User-Friendly Covariance Estimation for Heavy-Tailed Distributions

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Abstract

We offer a survey of recent results on covariance estimation for heavytailed distributions. By unifying ideas scattered in the literature, we propose user-friendly methods that facilitate practical implementation. Specifically, we introduce element-wise and spectrum-wise truncation operators, as well as their M-estimator counterparts, to robustify the sample covariance matrix. Different from the classical notion of robustness that is characterized by the breakdown property, we focus on the tail robustness which is evidenced by the connection between nonasymptotic deviation and confidence level. The key observation is that the estimators needs to adapt to the sample size, dimensionality of the data and the noise level to achieve optimal tradeoff between bias and robustness. Furthermore, to facilitate their practical use, we propose data-driven procedures that automatically calibrate the tuning parameters. We demonstrate their applications to a series of structured models in high dimensions, including the bandable and low-rank covariance matrices and sparse precision matrices. Numerical studies lend strong support to the proposed methods.

Keywords: Covariance estimation, heavy-tailed data, *M*-estimation, nonasymptotics, tail robustness, truncation.

1 Introduction

Covariance matrices are important in multivariate statistics. The estimation of covariance matrices, therefore, serves as a building block for many important statistical

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methods, including principal component analysis, discriminant analysis, clustering analysis and regression analysis, among many others. Recently, the problem of estimation of structured large covariance matrices, such as bandable, sparse and low-rank matrices, has attracted ever-growing attention in statistics and machine learning (Bickel and Levina, 2008a,b; Cai, Ren and Zhou, 2016; Fan, Liao and Liu, 2016). This problem has many applications, ranging from functional magnetic resonance imaging (fMRI), analysis of gene expression arrays to risk management and portfolio allocation.

Theoretical properties of large covariance estimators discussed in the literature often hinge heavily on the Gaussian or sub-Gaussian¹ assumptions (Vershynin, 2012). See, for example, Theorem 1 of Bickel and Levina (2008a). Such an assumption is typically very restrictive in practice. For example, a recent fMRI study by Eklund et al. (2016) reported that most of the common software packages, such as SPM and FSL, for fMRI analysis can result in inflated false-positive rates up to 70% under 5% nominal levels, and questioned a number of fMRI studies among approximately 40,000 studies according to PubMed. Their results suggested that

The principal cause of the invalid cluster inferences is spatial autocorrelation functions that do not follow the assumed Gaussian shape.

Eklund et al. (2016) plotted the empirical versus theoretical spatial autocorrelation functions for several datasets. The empirical autocorrelation functions have much heavier tails compared to their theoretical counterparts under the commonly used assumption of a Gaussian random field, which causes the failure of fMRI inferences (Eklund et al., 2016). Similar phenomenon has also been discovered in genomic studies (Liu et al., 2003; Purdom and Holmes, 2005) and in quantitative finance (Cont, 2001). It is therefore imperative to develop robust inferential procedures that are less sensitive to the distributional assumptions.

We are interested in constructing estimators that admit tight nonasymptotic deviation guarantees under weak moment assumptions. Heavy-tailed distribution is a viable model for data contaminated by outliers that are typically encountered in applications. Due to heavy tailedness, the probability that some observations are sampled far away from the "true" parameter of the population is non-negligible. We refer to these outlying data points as stochastic outliers. A procedure that is robust against such outliers, evidenced by its better finite-sample performance than a non-robust method, is called a *tail-robust* procedure. In this paper, by unifying ideas scattered in the literature, we provide a unified framework for constructing user-friendly tail-robust covariance estimators. Specifically, we propose element-wise and spectrum-wise truncation operators, as well as their *M*-estimator counterparts, with adaptively chosen robustification parameters. Theoretically, we establish nonasymptotic deviation bounds and demonstrate that the robustification parameters should adapt to the sample size, dimensionality and noise level for optimal tradeoff between bias and robustness. Our goal is to obtain estimators that

¹A random variable Z is said to have sub-Gaussian tails if there exists constants c_1 and c_2 such that $\mathbb{P}(|Z - \mathbb{E}Z| > t) \leq c_1 \exp(-c_2 t^2)$ for all $t \geq 0$.

are computationally efficient and easily implementable in practice. To this end, we propose data-driven schemes to calibrate the tuning parameters, making our proposal user-friendly. Finally, we discuss applications to several structured models in high dimensions, including bandable matrices, low-rank covariance matrices as well as sparse precision matrices. In the supplementary material, we further consider robust covariance estimation and inference under factor models, which might be of independent interest.

Our definition of robustness is different from the conventional perspective under Huber's ϵ -contamination model (Huber, 1964), where the focus has been on developing robust procedures with a high breakdown point. The breakdown point (Hampel, 1971) of an estimator is defined (informally) as the largest proportion of outliers in the data for which the estimator remains stable. Since the seminal work of Tukey (1975), a number of depth-based robust procedures have been developed; see, for example, the papers by Liu (1990), Zuo and Serfling (2000), Mizera (2002) and Salibian-Barrera and Zamar (2002), among others. Another line of work focuses on robust and resistant *M*-estimators, including the least median of squares and least trimmed squares (Rousseeuw, 1984), the S-estimator (Rousseeuw and Yohai, 1984) and the MM-estimator (Yohai, 1987). We refer to Portnoy and He (2000) for a literature review on classical robust statistics, and to Chen, Gao and Ren (2018) for recent developments on nonasymptotic analysis under contamination models.

The rest of the paper is organized as follows. We start with a motivating example in Section 2, which reveals the downsides of the sample covariance matrix. In Section 3, we introduce two types of generic robust covariance estimators and establish their deviation bounds under different norms of interest. The finite-sample performance of the proposed estimators, both element-wise and spectrum-wise, depends on a careful tuning of the robustification parameter, which should adapt to the noise level for bias-robustness tradeoff. We also discuss the median-of-means estimator, which is virtually tuning-free at the cost of slightly stronger assumptions. For practical implementation, in Section 4 we propose a data-driven scheme to choose the key tuning parameters. Section 5 presents various applications to estimating structured covariance and precision matrices. Numerical studies are provided in Section 6. We close this paper with a discussion in Section 7.

1.1 Overview of the previous work

In the past several decades, there has been a surge of work on robust covariance estimation in the absence of normality. Examples include the Minimum Covariance Determinant (MCD) estimator, the Minimum Volume Ellipsoid (MVE) estimator, Maronna's (Maronna, 1976) and Tyler's (Tyler, 1987) *M*-estimators of multivariate scatter matrices. We refer to Hubert, Rousseeuw and Van Aelst (2008) for a comprehensive review. Asymptotic properties of these methods have been established for the family of elliptically symmetric distributions; see, for example, Davies (1992), Butler, Davies and Jhun (1993) and Zhang, Cheng and Singer (2016), among others. However, the aforementioned estimators either rely on parametric assumptions, or impose a shape constraint on the sampling distribution. Under a general setting where neither of these assumptions are made, robust covariance estimation remains a challenging problem.

The work of Catoni (2012) triggered a growing interest in developing tail-robust estimators, which are characterized by tight nonasymptotic deviation analysis, rather than mean squared errors. The current state-of-the-art methods for covariance estimation with heavy-tailed data include those of Catoni (2016), Minsker (2018), Minsker and Wei (2018), Avella-Medina et al. (2018), Mendelson and Zhivotovskiy (2018). From a spectrum-wise perspective, Catoni (2016) constructed a robust estimator of the Gram and covariance matrices of a random vector $X \in \mathbb{R}^d$ via estimating the quadratic forms $\mathbb{E}\langle u, X \rangle^2$ uniformly over the unit sphere in \mathbb{R}^d , and proved error bounds under the operator norm. More recently, Mendelson and Zhivotovskiy (2018) proposed a different robust covariance estimator that admits tight deviation bounds under the finite kurtosis condition. Both constructions, however, involve brute-force search over every direction in a d-dimensional ε -net, and thus are computationally intractable. From an element-wise perspective, Avella-Medina et al. (2018) combined robust estimates of the first and second moments to obtain variance estimators. In practice, three potential drawbacks of this approach are: (i) the accumulated error consists of those from estimating the first and second moments, which may be significant; (ii) the diagonal variance estimators are not necessarily positive and therefore additional adjustments are required; and (iii) using the cross-validation to calibrate a total number of $O(d^2)$ tuning parameters is computationally expensive.

Building on the ideas of Minsker (2018) and Avella-Medina et al. (2018), we propose user-friendly tail-robust covariance estimators that enjoy desirable finite-sample deviation bounds under weak moment conditions. The constructed estimators only involve simple truncation techniques and are computationally friendly. Through a novel data-driven tuning scheme, we are able to efficiently compute these robust estimators for large-scale problems in practice. These two points distinguish our work from the literature on the topic. The proposed robust procedures serve as building blocks for estimating large structured covariance and precision matrices, and we illustrate their broad applicability in a series of problems.

1.2 Notation

We adopt the following notation throughout the paper. For any $0 \le r, s \le \infty$ and a $d \times d$ matrix $\mathbf{A} = (A_{k\ell})_{1 \le k, \ell \le d}$, we define the max norm $\|\mathbf{A}\|_{\max} = \max_{1 \le k, \ell \le d} |A_{k\ell}|$, the Frobenius norm $\|\mathbf{A}\|_{\mathrm{F}} = (\sum_{1 \le k, \ell \le d} A_{k\ell}^2)^{1/2}$ and the operator norm

$$\|\mathbf{A}\|_{r,s} = \sup_{\boldsymbol{u}=(u_1,\ldots,u_d)^{\mathsf{T}}:\|\boldsymbol{u}\|_r=1} \|\mathbf{A}\boldsymbol{u}\|_s,$$

where $\|\boldsymbol{u}\|_{r}^{r} = \sum_{k=1}^{d} |u_{k}|^{r}$ for $r \in (0,\infty)$, $\|\boldsymbol{u}\|_{0} = \sum_{k=1}^{d} I(|u_{k}| \neq 0)$ and $\|\boldsymbol{u}\|_{\infty} = \max_{1 \leq k \leq d} |u_{k}|$. In particular, it holds $\|\boldsymbol{A}\|_{1,1} = \max_{1 \leq \ell \leq d} \sum_{k=1}^{d} |A_{k\ell}|$ and $\|\boldsymbol{A}\|_{\infty,\infty} = \max_{1 \leq k \leq d} \sum_{\ell=1}^{d} |A_{k\ell}|$. Moreover, we write $\|\boldsymbol{A}\|_{2} := \|\boldsymbol{A}\|_{2,2}$ for the spectral norm and

use $r(\mathbf{A}) = tr(\mathbf{A})/||\mathbf{A}||_2$ to denote the effective rank of a nonnegative definite matrix \mathbf{A} , where $tr(\mathbf{A}) = \sum_{k=1}^{d} A_{kk}$ is the trace of \mathbf{A} . When \mathbf{A} is symmetric, it is well known that $||\mathbf{A}||_2 = \max_{1 \le k \le d} |\lambda_k(\mathbf{A})|$ where $\lambda_1(\mathbf{A}) \ge \lambda_2(\mathbf{A}) \dots \ge \lambda_d(\mathbf{A})$ are the eigenvalues of \mathbf{A} . For any matrix $\mathbf{A} \in \mathbb{R}^{d \times d}$ and an index set $J \subseteq \{1, \dots, d\}^2$, we use J^c to denote the complement of J, and \mathbf{A}_J to denote the submatrix of \mathbf{A} with entries indexed by J. For a real-valued random variable X, let kurt(X) be the kurtosis of X, defined as $kurt(X) = \mathbb{E}(X-\mu)^4/\sigma^4$, where $\mu = \mathbb{E}X$ and $\sigma^2 = var(X)$.

