|Pr\|_2 \leq \|P\tilde{X}\|_{\psi_2} \|\tilde{Y}\|_{\psi_2}$. Furthermore, since $r, \hat{r} \in \text{Im}(\Sigma)$, we can rewrite $\|Q\Delta_r\|_2 = \|U_Q\Delta_r\|_2$ and $\|P\Delta_r\|_2 = \|U_P\Delta_r\|_2$, where the rows of $U_Q \in \mathbb{R}^{d_Q \times D}$ and $U_P \in \mathbb{R}^{d_P \times D}$ contain orthonormal bases for $\text{Im}(Q \Sigma)$ and $\text{Im}(P \Sigma)$, respectively. Using Lemma 19 and $d_Q \lor d_P \leq \text{rank}(\Sigma)$, we have, whenever $N > C(\text{rank}(\Sigma) + u)(1 \lor \varepsilon^{-2})$ we have with probability at least $1 - \exp(-u)$

$$\|Q\Delta_r\|_2 \leq \min\{\tilde{\varepsilon}, 1\} \|Q\tilde{X}\|_{\psi_2} \|\tilde{Y}\|_{\psi_2}, \quad \text{and} \quad \|P\Delta_r\|_2 \leq \min\{\tilde{\varepsilon}, 1\} \|P\tilde{X}\|_{\psi_2} \|\tilde{Y}\|_{\psi_2}. \quad (47)$$

Furthermore, by Theorem 9 whenever $N > C(\text{rank}(\Sigma) + u)(\kappa(P, X) \lor \kappa(Q, X) \lor \varepsilon^{-2})$ we get with probability $1 - \exp(-u)$

$$\|P(\Sigma^t - \tilde{\Sigma}^t) B\|_2 \leq \tilde{\varepsilon} \|P\Sigma^t \tilde{X}\|_{\psi_2} \|B\Sigma^t \tilde{X}\|_{\psi_2}, \quad B \in \{P, Q\}. \quad (48)$$

Conditioned on all three events we now have

$$\|P(\Sigma^t - \tilde{\Sigma}^t) P\|_2 \|Pr\|_2 \leq \tilde{\varepsilon} \|\tilde{Y}\|_{\psi_2} \|P\Sigma^t \tilde{X}\|_{\psi_2} \sqrt{\kappa(P, X)},$$

$$\|P(\Sigma^t - \tilde{\Sigma}^t) Q\|_2 \|Qr\|_2 \leq \tilde{\varepsilon} \|\tilde{Y}\|_{\psi_2} \|P\Sigma^t \tilde{X}\|_{\psi_2} \sqrt{\kappa(Q, X)}.$$  

Moreover,

$$\|P\Sigma^t P\|_2 \|\Delta_r\|_2 \leq \left( \|P\Sigma^t P\|_2 + \|P(\tilde{\Sigma}^t - \Sigma^t) P\|_2 \right) \|\Delta_r\|_2 \leq K\tilde{\varepsilon} \|\tilde{Y}\|_{\psi_2} \|P\Sigma^t \tilde{X}\|_{\psi_2} \sqrt{\kappa(P, X)},$$

$$\|P\tilde{\Sigma}^t Q\|_2 \|Q\Delta_r\|_2 \leq \left( \|P\tilde{\Sigma}^t Q\|_2 + \|P(\tilde{\Sigma}^t - \Sigma^t) Q\|_2 \right) \|Q\Delta_r\|_2 \leq K\tilde{\varepsilon} \|\tilde{Y}\|_{\psi_2} \|P\Sigma^t \tilde{X}\|_{\psi_2} \sqrt{\kappa(Q, X)}.$$  

where we use property (3) in Lemma 15, with $K = 1 + C$, and $C$ being the implicit constant, by exploiting the identity $\Sigma^t = \Sigma^t \Sigma \Sigma^t$, and we use Lemma 16 in the second line. Combining the bounds and conditioning on the events above, we have that with probability at least $1 - 3\exp(-u)$

$$\|P(\Sigma^t r - \tilde{\Sigma}^t \hat{r})\|_2 \leq (4 + 2K)\tilde{\varepsilon} \|\tilde{Y}\|_{\psi_2} \|P\Sigma^t \tilde{X}\|_{\psi_2} \sqrt{\kappa(P, X) \lor \kappa(Q, X)},$$

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if $N > C(\text{rank}(\Sigma) + u)(\kappa(P, X) \lor \kappa(Q, X) \lor \bar{\varepsilon}^{-2})$. Setting $\bar{\varepsilon} = \frac{\bar{\varepsilon}}{\sqrt{4K}}$ and adjusting the constant $C$ to account for the change in the probability constant and the requirement on $N$, the claim follows. The proof for the bound on $\|Q\Sigma^\dagger X\|_2$ follows analogous lines or argument.