2 Motivating example: a challenge of heavy-tailedness

Suppose that we observe a sample of independent and identically distributed (i.i.d.) copies X_1, \ldots, X_n of a random vector $X = (X_1, \ldots, X_d)^{\intercal} \in \mathbb{R}^d$ with mean μ and covariance matrix $\Sigma = (\sigma_{k\ell})_{1 \leq k, \ell \leq d}$. To assess the difficulty of mean and covariance estimation for heavy-tailed distributions, we first provide a lower bound for the deviation of the empirical mean under the ℓ_{∞} -norm in \mathbb{R}^d .

Proposition 2.1. For any $\sigma > 0$ and $0 < \delta < (2e)^{-1}$, there exists a distribution in \mathbb{R}^d with mean μ and covariance matrix $\sigma^2 \mathbf{I}_d$ such that the empirical mean $\bar{\mathbf{X}} = (1/n) \sum_{i=1}^n \mathbf{X}_i$ of i.i.d. observations $\mathbf{X}_1, \ldots, \mathbf{X}_n$ from this distribution satisfies, with probability at least δ ,

$$\|\bar{\boldsymbol{X}} - \boldsymbol{\mu}\|_{\infty} \ge \sigma \sqrt{\frac{d}{n\delta}} \left(1 - \frac{2e\delta}{n}\right)^{(n-1)/2}.$$
(2.1)

The above proposition is a multivariate extension of Proposition 6.2 of Catoni (2012). It provides a lower bound under the ℓ_{∞} -norm for estimating a mean vector via the empirical mean. On the other hand, combining the union bound with Chebyshev's inequality, we obtain that with probability at least $1 - \delta$,

$$\|\bar{\boldsymbol{X}} - \boldsymbol{\mu}\|_{\infty} \le \sigma \sqrt{\frac{d}{n\delta}}$$

Together, this upper bound and inequality (2.1) show that the worst case deviations of the empirical means grow polynomially in $1/\delta$ under the ℓ_{∞} -norm in the presence of heavy-tailed distributions. As we will see later, a more robust estimator can achieve an exponential-type deviation bound under weak moment conditions.

To demonstrate the practical implications of Proposition 2.1, we perform a toy numerical study on covariance matrix estimation. Let X_1, \ldots, X_n be i.i.d. copies of $\mathbf{X} = (X_1, \ldots, X_d) \in \mathbb{R}^d$, where X_k 's are independent and have centered Gamma(3, 1) distribution so that $\boldsymbol{\mu} = \mathbf{0}$ and $\boldsymbol{\Sigma} = 3\mathbf{I}_d$. We compare the performance of three methods: the sample covariance matrix, the element-wise truncated covariance matrix and the spectrum-wise truncated covariance matrix. The latter two are tail-robust covariance estimators that will be introduced in Sections 3.1 and 3.2 respectively. We report the estimation errors under the max norm. We take n = 200and let d increase from 50 to 500 with a step size of 50. The results are based on 50 simulations. Figure 1 displays the average (line) and the spread (dots) of estimation

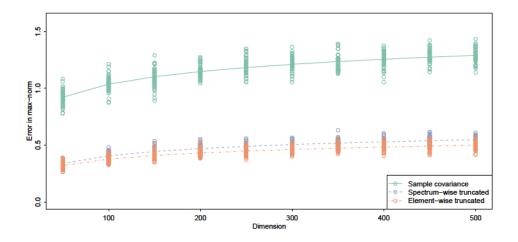


Figure 1: Plots of estimation error under max norm versus dimension.

errors for each method as the dimension increases. We see that the sample covariance estimator has not only the largest average error but also the highest variability in all the settings. This example demonstrates that the sample covariance matrix suffers from poor finite-sample performance when data are heavy-tailed.

3 Tail-robust covariance estimation

3.1 Element-wise truncated estimator

We consider the same setting as in the previous section. For mean estimation, the suboptimality of deviations of $\bar{X} = (\bar{X}_1, \ldots, \bar{X}_d)^{\mathsf{T}}$ under ℓ_{∞} -norm is due to the fact that the tail probability of $|\bar{X}_k - \mu_k|$ decays only polynomially. A simple yet natural idea for improvement is to truncate the data to eliminate outliers introduced by heavy-tailed noises, so that each entry of the resulting estimator has sub-Gaussian tails. To implement this idea, we introduce the following truncation operator, which is closely related to the Huber loss.

Definition 3.1 (Truncation operator). Let $\psi_{\tau}(\cdot)$ be a truncation operator given by

$$\psi_{\tau}(u) = (|u| \wedge \tau) \operatorname{sign}(u), \quad u \in \mathbb{R},$$
(3.1)

where the truncation parameter $\tau > 0$ is also referred to as the *robustification* parameter that trades off bias for robustness.

As an illustration, we assume that $\mu = 0$ whence $\Sigma = \mathbb{E}(XX^{\intercal})$. We apply the truncation operator above to each entry of $X_i X_i^{\intercal}$, and then take the average to obtain

$$\widehat{\sigma}_{0,k\ell}^{\mathcal{T}} = \frac{1}{n} \sum_{i=1}^{n} \psi_{\tau_{k\ell}}(X_{ik} X_{i\ell}), \quad 1 \le k, \ell \le d,$$

where $\tau_{k\ell} > 0$ are robustification parameters. When the mean vector $\boldsymbol{\mu}$ is unspecified, a straightforward approach is to first estimate the mean vector using existing robust methods (Minsker, 2015; Lugosi and Mendelson, 2019), and then to employ $\hat{\sigma}_{0,k\ell}^{\mathcal{T}}$ as robust estimates of the second moments. Estimating the first and second moments separately will unavoidably introduce additional tuning parameters, which increases both statistical variability and computational complexity. In what follows, we propose to use the pairwise difference approach, which is free of mean estimation. To the best of our knowledge, the difference-based techniques can be traced back to Rice (1984) and Hall, Kay and Titterington (1990) in the context of bandwidth selection and variance estimation for nonparametric regression.

Let N := n(n-1)/2 and define the paired data

$$\{Y_1, Y_2, \dots, Y_N\} = \{X_1 - X_2, X_1 - X_3, \dots, X_{n-1} - X_n\},$$
 (3.2)

which are identically distributed from a random vector \boldsymbol{Y} with mean $\boldsymbol{0}$ and covariance matrix $\operatorname{cov}(\boldsymbol{Y}) = 2\boldsymbol{\Sigma}$. It is easy to check that the sample covariance matrix, $\widehat{\boldsymbol{\Sigma}}^{\operatorname{sam}} = (1/n) \sum_{i=1}^{n} (\boldsymbol{X}_{i} - \bar{\boldsymbol{X}}) (\boldsymbol{X}_{i} - \bar{\boldsymbol{X}})^{\mathsf{T}}$ with $\bar{\boldsymbol{X}} = (1/n) \sum_{i=1}^{n} \boldsymbol{X}_{i}$, can be expressed as a U-statistic

$$\widehat{\boldsymbol{\Sigma}}^{\mathrm{sam}} = \frac{1}{N} \sum_{i=1}^{N} \boldsymbol{Y}_{i} \boldsymbol{Y}_{i}^{\mathsf{T}} / 2.$$

Following the argument from the last section, we apply the truncation operator ψ_{τ} to $Y_i Y_i^{\intercal}/2$ entry-wise, and then take the average to obtain

$$\widehat{\sigma}_{1,k\ell}^{\mathcal{T}} = \frac{1}{N} \sum_{i=1}^{N} \psi_{\tau_{k\ell}}(Y_{ik}Y_{i\ell}/2), \quad 1 \le k, \ell \le d.$$

Concatenating these estimators, we define the element-wise truncated covariance matrix estimator via

$$\widehat{\Sigma}_{1}^{\mathcal{T}} = \widehat{\Sigma}_{1}^{\mathcal{T}}(\Gamma) = (\widehat{\sigma}_{1,k\ell}^{\mathcal{T}})_{1 \le k,\ell \le d}, \qquad (3.3)$$

where $\mathbf{\Gamma} = (\tau_{k\ell})_{1 \leq k,\ell \leq d}$ is a symmetric matrix of parameters. $\widehat{\mathbf{\Sigma}}_1^{\mathcal{T}}$ can be viewed as a truncated version of the sample covariance matrix $\widehat{\mathbf{\Sigma}}^{\text{sam}}$. We assume that $n \geq 2, d \geq 1$ and define $m = \lfloor n/2 \rfloor$, the largest integer not exceeding n/2. Moreover, let $\mathbf{V} = (v_{k\ell})_{1 \leq k,\ell \leq d}$ be a symmetric $d \times d$ matrix such that

$$v_{k\ell}^2 = \mathbb{E}(Y_{1k}Y_{1\ell}/2)^2 = \mathbb{E}\{(X_{1k} - X_{2k})(X_{1\ell} - X_{2\ell})\}^2/4.$$

Theorem 3.1. For any $0 < \delta < 1$, the estimator $\widehat{\Sigma}_1^{\mathcal{T}} = \widehat{\Sigma}_1^{\mathcal{T}}(\Gamma)$ defined in (3.3) with

$$\Gamma = \sqrt{m/(2\log d + \log \delta^{-1})} \mathbf{V}$$
(3.4)

satisfies

$$\mathbb{P}\left(\|\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{T}} - \mathbf{\Sigma}\|_{\max} \ge 2\|\mathbf{V}\|_{\max}\sqrt{\frac{2\log d + \log \delta^{-1}}{m}}\right) \le 2\delta.$$
(3.5)

Theorem 3.1 indicates that, with properly calibrated parameter matrix Γ , the resulting covariance matrix estimator achieves element-wise tail robustness against heavy-tailed distributions: provided the fourth moments are bounded, each entry of $\widehat{\Sigma}_1^{\mathcal{T}}$ concentrates tightly around its mean so that the maximum error scales as $\sqrt{\log(d)/n} + \sqrt{\log(\delta^{-1})/n}$. Element-wise, we are able to accurately estimate Σ at high confidence levels under the constraint that $\log(d)/n$ is small. Implicitly, the dimension d = d(n) is regarded as a function of n, and we shall use array asymptotics " $n, d \to \infty$ " to characterize large sample behaviors. The finite sample performance, on the other hand, is characterized via nonasymptotic probabilistic bounds with explicit dependence on n and d.

Remark 1. It is worth mentioning that the estimator given in (3.3) and (3.4) is not a genuine sub-Gaussian estimator, in a sense that it depends on the confidence level $1 - \delta$ at which one aims to control the error. More precisely, following the terminology used by Devroye et al. (2016), it is called a δ -dependent sub-Gaussian estimator (under the max norm). Estimators of a similar type include those of Catoni (2012), Minsker (2015), Brownlees, Joly and Lugosi (2015), Hsu and Sabato (2016), Minsker (2018) and Avella-Medina et al. (2018), among others. For univariate mean estimation, Devroye et al. (2016) proposed multiple- δ mean estimators that satisfy exponential-type concentration bounds uniformly over $\delta \in [\delta_{\min}, 1)$. The idea is to combine a sequence of δ -dependent estimators in a way very similar to Lepski's method (Lepski, 1990).

Remark 2. Since the element-wise truncated estimator is obtained by treating each covariance $\sigma_{k\ell}$ separately as a univariate parameter, the problem is equivalent to estimation of a large vector given by the concatenation of the columns of Σ . These type of results are particularly useful for proving upper bounds for sparse covariance and precision estimators in high dimensions; see Section 5. Integrated with ℓ_{∞} -type perturbation bounds, it can also be applied to principle component analysis and factor analysis for heavy-tailed data (Fan et al., 2018). However, when dealing with large covariance matrices with bandable or low-rank structure, controlling the estimation error under spectral norm is arguably more relevant. A natural idea is then to truncate the spectrum of the sample covariance matrix instead of its entries, which leads to the spectrum-wise truncated estimator defined in the following section.

3.2 Spectrum-wise truncated estimator

In this section, we propose and study a covariance estimator that is tail-robust in the spectral norm. To this end, we directly apply the truncation operator to matrices in their spectrum domain. We need the following standard definition of a matrix functional.

Definition 3.2 (Matrix functional). Given a real-valued function f defined on \mathbb{R} and a symmetric $\mathbf{A} \in \mathbb{R}^{K \times K}$ with eigenvalue decomposition $\mathbf{A} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^{\mathsf{T}}$ such

that $\mathbf{\Lambda} = \operatorname{diag}(\lambda_1, \ldots, \lambda_K)$, $f(\mathbf{\Lambda})$ is defined as $f(\mathbf{\Lambda}) = \mathbf{U}f(\mathbf{\Lambda})\mathbf{U}^{\intercal}$, where $f(\mathbf{\Lambda}) = \operatorname{diag}(f(\lambda_1), \ldots, f(\lambda_K))$.

Following the same rational as in the previous section, we propose a spectrumwise truncated covariance estimator based on the pairwise difference approach:

$$\widehat{\boldsymbol{\Sigma}}_{2}^{\mathcal{T}} = \widehat{\boldsymbol{\Sigma}}_{2}^{\mathcal{T}}(\tau) = \frac{1}{N} \sum_{i=1}^{N} \psi_{\tau}(\boldsymbol{Y}_{i}\boldsymbol{Y}_{i}^{\mathsf{T}}/2), \qquad (3.6)$$

where Y_i are given in (3.2). Note that $Y_i Y_i^{\mathsf{T}}/2$ is a rank-one matrix with eigenvalue $\|Y_i\|_2^2/2$ and the corresponding eigenvector $Y_i/\|Y_i\|_2$. By Definition 3.2, $\hat{\Sigma}_2^{\mathcal{T}}$ can be rewritten as

$$\frac{1}{N} \sum_{i=1}^{N} \psi_{\tau} \left(\frac{1}{2} \| \mathbf{Y}_i \|_2^2 \right) \frac{\mathbf{Y}_i \mathbf{Y}_i^{\mathsf{T}}}{\| \mathbf{Y}_i \|_2^2}$$

=
$$\frac{1}{\binom{n}{2}} \sum_{1 \le i < j \le n} \psi_{\tau} \left(\frac{1}{2} \| \mathbf{X}_i - \mathbf{X}_j \|_2^2 \right) \frac{(\mathbf{X}_i - \mathbf{X}_j) (\mathbf{X}_i - \mathbf{X}_j)^{\mathsf{T}}}{\| \mathbf{X}_i - \mathbf{X}_j \|_2^2}$$

This alternative expression renders the computation almost effortless. The following theorem provides an exponential-type concentration inequality for $\hat{\Sigma}_2^{\mathcal{T}}$ under operator norm, which is a useful complement to the Remark 8 of Minsker (2018). Similarly to Theorem 3.1, our next result shows that $\hat{\Sigma}_2^{\mathcal{T}}$ achieves exponential-type concentration in the operator norm for heavy-tailed data with finite operator-wise fourth moment, meaning that

$$v^{2} = \frac{1}{4} \|\mathbb{E}\{(X_{1} - X_{2})(X_{1} - X_{2})^{\mathsf{T}}\}^{2}\|_{2}$$
(3.7)

is finite.

Theorem 3.2. For any $0 < \delta < 1$, the estimator $\widehat{\Sigma}_2^{\mathcal{T}} = \widehat{\Sigma}_2^{\mathcal{T}}(\tau)$ with

$$\tau = v \sqrt{\frac{m}{\log(2d) + \log \delta^{-1}}} \tag{3.8}$$

satisfies, with probability at least $1 - \delta$,

$$\|\widehat{\boldsymbol{\Sigma}}_{2}^{\mathcal{T}} - \boldsymbol{\Sigma}\|_{2} \le 2v\sqrt{\frac{\log(2d) + \log\delta^{-1}}{m}}.$$
(3.9)

To better understand this result, note that v^2 can be written as

$$\frac{1}{2} \|\mathbb{E}\{(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^{\mathsf{T}}\}^{2} + \operatorname{tr}(\boldsymbol{\Sigma})\boldsymbol{\Sigma} + 2\boldsymbol{\Sigma}^{2}\|_{2}$$

which is well-defined if the fourth moments $\mathbb{E}(X_k^4)$ are finite. Let

$$K = \sup_{\boldsymbol{u} \in \mathbb{R}^d} \operatorname{kurt}(\boldsymbol{u}^{\intercal} \boldsymbol{X})$$

be the maximal kurtosis of the one-dimensional projections of X. Then

$$v^2 \leq \|\mathbf{\Sigma}\|_2 \{ (K+1) \operatorname{tr}(\mathbf{\Sigma})/2 + \|\mathbf{\Sigma}\|_2 \}.$$

The following result is a direct consequence of Theorem 3.2: $\widehat{\Sigma}_2^{\mathcal{T}}$ admits exponentialtype concentration for data with finite kurtoses. **Corollary 3.1.** Assume that $K = \sup_{\boldsymbol{u} \in \mathbb{R}^d} \operatorname{kurt}(\boldsymbol{u}^{\mathsf{T}} \boldsymbol{X})$ is finite. Then, for any $0 < \delta < 1$, the estimator $\widehat{\boldsymbol{\Sigma}}_2^{\mathcal{T}} = \widehat{\boldsymbol{\Sigma}}_2^{\mathcal{T}}(\tau)$ defined in Theorem 3.2 satisfies

$$\|\widehat{\boldsymbol{\Sigma}}_{2}^{\mathcal{T}} - \boldsymbol{\Sigma}\|_{2} \lesssim K^{1/2} \|\boldsymbol{\Sigma}\|_{2} \sqrt{\frac{\operatorname{r}(\boldsymbol{\Sigma})(\log d + \log \delta^{-1})}{n}}$$
(3.10)

with probability at least $1 - \delta$.

Remark 3. An estimator proposed by Mendelson and Zhivotovskiy (2018) achieves a more refined deviation bound, namely, with $\|\Sigma\|_2 \sqrt{r(\Sigma)(\log d + \log \delta^{-1})}$ in (3.10) improved to $\|\Sigma\|_2 \sqrt{r(\Sigma) \log r(\Sigma)} + \|\Sigma\|_2 \sqrt{\log \delta^{-1}}$; in particular, the deviations are controlled by the spectral norm $\|\Sigma\|_2$ instead of the (possibly much larger) trace $tr(\Sigma)$. Estimators admitting such deviations guarantees are often called "sub-Gaussian" as they achieve performance similar to the sample covariance obtained from data with multivariate normal distributions. Unfortunately, the aforementioned estimator is computationally intractable. The question of computational tractability was subsequently resolved by Hopkins (2018) and Cherapanamjeri, Flammarion and Bartlett (2019). The former showed that a polynomial-time algorithm achieves statistically optimal rate under the ℓ_2 -norm, and the latter proposed an estimator that has a significantly faster runtime and has sub-Gaussian error bounds; in particular, these results apply to covariance estimation in Frobenius norm. Yet it remains an open problem to design a polynomial-time algorithm capable of efficiently computing the estimator proposed by Mendelson and Zhivotovskiy (2018) that achieves near-optimal deviation in the spectral norm.

3.3 An *M*-estimation viewpoint

In this section, we discuss alternative tail-robust covariance estimators from an Mestimation perspective, and study both the element-wise and spectrum-wise truncated estimators. The connection with truncated covariance estimators is discussed at the end of this section. To proceed, we revisit the definition of Huber loss.

Definition 3.3 (Huber loss). The Huber loss $\ell_{\tau}(\cdot)$ (Huber, 1964) is defined as

$$\ell_{\tau}(u) = \begin{cases} u^2/2, & \text{if } |u| \le \tau, \\ \tau |u| - \tau^2/2, & \text{if } |u| > \tau, \end{cases}$$
(3.11)

where $\tau > 0$ is a robustification parameter similar to that in Definition 3.1.

Compared with the squared error loss, large values of u are down-weighted in the Huber loss, yielding robustness. Generally speaking, minimizing Huber's loss produces a biased estimator of the mean, and parameter τ can be chosen to control the bias. In other words, τ quantifies the tradeoff between bias and robustness. As observed by Sun, Zhou and Fan (2018), in order to achieve an optimal tradeoff, τ should adapt to the sample size, dimension and the noise level of the problem.