**Proof of Corollary 12.** Assume for the moment $b^\top b > 0$. In this case $b$ and $P\hat{b}$ are co-linear since $P\hat{b} = \frac{b^\top b}{\|b\|_2^2} b$. Therefore $a = \frac{b}{\|b\|_2} = \frac{\hat{b}}{\|\hat{b}\|_2}$, which implies

$$\|P(\hat{a} - a)\|_2 = \left\| \frac{P\hat{b}}{\|b\|_2} - \frac{P\hat{b}}{\|\hat{b}\|_2} \right\|_2 = \left\| \frac{P\hat{b}}{\|b\|_2} \right\|_2 - \frac{1}{\|\hat{b}\|_2} \left\| \frac{P\hat{b}}{\|\hat{b}\|_2} \right\|_2 \leq \sqrt{\frac{\|\hat{b}\|_2}{\|b\|_2} - \|P(b - \hat{b})\|_2}.$$

Since $Qa = 0$ we now have

$$\|\hat{a} - a\|_2 = \sqrt{\|P(\hat{a} - a)\|_2^2 + \|Q\hat{a}\|_2^2} \leq \sqrt{2\left\| \frac{Q\hat{b}}{\|b\|_2} \right\|_2} \leq \sqrt{2\frac{\|\hat{b}\|_2}{\|b\|_2} - \|P(b - \hat{b})\|_2}.$$

Therefore, it suffices to ensure $\|P(\hat{b} - b)\|_2 < \frac{1}{2}\|b\|_2$, which would also give $b^\top b > 0$. To that end, Lemma 11 gives that $\|P(\hat{b} - b)\|_2 \leq \frac{1}{2}\|b\|_2$ holds with probability at least $1 - \exp(-u)$ provided

$$N > C(\text{rank}(\Sigma) + u) \left( \kappa(P, X) \lor \kappa(Q, X) \lor \frac{\|Y\|_2^2}{\|P\Sigma^\dagger X\|_2} \right) \left( \frac{\|P\Sigma^\dagger X\|_2}{\|b\|_2^2} \right).$$

The result follows by bounding $\|Q\hat{b}\|_2$ through Lemma 11.

**Lemma 20.** If $Z$ is sub-Gaussian and $E$ an event with $P(E) > 0$, then $Z|E$ is also sub-Gaussian.

**Proof.** Assume without loss of generality that $Z \in \mathbb{R}$. The argument for vectors then follows by the definition. We use the characterization of sub-Gaussianity by the moment bound [35, Proposition 2.5.2, b)]. Let $p \geq 1$. By the law of total expectation it follows

$$\mathbb{E}[|Z|^p] = \mathbb{E}[|Z|^p|E]\mathbb{P}(E) + \mathbb{E}[|Z|^p|E^c]\mathbb{P}(E^c) \geq \mathbb{E}[|Z|^p|E]\mathbb{P}(E).$$

Dividing by $\mathbb{P}(E)$ and using the monotonicity of the $p$-th root yields

$$(\mathbb{E}[|Z|^p|E])^{1/p} \leq \left( \frac{\mathbb{E}[|Z|^p]}{\mathbb{P}(E)} \right)^{1/p} \leq C \frac{\|Z\|_p^{1/p} \sqrt{p}}{\mathbb{P}(E)},$$

where $C > 0$ is some universal constant, and we used $\mathbb{P}(E) \leq 1$ and the sub-Gaussianity of $Z$ in the last inequality. Thus, the claim follows.

**Proof of Theorem 14.** Using $0 \leq \max_{s=\pm 1} \left\langle su_1(M_J), a \right\rangle \leq 1$, we first compute

$$\min_{s=\pm 1} \left\| su_1(M_J) - a \right\|_2^2 = \min_{s=\pm 1} 2 \left( 1 - \left\langle su_1(M_J), a \right\rangle \right) \leq 2(1 - \left\langle u_1(M_J), a \right\rangle^2) \leq 2 \left\| Q u_1(M_J) \right\|_2^2.$$