Starting with the element-wise method, we define the entry-wise estimators

$$\widehat{\sigma}_{1,k\ell}^{\mathcal{H}} = \underset{\theta \in \mathbb{R}}{\operatorname{argmin}} \sum_{i=1}^{N} \ell_{\tau_{k\ell}} (Y_{ik} Y_{i\ell}/2 - \theta), \quad 1 \le k, \ell \le d,$$
(3.12)

where $\tau_{k\ell}$ are robustification parameters satisfying $\tau_{k\ell} = \tau_{\ell k}$. When $k = \ell$, even though the minimization is over \mathbb{R} , it turns out the solution $\widehat{\sigma}_{1,kk}^{\mathcal{H}}$ is still positive almost surely and therefore provides a reasonable estimator of $\sigma_{1,kk}^{\mathcal{H}}$. To see this, for each $1 \leq k \leq d$, define $\theta_{0k} = \min_{1 \leq i \leq N} Y_{ik}^2/2$ and note that for any $\tau > 0$ and $\theta \leq \theta_{0k}$,

$$\sum_{i=1}^{N} \ell_{\tau}(Y_{ik}^2/2 - \theta) \ge \sum_{i=1}^{N} \ell_{\tau}(Y_{ik}^2/2 - \theta_{0k}).$$

It implies that $\widehat{\sigma}_{1,kk}^{\mathcal{H}} \geq \theta_{0k}$, which is strictly positive as long as there are no tied observations. Again, concatenating these marginal estimators, we obtain a Huber-type *M*-estimator

$$\widehat{\Sigma}_{1}^{\mathcal{H}} = \widehat{\Sigma}_{1}^{\mathcal{H}}(\Gamma) = (\widehat{\sigma}_{1,k\ell}^{\mathcal{H}})_{1 \le k,\ell \le d}, \qquad (3.13)$$

where $\Gamma = (\tau_{k\ell})_{1 \leq k,\ell \leq d}$. The following main result of this section indicates that $\widehat{\Sigma}_1^{\mathcal{H}}$ achieves tight concentration under the max norm for data with finite fourth moments.

Theorem 3.3. Let $\mathbf{V} = (v_{k\ell})_{1 \le k, \ell \le d}$ be a symmetric matrix with entries

$$v_{k\ell}^2 = \operatorname{var}((X_{1k} - X_{2k})(X_{1\ell} - X_{2\ell})/2).$$
(3.14)

For any $0 < \delta < 1$, the covariance estimator $\widehat{\Sigma}_{1}^{\mathcal{H}}$ given in (3.13) with

$$\mathbf{\Gamma} = \sqrt{\frac{m}{2\log d + \log \delta^{-1}}} \mathbf{V}$$
(3.15)

satisfies

$$\mathbb{P}\left(\|\widehat{\boldsymbol{\Sigma}}_{1}^{\mathcal{H}} - \boldsymbol{\Sigma}\|_{\max} \ge 4\|\mathbf{V}\|_{\max}\sqrt{\frac{2\log d + \log \delta^{-1}}{m}}\right) \le 2\delta \tag{3.16}$$

as long as $m \ge 8 \log(d^2 \delta^{-1})$.

The *M*-estimator counterpart of the spectrum-truncated covariance estimator was first proposed by Minsker (2018) using a different robust loss function, and extended by Minsker and Wei (2018) to more general framework of *U*-statistics. In line with the previous element-wise *M*-estimator, we restrict our attention to the Huber loss and consider

$$\widehat{\Sigma}_{2}^{\mathcal{H}} \in \operatorname*{argmin}_{\mathbf{M} \in \mathbb{R}^{d \times d} : \mathbf{M} = \mathbf{M}^{\intercal}} \operatorname{tr} \bigg\{ \frac{1}{N} \sum_{i=1}^{N} \ell_{\tau} (\boldsymbol{Y}_{i} \boldsymbol{Y}_{i}^{\intercal} / 2 - \mathbf{M}) \bigg\},$$
(3.17)

which is a natural robust variant of the sample covariance matrix

$$\widehat{\boldsymbol{\Sigma}}^{\text{sam}} = \operatorname*{argmin}_{\mathbf{M} \in \mathbb{R}^{d \times d}: \mathbf{M} = \mathbf{M}^{\intercal}} \operatorname{tr} \left\{ \frac{1}{N} \sum_{i=1}^{N} (\boldsymbol{Y}_{i} \boldsymbol{Y}_{i}^{\intercal} / 2 - \mathbf{M})^{2} \right\}$$

Define the $d \times d$ matrix $\mathbf{S}_0 = \mathbb{E}\{(\mathbf{X}_1 - \mathbf{X}_2)(\mathbf{X}_1 - \mathbf{X}_2)^{\intercal}/2 - \mathbf{\Sigma}\}^2$ that satisfies

$$\mathbf{S}_0 = \frac{\mathbb{E}\{(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^{\mathsf{T}}\}^2 + \operatorname{tr}(\boldsymbol{\Sigma})\boldsymbol{\Sigma}}{2}$$

The following result is modified from Corollary 4.1 of Minsker and Wei (2018).

Theorem 3.4. Assume that there exists some K > 0 such that $\sup_{\boldsymbol{u} \in \mathbb{R}^d} \operatorname{kurt}(\boldsymbol{u}^{\mathsf{T}}\boldsymbol{X}) \leq K$. Then for any $0 < \delta < 1$ and $v \geq \|\mathbf{S}_0\|_2^{1/2}$, the *M*-estimator $\widehat{\boldsymbol{\Sigma}}_2^{\mathcal{H}}$ with $\tau = v\sqrt{m/(2\log d + 2\log \delta^{-1})}$ satisfies

$$\|\widehat{\boldsymbol{\Sigma}}_{2}^{\mathcal{H}} - \boldsymbol{\Sigma}\|_{2} \le C_{1} v \sqrt{\frac{\log d + \log \delta^{-1}}{m}}$$
(3.18)

with probability at least $1 - 5\delta$ as long as $n \ge C_2 K \cdot r(\mathbf{\Sigma})(\log d + \log \delta^{-1})$, where $C_1, C_2 > 0$ are absolute constants.

To solve the convex optimization problem (3.17), Minsker and Wei (2018) propose the following gradient descent algorithm: starting with an initial estimator $\hat{\Sigma}^{(0)}$, at iteration t = 1, 2, ..., compute

$$\widehat{\boldsymbol{\Sigma}}^{(t)} = \widehat{\boldsymbol{\Sigma}}^{(t-1)} - \frac{1}{N} \sum_{i=1}^{N} \psi_{\tau} \Big(\boldsymbol{Y}_{i} \boldsymbol{Y}_{i}^{\mathsf{T}} / 2 - \widehat{\boldsymbol{\Sigma}}^{(t-1)} \Big),$$

where ψ_{τ} is given in (3.1). From this point of view, the truncated estimator $\widehat{\Sigma}_{2}^{\mathcal{T}}$ given in (3.6) can be viewed as the first step of the gradient descent iteration for solving optimization problem (3.17) initiated at $\widehat{\Sigma}^{(0)} = \mathbf{0}$. This procedure enjoys a nice contraction property, as demonstrated by Lemma 3.2 of Minsker and Wei (2018). However, since the difference matrix $\mathbf{Y}_i \mathbf{Y}_i^{\mathsf{T}}/2 - \widehat{\Sigma}^{(t-1)}$ for each t is no longer rank-one, we need to perform a singular value decomposition to compute the matrix $\psi_{\tau}(\mathbf{Y}_i\mathbf{Y}_i^{\mathsf{T}}/2 - \widehat{\Sigma}^{(t-1)})$ for $i = 1, \ldots, N$.

We end this section with a discussion of the similarities and differences between M-estimators and estimators defined via truncation. Both types of estimators achieve tail robustness through a bias-robustness tradeoff, either element-wise or spectrum-wise. However (informally speaking), M-estimators truncate symmetrically around the true expectation as shown in (3.12) and (3.17), while the truncationbased estimators truncate around zero as in (3.3) and (3.6). Due to smaller bias, M-estimators are expected to outperform the simple truncation estimators. However, since the optimal choice of the robustification parameter is often much larger than the population moments in magnitude, either element-wise or spectrum-wise, the difference between truncation estimators and M-estimators becomes insignificant when the sample size n is large. Therefore, we advocate using the simple truncated estimator primarily due to its simplicity and computational efficiency.

3.4 Median-of-means estimator

Truncation-based approaches described in the previous sections require knowledge of robustification parameters $\tau_{k\ell}$. Adaptation and tuning of these parameters will be discussed in Section 4 below. Here, we suggest another method that does not need any tuning but requires stronger assumptions, namely, existence of moments of order six. This method is based on the median-of-means (MOM) technique (Nemirovsky and Yudin, 1983; Devroye et al., 2016; Minsker and Strawn, 2017). To this end, assume that the index set $\{1, \ldots, n\}$ is partitioned into k disjoint groups G_1, \ldots, G_k (partitioning scheme is assumed to be independent of X_1, \ldots, X_n) such that the cardinalities $|G_j|$ satisfy $||G_j| - \frac{n}{k}| \leq 1$ for $j = 1, \ldots, k$. For each $j = 1, \ldots, k$, let $\bar{X}_{G_j} = (1/|G_j|) \sum_{i \in G_j} X_i$ and

$$\widehat{\boldsymbol{\Sigma}}^{(j)} = \frac{1}{|G_j|} \sum_{i \in G_j} (\boldsymbol{X}_i - \bar{\boldsymbol{X}}_{G_j}) (\boldsymbol{X}_i - \bar{\boldsymbol{X}}_{G_j})^{\mathsf{T}}$$

be the sample covariance evaluated over the data in group j. Then, for all $1 \leq \ell, m \leq d$, the MOM estimator of $\sigma_{\ell m}$ is defined via

$$\widehat{\sigma}_{\ell m}^{\text{MOM}} = \text{median} \{ \widehat{\sigma}_{\ell m}^{(1)}, \dots, \widehat{\sigma}_{\ell m}^{(k)} \},\,$$

where $\widehat{\sigma}_{\ell m}^{(j)}$ is the entry in the ℓ -th row and *m*-th column of $\widehat{\Sigma}^{(j)}$. This leads to

$$\widehat{\boldsymbol{\Sigma}}^{\text{MOM}} = \left(\widehat{\sigma}_{\ell m}^{\text{MOM}}\right)_{1 \leq \ell, m \leq d}$$

Let $\Delta_{\ell m}^2 = \operatorname{Var}((X_{\ell} - \mathbb{E}X_{\ell})(X_m - \mathbb{E}X_m))$ for $1 \leq \ell, m \leq d$. The following result provides a deviation bound for the MOM estimator $\widehat{\Sigma}^{\text{MOM}}$ under the max norm.

Theorem 3.5. Assume that $\min_{\ell,m} \Delta_{\ell m}^2 \ge c_\ell > 0$ and $\max_{1 \le k \le d} \mathbb{E}|X_k - \mathbb{E}X_k|^6 \le c_u < \infty$. Then, there exists $C_0 > 0$ depending only on (c_ℓ, c_u) such that

$$\mathbb{P}\left(\|\widehat{\mathbf{\Sigma}}^{\text{MOM}} - \mathbf{\Sigma}\|_{\max} \ge 3 \max_{\ell, m} \Delta_{\ell m} \left\{ \sqrt{\frac{\log(d+1) + \log \delta^{-1}}{n}} + C_0 \frac{k}{n} \right\} \right) \le 2\delta \quad (3.19)$$

for all δ satisfying $\sqrt{\{\log(d+1) + \log \delta^{-1}\}/k} + C_0 \sqrt{k/n} \le 0.33.$

Remark 4.

- 1. The only user-defined parameter in the definition of $\widehat{\Sigma}^{\text{MOM}}$ is the number of subgroups k. The bound above shows that, provided $k \ll \sqrt{n}$ (say, one could set $k = \frac{\sqrt{n}}{\log n}$), the term $C_0 \frac{k}{n}$ in (3.19) is of smaller order, and we obtain an estimator that admits tight deviation bounds for a wide range of δ . In this sense, estimator $\widehat{\Sigma}^{\text{MOM}}$ is essentially a multiple- δ estimator (Devroye et al., 2016); see Remark 1.
- 2. Application of the MOM construction to large covariance estimation problems has been explored by Avella-Medina et al. (2018). However, the results obtained therein are insufficient to conclude that MOM estimators are truly "tuning-free". Under a bounded fourth moment assumption, Avella-Medina et al. (2018) derived a deviation bound (under max norm) for the elementwise median-of-means estimator with the number of partitions depending on a prespecified confidence level parameter. See Proposition 5 therein.

4 Automatic tuning of robustification parameters

For all the proposed tail-robust estimators besides the median-of-means, the robustification parameter needs to adapt properly to the sample size, dimensionality and noise level in order to achieve optimal tradeoff between bias and robustness in finite samples. An intuitive yet computationally expensive idea is to use cross-validation. Another approach is based on Lepski's method (Lepski and Spokoiny, 1997); this approach yields adaptive estimators with provable guarantees (Minsker, 2018; Minsker and Wei, 2018), however, it is also not computationally efficient. In this section, we propose tuning-free approaches for constructing both truncated and *M*-estimators that have low computational costs. Our nonasymptotic analysis provides useful guidance on the choice of key tuning parameters.

4.1 Adaptive truncated estimator

In this section we introduce a data-driven procedure that automatically tunes the robustification parameters in the element-wise truncated covariance estimator. Practically, each individual parameter can be tuned by cross-validation from a grid search. This, however, will incur extensive computational cost even when the dimension dis moderately large. Instead, we propose a data-driven procedure that automatically calibrates the d(d + 1)/2 parameters. This procedure is motivated by the theoretical properties established in Theorem 3.1. To avoid notational clutter, we fix $1 \le k \le \ell \le d$ and define $\{Z_1 \ldots, Z_N\} = \{Y_{1k}Y_{1\ell}/2, \ldots, Y_{Nk}Y_{N\ell}/2\}$ such that $\sigma_{k\ell} = \mathbb{E}Z_1$. Then $\widehat{\sigma}_{1,k\ell}^{\mathcal{T}}$ can be written as $(1/N) \sum_{i=1}^N \psi_{\tau_{k\ell}}(Z_i)$. In view of (3.4), an "ideal" choice of $\tau_{k\ell}$ is

$$\tau_{k\ell} = v_{k\ell} \sqrt{\frac{m}{2\log d + t}} \quad \text{with} \quad v_{k\ell}^2 = \mathbb{E}Z_1^2, \tag{4.1}$$

where $t = \log \delta^{-1} \ge 1$ is prespecified to control the confidence level and will be discussed later. A naive estimator of $v_{k\ell}^2$ is the empirical second moment $(1/N) \sum_{i=1}^N Z_i^2$, which tends to overestimate the true value when data have high kurtosis. Intuitively, a well-chosen $\tau_{k\ell}$ makes $(1/N) \sum_{i=1}^N \psi_{\tau_{k\ell}}(Z_i)$ a good estimator of $\mathbb{E}Z_1$, and meanwhile, we expect the empirical truncated second moment $(1/N) \sum_{i=1}^N \psi_{\tau_{k\ell}}^2(Z_i) =$ $(1/N) \sum_{i=1}^N (Z_i^2 \wedge \tau_{k\ell}^2)$ to be a reasonable estimate of $\mathbb{E}Z_1^2$ as well. Plugging this empirical truncated second moment into (4.1) yields

$$\frac{1}{N}\sum_{i=1}^{N}\frac{(Z_i^2 \wedge \tau^2)}{\tau^2} = \frac{2\log d + t}{m}, \quad \tau > 0.$$
(4.2)

We then solve the above equation to obtain $\hat{\tau}_{k\ell}$, a data-driven choice of $\tau_{k\ell}$. By Proposition 3 in Wang et al. (2018), equation (4.2) has a unique solution as long as $2 \log d + t < (m/N) \sum_{i=1}^{N} I\{Z_i \neq 0\}$. We characterize the theoretical properties of this tuning method in a companion paper (Wang et al., 2018).

Regarding the choice of $t = \log \delta^{-1}$: on the one hand, as it controls the confidence level according to (3.5), we should let $t = t_n$ be sufficiently large so that the estimator is concentrated around the true value with high probability. On the other hand, talso appears in the deviation bound that corresponds to the width of the confidence interval, so it should not grow too fast as a function of n. In practice, we recommend using $t = \log n$ (or equivalently, $\delta = n^{-1}$), a typical slowly varying function of n. To implement the spectrum-wise truncated covariance estimator in practice, note that there is only one tuning parameter whose theoretically optimal scale is

$$\frac{1}{2} \|\mathbb{E}\{(\boldsymbol{X}_1 - \boldsymbol{X}_2)(\boldsymbol{X}_1 - \boldsymbol{X}_2)^{\mathsf{T}}\}^2\|_2^{1/2} \sqrt{\frac{m}{\log(2d) + t}}$$

Motivated by the data-driven tuning scheme for the element-wise estimator, we choose τ by (approximately) solving the equation

$$\left\|\frac{1}{\tau^2 N} \sum_{i=1}^N \left(\frac{\|\boldsymbol{Y}_i\|_2^2}{2} \bigwedge \tau\right)^2 \frac{\boldsymbol{Y}_i \boldsymbol{Y}_i^{\mathsf{T}}}{\|\boldsymbol{Y}_i\|_2^2}\right\|_2 = \frac{\log(2d) + t}{m},$$

where as before we take $t = \log n$.

4.2 Adaptive Huber-type *M*-estimator

To construct a data-driven approach for automatically tuning the adaptive Huber estimator, we follow the same rationale from the previous subsection. Since the optimal $\tau_{k\ell}$ now depends on $\operatorname{var}(Z_1)$ instead of the second moment $\mathbb{E}Z_1^2$, it is therefore conservative to directly apply the above data-driven method in this case. Instead, we propose to estimate $\tau_{k\ell}$ and $\sigma_{k\ell}$ simultaneously by solving the following system of equations

$$f_1(\theta,\tau) = \frac{1}{N} \sum_{i=1}^N \frac{\{(Z_i - \theta)^2 \wedge \tau^2\}}{\tau^2} - \frac{2\log d + t}{n} = 0,$$
(4.3a)

$$f_2(\theta, \tau) = \sum_{i=1}^{N} \psi_\tau(Z_i - \theta) = 0,$$
 (4.3b)

for $\theta \in \mathbb{R}$ and $\tau > 0$. Via a similar argument, it can be shown that the equation $f_1(\theta, \cdot) = 0$ has a unique solution as long as $2 \log d + t < (n/N) \sum_{i=1}^N I\{Z_i \neq \theta\}$; for any $\tau > 0$, the equation $f_2(\cdot, \tau) = 0$ also has a unique solution. Starting with an initial estimate $\theta^{(0)} = (1/N) \sum_{i=1}^N Z_i$, which is the sample variance estimator of $\sigma_{k\ell}$, we iteratively solve $f_1(\theta^{(s-1)}, \tau^{(s)}) = 0$ and $f_2(\theta^{(s)}, \tau^{(s)}) = 0$ for $s = 1, 2, \ldots$ until convergence. The resultant estimator, denoted by $\widehat{\sigma}_{3,k\ell}^{\mathcal{H}}$ with slight abuse of notation, is then referred to as the adaptive Huber estimator of $\sigma_{k\ell}$. We then obtain the data-adaptive Huber covariance matrix estimator as $\widehat{\Sigma}_3^{\mathcal{H}} = (\widehat{\sigma}_{3,k\ell}^{\mathcal{H}})_{1 \leq k,\ell \leq d}$. Algorithm 1 presents the summary of this data-driven approach.

5 Applications to structured matrix estimation

The robustness properties of the element-wise and spectrum-wise truncation estimators are demonstrated in Theorems 3.1 and 3.2. In particular, the exponential-type concentration bounds are essential for establishing reasonable estimators for highdimensional structured covariance and precision matrices. In this section, we apply the proposed generic robust methods to the estimation of bandable and low-rank covariance matrices as well as sparse precision matrix. Algorithm 1 Data-Adaptive Huber Covariance Matrix Estimation

Input Data vectors $X_i \in \mathbb{R}^d$ (i = 1, ..., n), tolerance level ϵ and maximum iteration S_{max} .

Output Data-adaptive Huber covariance matrix estimator $\widehat{\Sigma}_{3}^{\mathcal{H}} = (\widehat{\sigma}_{3,k\ell}^{\mathcal{H}})_{1 \leq k,\ell \leq d}$.