The Davis-Kahan Theorem [4, Theorem 7.3.1] for $M_J$ and $P = aa^\top$ then gives

$$2 \left\| Qu_1(M_J) \right\|_2^2 = 2 \left\| Qu_1(M_J)u_1(M_J)^\top \right\|_F^2 \leq 2 \frac{\left\| Q(M_J) - \hat{M}_J \right\|_F^2}{\lambda_1(M_J)^2} = 2 \frac{\left\| Q \hat{M}_J \right\|_F^2}{\lambda_1(M_J)^2}.$$
It remains to find a concentration bound for the matrix \( Q\hat{M}_J \) around zero. Let \( \pi : \{I_J\} \to I_K \) be bijective and introduce the matrix
\[
\hat{B}_J = \left[ \sqrt{\hat{\rho}_{J,\pi(1)}b_{J,\pi(1)}} \cdots \sqrt{\hat{\rho}_{J,\pi(|I_J|)}b_{J,\pi(|I_J|)}} \right] \in \mathbb{R}^{D \times |I_J|},
\]
satisfying \( \hat{M}_J = \hat{B}_J\hat{B}_J^\top \), and thus \( \lambda_1(\hat{M}_J) = \lambda_1(\hat{B}_J\hat{B}_J^\top) \). Using \( \|GH\|_F \leq \|G\|_2 \|H\|_F \) and \( \|G\|_F = \|G^\top\|_F \), which hold for arbitrary matrices \( G \) and \( H \), yields
\[
\|QM_J\|_F^2 = \|QB_J\hat{B}_J^\top\|_F^2 \leq \|B_J\|_2^2 \|QB_J\|_F^2 \leq \lambda_1(M_J) \|QB_J\|_F^2.
\]
By Lemma 20, conditioning on a sub-Gaussian random vector gives a sub-Gaussian random vector. Thus, by (27) we have
\[
\mathbb{P}\left( \forall \ell \in I_J : \|Q\hat{b}_{J,\ell}\|_2^2 \leq \varepsilon^2 \|\bar{Y}|Y \in \mathcal{R}_{J,\ell}\|_{\psi_2}^2 \|Q\Sigma_{J,\ell}^{\dagger}\tilde{X}|Y \in \mathcal{R}_{J,\ell}\|_{\psi_2}^2 \|\lambda_{J,\ell} \right) > 1 - \exp(-u), \quad (49)
\]
provided \( N_{J,\ell} > C(\text{rank}(\Sigma_{J,\ell}) + u + \log(|I_J|))(\kappa_{J,\ell}^2 \vee \varepsilon^{-2}) \) for all \( \ell \in I_J \). By definition of \( I_J \), we have \( N_{J,\ell} > \alpha NJ^{-1} \), and thus the previous condition is satisfied whenever for all \( \ell \in I_J \)
\[
\frac{N}{J} > \frac{C(\text{rank}(\Sigma) + u)(\max_{\ell \in I_J} \kappa_{J,\ell} \vee \varepsilon^{-2})}{\alpha},
\]
which is implied by
\[
\frac{N}{(1 + \log(J))J} > \frac{C(\text{rank}(\Sigma) + u)(\max_{\ell \in I_J} \kappa_{J,\ell} \vee \varepsilon^{-2})}{\alpha}.
\]
Under the same conditions and with similar probability we obtain
\[
\|QM_J\|_F^2 \leq \lambda_1(M_J) \sum_{\ell \in I_J} \hat{\rho}_{J,\ell} \|Q\hat{b}_{J,\ell}\|_2^2 \leq \varepsilon^2 \lambda_1(M_J) \sum_{\ell \in I_J} \hat{\rho}_{J,\ell} \|\bar{Y}|Y \in \mathcal{R}_{J,\ell}\|_{\psi_2}^2 \|Q\Sigma_{J,\ell}^{\dagger}\tilde{X}|Y \in \mathcal{R}_{J,\ell}\|_{\psi_2}^2 \kappa_{J,\ell}
\]
\[
\leq C' \frac{\varepsilon^2}{J^2} \lambda_1(M_J) \sum_{\ell \in I_J} \hat{\rho}_{J,\ell} \|Q\Sigma_{J,\ell}^{\dagger}\tilde{X}|Y \in \mathcal{R}_{J,\ell}\|_{\psi_2}^2 \kappa_{J,\ell},
\]
where we used \( \mathcal{R}_{J,\ell} = [(\ell - 1)J^{-1}, \ell J^{-1}] \) and thus \( \|\bar{Y}|Y \in \mathcal{R}_{J,\ell}\|_{\psi_2} \leq C' \|\mathcal{R}_{J,\ell}\| = C' J^{-1} \) in the last inequality. The result follows after taking the square root.

\[\square\]

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