- 1: Compute pairwise differences $Y_1 = X_1 X_2$, $Y_2 = X_1 X_3$, ..., $Y_N = X_{n-1} X_n$, where N = n(n-1)/2.
- 2: **for** $1 \le k \le \ell \le d$ **do**
- 3: $\theta^{(0)} = (2N)^{-1} \sum_{i=1}^{N} Y_{ik} Y_{i\ell}.$
- 4: for $s = 1, \dots S_{\max}$ do
- 5: $\tau^{(s)} \leftarrow \text{solution of } f_1(\theta^{(s-1)}, \cdot) = 0.$
- 6: $\theta^{(s)} \leftarrow \text{solution of } f_2(\cdot, \tau^{(s)}) = 0.$
- 7: if $|\theta^{(s)} \theta^{(s-1)}| < \epsilon$ break
- 8: **stop** $\widehat{\sigma}_{3,\ell k}^{\mathcal{H}} = \widehat{\sigma}_{3,k\ell}^{\mathcal{H}} = \theta^{(S_{\max})}.$
- 9: **stop**

10: return $\widehat{\Sigma}_{3}^{\mathcal{H}} = (\widehat{\sigma}_{3,k\ell}^{\mathcal{H}})_{1 \leq k,\ell \leq d}.$

5.1 Bandable covariance matrix estimation

Motivated by applications to climate studies and spectroscopy in which the index set of variables $\mathbf{X} = (X_1, \ldots, X_d)^{\mathsf{T}}$ admits a natural order, one can expect that a large "distance" $|k - \ell|$ implies near-independence. We characterize this feature by the following class of bandable covariance matrices considered by Bickel and Levina (2008a) and by Cai, Zhang and Zhou (2010):

$$\mathcal{F}_{\alpha}(M_{0}, M) = \left\{ \boldsymbol{\Sigma} = (\sigma_{k\ell})_{1 \leq k, \ell \leq d} \in \mathbb{R}^{d \times d} : \lambda_{1}(\boldsymbol{\Sigma}) \leq M_{0}, \\ \max_{1 \leq \ell \leq d} \sum_{k: |k-\ell| > m} |\sigma_{k\ell}| \leq \frac{M}{m^{\alpha}} \text{ for all } m \right\}.$$
(5.1)

Here M_0, M are regarded as universal constants and the parameter α specifies the decay rate of $\sigma_{k\ell}$ to zero as $\ell \to \infty$ for each row.

When X follows sub-Gaussian distribution, Cai, Zhang and Zhou (2010) proposed a minimax-optimal estimator over $\mathcal{F}_{\alpha}(M_0, M)$ under the spectral norm. Specifically, they proposed a tapering estimator $\widehat{\Sigma}_m^{\text{tap}} = (\widehat{\sigma}_{k\ell} \cdot \omega_{|k-\ell|})$, where the positive integer $m \leq d$ specifies the bandwidth, $\omega_q = 1$, 2 - 2q/m, 0, when $q \leq m/2$, $m/2 < q \leq m$, q > m, respectively. $\widehat{\Sigma}^{\text{sam}} = (\widehat{\sigma}_{k\ell})_{1 \leq k,\ell \leq d}$ denotes the sample covariance. With the optimal choice of bandwidth $m \approx \min\{n^{1/(2\alpha+1)}, d\}$, Cai, Zhang and Zhou (2010) showed that $\widehat{\Sigma}_m^{\text{tap}}$ achieves the minimax rate of convergence $\{\sqrt{\log(d)/n} + n^{-\alpha/(2\alpha+1)}\} \land \sqrt{d/n}$ under the spectral norm.

To obtain a root-*n* consistent covariance estimator, we expect the coordinates of X to have at least finite fourth moments. Under this condition, it is unclear whether the optimal rate can be achieved over $\mathcal{F}_{\alpha}(M_0, M)$ without imposing additional distributional assumptions, such as the elliptical symmetry (Mitra and Zhang, 2014; Chen, Gao and Ren, 2018). Estimators that naively use the sample covariance will inherit its sensitivity to outliers. Recall the definition of $\widehat{\Sigma}_2^{\mathcal{T}}$ in (3.6); a simple idea is to replace the sample covariance by a spectrum-wise truncated estimator $\widehat{\Sigma}_2^{\mathcal{T}}$ in the first step, to which the tapering procedure can be applied. However, such an estimator is not optimal: indeed, the analysis of a tapering estimator requires each small principal submatrix of the initial estimator to be highly concentrated around the population object. Suppose that we truncate the ℓ_2 -norm of the entire vector Y_i at a level τ scaling with tr(Σ). For each subset $J \subseteq \{1, \ldots, d\}$, let Y_{iJ} be the subvector of Y_i indexed by J. Then the corresponding principal submatrix

$$\frac{1}{N}\sum_{i=1}^{N}\psi_{\tau}\left(\frac{1}{2}\|\boldsymbol{Y}_{i}\|_{2}^{2}\right)\frac{\boldsymbol{Y}_{iJ}\boldsymbol{Y}_{iJ}^{\mathsf{T}}}{\|\boldsymbol{Y}_{i}\|_{2}^{2}}$$

is not an ideal robust estimator of Σ_{JJ} because the "optimal" τ in this case should scale with tr(Σ_{JJ}) rather than tr(Σ). This explains why directly applying the tapering procedure to $\widehat{\Sigma}_{2}^{\mathcal{T}}$ is not ideal.

In what follows, we propose an optimal robust covariance estimator based on the spectrum-wise truncation technique introduced in Section 3.2. First we introduce some notation. Let $\mathbf{Z}_{i}^{(p,q)} = (Y_{i,p}, Y_{i,p+1}, \ldots, Y_{i,p+q-1})^{\mathsf{T}}$ be a subvector of \mathbf{Y}_{i} given

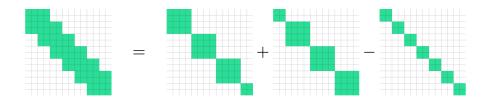


Figure 2: Motivation of our estimator of bandable covariance matrices

in (3.2). Accordingly, define the truncated estimator of the principal submatrix of Σ as

$$\widehat{\Sigma}_{2}^{(p,q),\mathcal{T}} = \widehat{\Sigma}_{2}^{(p,q),\mathcal{T}}(\tau) = \frac{1}{N} \sum_{i=1}^{N} \psi_{\tau}(\mathbf{Z}_{i}^{(p,q)} \mathbf{Z}_{i}^{(p,q)\mathsf{T}}/2),$$
(5.2)

where τ is as in (3.8) with d replaced by q and $v = \|\mathbb{E}\{Z_1^{(p,q)}Z_1^{(p,q)\mathsf{T}}\}^2\|_2/4$. Moreover, we define an operator that embeds a small matrix into a large zero matrix: for a $q \times q$ matrix $\mathbf{A} = (a_{k\ell})_{1 \leq k,\ell \leq q}$, define the $d \times d$ matrix $\mathbf{E}_p^d(\mathbf{A}) = (b_{k\ell})_{1 \leq k,\ell \leq d}$, where p indicates the location and

$$b_{k\ell} = \begin{cases} a_{k-p+1,\ell-p+1} & \text{if } p \le k, \ell \le p+q-1, \\ 0 & \text{otherwise.} \end{cases}$$

Our final robust covariance estimator is then defined as

$$\widehat{\Sigma}_{q} = \sum_{j=-1}^{\lceil (d-1)/q \rceil} \mathbf{E}_{jq+1}^{d} (\widehat{\Sigma}_{2}^{(jq+1,2q),\mathcal{T}}) - \sum_{j=0}^{\lceil (d-1)/q \rceil} \mathbf{E}_{jq+1}^{d} (\widehat{\Sigma}_{2}^{(jq+1,q),\mathcal{T}}).$$
(5.3)

The idea behind the construction above is that a bandable covariance matrix in $\mathcal{F}_{\alpha}(M_0, M)$ can be approximately decomposed into several principal submatrices of size 2q and q, as shown in Figure 2. Using spectrum-wise truncated estimators $\widehat{\Sigma}_2^{(p,q),\mathcal{T}}$ and $\widehat{\Sigma}_2^{(p,2q),\mathcal{T}}$ to estimate the corresponding principal submatrices in this decomposition leads to the proposed estimator $\widehat{\Sigma}_q$.

This construction is different from the literature where the banding or tapering procedure is directly applied to an initial estimator, say the sample covariance matrix (Bickel and Levina, 2008a; Cai, Zhang and Zhou, 2010). It is worth mentioning that a similar robust estimator can be constructed following the idea of Cai, Zhang and Zhou (2010), which differs from our proposal. Computationally, our estimator evaluates as many as O(d/q) matrices of size $q \times q$ (or $2q \times 2q$), while the method developed by Cai, Zhang and Zhou (2010) computes as many as O(d) such matrices.

The following result shows that the estimator defined in (5.3) achieves nearoptimal rate of convergence under the spectral norm as long as X has uniformly bounded fourth moments. The proof is deferred to the supplementary material.

Theorem 5.1. Assume that $\Sigma \in \mathcal{F}_{\alpha}(M_0, M)$ and $\sup_{\boldsymbol{u} \in \mathbb{S}^{d-1}} \operatorname{kurt}(\boldsymbol{u}^{\mathsf{T}}\boldsymbol{X}) \leq M_1$ for some constant $M_1 > 0$. For any $c_0 > 0$, take $\delta = (n^{c_0}d)^{-1}$ in the definition of

 τ for constructing principal submatrix estimators $\widehat{\Sigma}_{2}^{(p,q),\tau}$ in (5.2). Then, with a bandwidth $q \simeq \{n/\log(nd)\}^{1/(2\alpha+1)} \wedge d$, the estimator $\widehat{\Sigma}_{q}$ defined in (5.3) is such that with probability at least $1 - 2n^{-c_0}$,

$$\|\widehat{\Sigma}_q - \Sigma\|_2 \le C \min\left\{\left(\frac{\log(nd)}{n}\right)^{\alpha/(2\alpha+1)}, \sqrt{\frac{d \cdot \log(nd)}{n}}\right\},\$$

where C > 0 is a constant depending only on M, M_0, M_1, c_0 .

According to the minimax lower bounds established by Cai, Zhang and Zhou (2010), up to a logarithmic term our robust estimator achieves the optimal rate of convergence that is enjoyed by the tapering estimator when the data are sub-Gaussian. The logarithmic term is not easy to remove: for instance, one cannot improve the rate of convergence by replacing each principal submatrix estimator in (5.2) with the theoretically more refined but computationally intractable estimator proposed by Mendelson and Zhivotovskiy (2018) (see Remark 3).

Remark 5. To achieve the near-optimal convergence rate shown in Theorem 5.1, the ideal choice of the bandwidth q depends on the knowledge of α . A fully datadriven and adaptive estimator can be obtained by selecting the optimal bandwidth via Lepski's method (Lepski and Spokoiny, 1997). We refer to Liu and Ren (2018) for constructing a similar adaptive estimator for a precision matrix with bandable Cholesky factor.

5.2 Low-rank covariance matrix estimation

In this section, we consider a structured model where $\Sigma = \text{cov}(X)$ is approximately low-rank. Using the trace-norm as a convex relaxation of the rank, our estimator is the solution to the following trace-norm penalized optimization program:

$$\widehat{\boldsymbol{\Sigma}}_{2,\gamma}^{\mathcal{T}} \in \operatorname*{argmin}_{\boldsymbol{A} \in \mathcal{S}_d} \left\{ \frac{1}{2} \| \boldsymbol{A} - \widehat{\boldsymbol{\Sigma}}_2^{\mathcal{T}} \|_{\mathrm{F}}^2 + \gamma \| \boldsymbol{A} \|_{\mathrm{tr}} \right\},$$
(5.4)

where S_d denotes the set of $d \times d$ positive semi-definite matrices, $\gamma > 0$ is a regularization parameter and $\widehat{\Sigma}_2^{\mathcal{T}}$, defined in (3.6), serves as a pilot estimator. This trace-penalized method was first proposed by Lounici (2014) with the initial estimator taken to be the sample covariance matrix, and later studied by Minsker (2018) using a different initial estimator. In fact, given the initial estimator $\widehat{\Sigma}_2^{\mathcal{T}}$, the estimator given in (5.4) has the following closed-form expression (Lounici, 2014):

$$\widehat{\boldsymbol{\Sigma}}_{2,\gamma}^{\mathcal{T}} = \sum_{k=1}^{d} \max\{\lambda_k(\widehat{\boldsymbol{\Sigma}}_2^{\mathcal{T}}) - \gamma, 0\} \boldsymbol{v}_k(\widehat{\boldsymbol{\Sigma}}_2^{\mathcal{T}}) \boldsymbol{v}_k(\widehat{\boldsymbol{\Sigma}}_2^{\mathcal{T}})^{\mathsf{T}},$$
(5.5)

where $\lambda_1(\widehat{\Sigma}_2^{\mathcal{T}}) \geq \cdots \geq \lambda_d(\widehat{\Sigma}_2^{\mathcal{T}})$ are the eigenvalues of $\widehat{\Sigma}_2^{\mathcal{T}}$ in an non-increasing order and $v_1(\widehat{\Sigma}_2^{\mathcal{T}}), \ldots, v_d(\widehat{\Sigma}_2^{\mathcal{T}})$ are the associated orthonormal eigenvectors. The following theorem provides a deviation bound for $\widehat{\Sigma}_{2,\gamma}^{\mathcal{T}}$ under the Frobenius norm. The proof follows directly from Theorem 3.2 and Theorem 1 of Lounici (2014), and therefore is omitted. **Theorem 5.2.** For any t > 0 and v > 0 satisfying (3.7), let

$$au = v \sqrt{\frac{m}{\log(2d) + t}}$$
 and $\gamma \ge 2v \sqrt{\frac{\log(2d) + t}{m}}$.

Then with probability at least $1 - e^{-t}$, the trace-penalized estimator $\widehat{\Sigma}_{2,\gamma}^{\mathcal{T}}$ satisfies

$$\begin{split} \|\widehat{\boldsymbol{\Sigma}}_{2,\gamma}^{\mathcal{T}} - \boldsymbol{\Sigma}\|_{\mathrm{F}}^{2} &\leq \inf_{\mathbf{A} \in \mathcal{S}_{d}} \left[\|\boldsymbol{\Sigma} - \mathbf{A}\|_{\mathrm{F}}^{2} + \min\{4\gamma \|\mathbf{A}\|_{\mathrm{tr}}, 3\gamma^{2} \mathrm{rank}(\mathbf{A})\} \right] \\ &\text{and} \quad \|\widehat{\boldsymbol{\Sigma}}_{2,\gamma}^{\mathcal{T}} - \boldsymbol{\Sigma}\|_{2} \leq 2\gamma. \end{split}$$

In particular, if rank(Σ) $\leq r_0$, then with probability at least $1 - e^{-t}$,

$$\|\widehat{\boldsymbol{\Sigma}}_{2,\gamma}^{\mathcal{T}} - \boldsymbol{\Sigma}\|_{\mathrm{F}}^{2} \le \min\{4\|\boldsymbol{\Sigma}\|_{2}\gamma, 3\gamma^{2}\}r_{0}.$$
(5.6)

5.3 Sparse precision matrix estimation

Our third example is related to sparse precision matrix estimation in high dimensions. Recently, Avella-Medina et al. (2018) showed that minimax optimality is achievable within a larger class of distributions if the sample covariance matrix is replaced by a robust pilot estimator, and also provided a unified theory for covariance and precision matrix estimation based on general pilot estimators. Specifically, Avella-Medina et al. (2018) robustifed the CLIME estimator (Cai, Liu and Luo, 2011) using three different pilot estimators: adaptive Huber, median-of-means and rank-based estimators. Based on the element-wise truncation procedure and the difference of trace (D-trace) loss proposed by Zhang and Zou (2014), we further consider a robust method for estimating the precision matrix $\Theta^* = \Sigma^{-1}$ under sparsity, which represents a useful complement to the methods developed by Avella-Medina et al. (2018).

The advantage of using the D-trace loss is that it automatically gives rise to a symmetric solution. Specifically, using the element-wise truncated estimator $\widehat{\Sigma}_1^{\mathcal{T}} = \widehat{\Sigma}_1^{\mathcal{T}}(\Gamma)$ in (3.3) as an initial estimate of Σ , we propose to solve

$$\widehat{\boldsymbol{\Theta}} \in \operatorname*{argmin}_{\boldsymbol{\Theta} \in \mathbb{R}^{d \times d}} \bigg\{ \underbrace{\frac{1}{2} \langle \boldsymbol{\Theta}^2, \widehat{\boldsymbol{\Sigma}}_1^{\mathcal{T}} \rangle - \operatorname{tr}(\boldsymbol{\Theta})}_{\mathcal{L}(\boldsymbol{\Theta})} + \lambda \|\boldsymbol{\Theta}\|_{\ell_1} \bigg\}.$$
(5.7)

where $\|\Theta\|_{\ell_1} = \sum_{k \neq \ell} |\Theta_{k\ell}|$ for $\Theta = (\Theta_{k\ell})_{1 \leq k,\ell \leq d}$. For simplicity, we write $\mathcal{L}(\Theta) = \langle \Theta^2, \widehat{\Sigma}_1^T \rangle - \operatorname{tr}(\Theta)$. Zhang and Zou (2014) imposed a positive definiteness constraint on Θ , and proposed an alternating direction method of multipliers (ADMM) algorithm to solve the constrained D-trace loss minimization. However, with the positive definiteness constraint, the ADMM algorithm at each iteration computes the singular value decomposition of a $d \times d$ matrix, and therefore is computationally intensive for large-scale data. In (5.7), we impose no constraint on Θ primarily for computational simplicity.

Before presenting the main theorem, we need to introduce an assumption on the restricted eigenvalue of the Hessian matrix of \mathcal{L} . First, note that the Hessian of \mathcal{L}

can be written as

$$\mathbf{H}_{\mathbf{\Gamma}} = rac{1}{2} (\mathbf{I} \otimes \widehat{\mathbf{\Sigma}}_{1}^{\mathcal{T}} + \widehat{\mathbf{\Sigma}}_{1}^{\mathcal{T}} \otimes \mathbf{I}),$$

where Γ is the tuning parameter matrix in (3.3). For matrices $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{d^2 \times d^2}$, we define $\langle \mathbf{A}, \mathbf{A} \rangle_{\mathbf{B}} = \operatorname{vec}(\mathbf{A})^{\mathsf{T}} \mathbf{B} \operatorname{vec}(\mathbf{A})$, where $\operatorname{vec}(\mathbf{A})$ designates the d^2 -dimensional vector concatenating the columns of \mathbf{A} . Let $\mathcal{S} = \operatorname{supp}(\mathbf{\Theta}^*) \subseteq \{1, \ldots, d\}^2$, the support set of $\mathbf{\Theta}^*$.

Definition 5.1. (Restricted Eigenvalue for Matrices) For any $\xi > 0$ and $m \ge 1$, we define the maximal and minimal restricted eigenvalues of the Hessian matrix \mathbf{H}_{Γ} as

$$\begin{aligned} \kappa_{-}(\mathbf{\Gamma},\xi,m) &= \inf_{\mathbf{W}} \left\{ \frac{\langle \mathbf{W},\mathbf{W} \rangle_{\mathbf{H}_{\mathbf{\Gamma}}}}{\|\mathbf{W}\|_{\mathrm{F}}^{2}} : \mathbf{W} \in \mathbb{R}^{d \times d}, \mathbf{W} \neq 0, \exists J \text{ such that } \mathcal{S} \subseteq J, \\ |J| \leq m, \|\mathbf{W}_{J^{\mathrm{c}}}\|_{\ell_{1}} \leq \xi \|\mathbf{W}_{J}\|_{\ell_{1}} \right\}; \\ \kappa_{+}(\mathbf{\Gamma},\xi,m) &= \sup_{\mathbf{W}} \left\{ \frac{\langle \mathbf{W},\mathbf{W} \rangle_{\mathbf{H}_{\mathbf{\Gamma}}}}{\|\mathbf{W}\|_{\mathrm{F}}^{2}} : \mathbf{W} \in \mathbb{R}^{d \times d}, \mathbf{W} \neq 0, \exists J \text{ such that } \mathcal{S} \subseteq J, \\ |J| \leq m, \|\mathbf{W}_{J^{\mathrm{c}}}\|_{\ell_{1}} \leq \xi \|\mathbf{W}_{J}\|_{\ell_{1}} \right\}. \end{aligned}$$

Condition 5.1. (Restricted Eigenvalue Condition) We say restricted eigenvalue condition with $(\Gamma, 3, k)$ holds if $0 < \kappa_{-} = \kappa_{-}(\Gamma, 3, k) \le \kappa_{+}(\Gamma, 3, k) = \kappa_{+} < \infty$.

Condition 5.1 is a form of the localized restricted eigenvalue condition (Fan et al., 2018). Moreover, we assume that the true precision matrix Θ^* lies in the following class of matrices:

$$\mathcal{U}(s,M) = \bigg\{ \mathbf{\Omega} \in \mathbb{R}^{d \times d} : \mathbf{\Omega} = \mathbf{\Omega}^{\mathsf{T}}, \mathbf{\Omega} \succ 0, \|\mathbf{\Omega}\|_{1} \le M, \sum_{k,\ell} I(\Omega_{k\ell} \neq 0) \le s \bigg\}.$$

A similar class of precision matrices has been studied in the literature; see, for example, Zhang and Zou (2014), Cai, Ren and Zhou (2016) and Sun et al. (2018). Recall the definition of \mathbf{V} in Theorem 3.1. We are ready to present the main result, with the proof deferred to the supplementary material.

Theorem 5.3. Assume that $\Theta^* = \Sigma^{-1} \in \mathcal{U}(s, M)$. Let $\Gamma \in \mathbb{R}^{d \times d}$ be as in Theorem 3.1 and let λ satisfy

$$\lambda = 4C \|\mathbf{V}\|_{\max} \sqrt{\frac{2\log d + \log \delta^{-1}}{\lfloor n/2 \rfloor}} \text{ for some } C \ge M.$$

Assume Condition 5.1 is fulfilled with k = s and Γ specified above. Then with probability at least $1 - 2\delta$, we have

$$\|\widehat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}^*\|_{\mathrm{F}} \le 6 C \kappa_{-}^{-1} \|\mathbf{V}\|_{\max} s^{1/2} \sqrt{\frac{2 \log d + \log \delta^{-1}}{\lfloor n/2 \rfloor}}$$

Remark 6. The nonasymptotic probabilistic bound in Theorem 5.3 is established under the assumption that Condition 5.1 holds. It can be shown that Condition 5.1 is satisfied with high probability as long as the coordinates of X have bounded fourth moments. The proof is based on an argument similar to that in the proof of Lemma 4 in the work of Sun, Zhou and Fan (2018), and thus is omitted here.

6 Numerical study

In this section, we assess the numerical performance of proposed tail-robust covariance estimators. We consider the element-wise truncated covariance estimator $\hat{\Sigma}_1^{\mathcal{T}}$ defined in (3.3), the spectrum-wise truncated covariance estimator $\hat{\Sigma}_2^{\mathcal{T}}$ defined in (3.6), the Huber-type *M*-estimator $\hat{\Sigma}_1^{\mathcal{H}}$ given in (3.13) and the adaptive Huber *M*-estimator $\hat{\Sigma}_3^{\mathcal{H}}$ in Section 4.2.

Throughout this section, we let $\{\tau_{k\ell}\}_{1 \leq k,\ell \leq d} = \tau$ for $\widehat{\Sigma}_1^{\mathcal{H}}$. To compute $\widehat{\Sigma}_2^{\mathcal{T}}$ and $\widehat{\Sigma}_1^{\mathcal{H}}$, the robustification parameter τ is selected by five-fold cross-validation. The robustification parameters $\{\tau_{k\ell}\}_{1 \leq k,\ell \leq d}$ for $\widehat{\Sigma}_1^{\mathcal{T}}$ are tuned by solving the equation (4.2), and thus is an adaptive elementwise-truncated estimator. To implement the *adaptive Huber M-estimator* $\widehat{\Sigma}_3^{\mathcal{H}}$, we calibrate $\{\tau_{k\ell}\}_{1 \leq k,\ell \leq d}$ and estimate $\{\sigma_{k\ell}\}_{1 \leq k,\ell \leq d}$ simultaneously by solving the equation system (4.3) as described in Algorithm 1.

We first generate a data matrix $\mathbf{Y} \in \mathbb{R}^{n \times d}$ with rows being i.i.d. vectors from a distribution with mean **0** and covariance matrix \mathbf{I}_d . We then rescaled the data and set $\mathbf{X} = \mathbf{Y} \mathbf{\Sigma}^{1/2}$ as the final data matrix, where $\mathbf{\Sigma} \in \mathbb{R}^{d \times d}$ is a structured covariance matrix. We consider four distribution models outlined below:

- (1) (Normal model). The rows of **Y** are i.i.d. generated from the standard normal distribution.
- (2) (Student's t model). $\mathbf{Y} = \mathbf{Z}/\sqrt{3}$, where the entries of \mathbf{Z} are i.i.d. with Student's distribution with 3 degrees of freedom.
- (3) (Pareto model). $\mathbf{Y} = 4\mathbf{Z}/3$, where the entries of \mathbf{Z} are i.i.d. with Pareto distribution with shape parameter 3 and scale parameter 1.
- (4) (Log-normal model). $\mathbf{Y} = \exp\{0.5 + \mathbf{Z}\}/(e^3 e^2)$, where the entries of \mathbf{Z} are i.i.d. with standard normal distribution.

The covariance matrix Σ has one of the following three structures:

- (a) (Diagonal structure). $\Sigma = \mathbf{I}_d$;
- (b) (Equal correlation structure). $\sigma_{k\ell} = 1$ for $k = \ell$ and $\sigma_{k\ell} = 0.5$ when $k \neq \ell$;
- (c) (Power decay structure). $\sigma_{k\ell} = 1$ for $k = \ell$ and $\sigma_{k\ell} = 0.5^{|k-\ell|}$ when $k \neq \ell$.

In each setting, we choose (n, d) as (50, 100), (50, 200) and (100, 200), and simulate 200 replications for each scenario. The performance is assessed by the relative mean error (RME) under spectral, max or Frobenius norm:

$$\text{RME} = \frac{\sum_{i=1}^{200} \|\widehat{\boldsymbol{\Sigma}}_i - \boldsymbol{\Sigma}\|_{2,\text{max},\text{F}}}{\sum_{i=1}^{200} \|\widetilde{\boldsymbol{\Sigma}}_i - \boldsymbol{\Sigma}\|_{2,\text{max},\text{F}}}$$

where $\widehat{\Sigma}_i$ is the estimate of Σ in the *i*th simulation using one of the four robust methods and $\widetilde{\Sigma}_i$ denotes the sample covariance estimate that serves as a benchmark. The smaller the RME is, the more improvement the robust method achieves.

Tables 1–3 summarize the simulation results, which indicate that all the robust estimators outperform the sample covariance matrix by a visible margin when data are generated from a heavy-tailed or an asymmetric distribution. On the other hand, the proposed estimators perform almost as good as the sample covariance matrix when the data follows a normal distribution, indicating high efficiency in this case. The performance of the four robust estimators are comparable in all scenarios: the spectrum-wise truncated covariance estimator $\hat{\Sigma}_2^{\mathcal{T}}$ has the smallest RME under spectral norm, while the other three estimators perform better under max and Frobenius norms. This outcome is inline with our intuition discussed in Section 3. Furthermore, the computationally efficient adaptive Huber M-estimator $\hat{\Sigma}_3^{\mathcal{H}}$ performs comparably as the Huber-type M-estimator $\hat{\Sigma}_1^{\mathcal{H}}$ where the robustification parameters are chosen by cross-validation.

Table 1: RME under diagonal structure.												
$n = 50, \ p = 100$												
		Norma	1	t_3			Pareto			Log-normal		
	2	max	F	2	max	F	2	\max	F	2	max	F
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}}$	0.97	0.95	0.98	0.37	0.39	0.65	0.27	0.21	0.47	0.27	0.21	0.51
$\widehat{\mathbf{\Sigma}}_{3}^{\mathcal{H}}$	0.97	0.90	0.96	0.37	0.36	0.59	0.29	0.24	0.45	0.24	0.19	0.49
$\widehat{\mathbf{\Sigma}}_1^\mathcal{T}$	0.97	0.91	0.96	0.40	0.38	0.62	0.27	0.23	0.42	0.25	0.18	0.50
$egin{array}{c} \widehat{\mathbf{\Sigma}}_3^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_2^{\mathcal{T}} \ \widehat{\mathbf{\Sigma}}_2^{\mathcal{T}} \end{array}$	0.96	0.99	0.98	0.34	0.41	0.67	0.26	0.25	0.44	0.25	0.26	0.56
n = 50, p = 200												
		Norma	1	t_3			Pareto			Log-normal		
	2	max	F	2	max	F	2	max	F	2	max	F
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}}$	0.98	0.95	0.98	0.32	0.29	0.60	0.29	0.23	0.41	0.24	0.20	0.43
$\widehat{\mathbf{\Sigma}}_3^{\mathcal{H}}$	0.98	0.96	0.97	0.31	0.26	0.54	0.27	0.20	0.42	0.24	0.19	0.38
$egin{array}{lll} \widehat{\mathbf{\Sigma}}_1^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_3^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_1^{\mathcal{T}} \ \widehat{\mathbf{\Sigma}}_2^{\mathcal{T}} \end{array}$	0.97	0.95	0.96	0.33	0.29	0.63	0.26	0.19	0.39	0.23	0.18	0.42
$\widehat{\mathbf{\Sigma}}_2^\mathcal{T}$	0.95	0.98	0.95	0.31	0.33	0.65	0.24	0.26	0.48	0.22	0.23	0.48
n = 100, p = 200												
		Norma	1	t_3			Pareto			Log-normal		
	2	\max	\mathbf{F}	2	\max	F	2	\max	F	2	\max	F
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}}$	0.99	0.98	0.99	0.40	0.47	0.58	0.46	0.49	0.51	0.32	0.20	0.47
$\widehat{\mathbf{\Sigma}}_3^\mathcal{H}$	0.95	0.99	0.98	0.39	0.47	0.59	0.45	0.45	0.48	0.28	0.21	0.49
$\widehat{\mathbf{\Sigma}}_1^\mathcal{T}$	0.97	0.94	0.97	0.38	0.45	0.57	0.46	0.49	0.51	0.26	0.27	0.47
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{3}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{2}^{\mathcal{T}}$	0.94	1.01	0.95	0.33	0.51	0.64	0.42	0.53	0.61	0.28	0.27	0.58

Mean relative errors of the the four robust estimators $\widehat{\Sigma}_1^{\mathcal{H}}$, $\widehat{\Sigma}_3^{\mathcal{H}}$, $\widehat{\Sigma}_1^{\mathcal{T}}$ and $\widehat{\Sigma}_2^{\mathcal{T}}$ over 200 replications when the true covariance matrix has a diagonal structure. 2, max and F denote the spectral, max and Frobenius norms, respectively.

7 Discussion

In this paper, we surveyed and unified selected recent results on covariance estimation for heavy-tailed distributions. More specifically, we proposed element-wise and

$n = 50, \ p = 100$													
	Normal				t_3			Pareto			Log-normal		
	2	\max	\mathbf{F}	2	\max	\mathbf{F}	2	\max	\mathbf{F}	2	\max	F	
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}}$	0.97	0.94	0.97	0.68	0.12	0.68	0.68	0.23	0.59	0.58	0.27	0.46	
$\widehat{\mathbf{\Sigma}}_3^{\mathcal{H}}$	0.96	0.95	0.96	0.69	0.15	0.64	0.62	0.21	0.59	0.52	0.27	0.44	
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{3}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{1}^{\mathcal{T}} \ \widehat{\mathbf{\Sigma}}_{2}^{\mathcal{T}}$	0.97	0.96	0.97	0.67	0.14	0.67	0.64	0.22	0.57	0.59	0.28	0.47	
$\widehat{\mathbf{\Sigma}}_2^\mathcal{T}$	0.95	0.99	1.02	0.56	0.26	0.71	0.62	0.27	0.60	0.50	0.33	0.51	
$n = 50, \ p = 200$													
Normal					t_3			Pareto			Log-normal		
	2	max	F	2	max	F	2	max	F	2	max	F	
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}}$	0.97	0.94	0.98	0.77	0.21	0.76	0.67	0.34	0.50	0.69	0.23	0.67	
$\widehat{\mathbf{\Sigma}}_{3}^{\mathcal{H}}$	1.00	0.97	0.98	0.77	0.22	0.73	0.63	0.31	0.50	0.70	0.23	0.68	
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{3}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{1}^{\mathcal{T}} \ \widehat{\mathbf{\Sigma}}_{2}^{\mathcal{T}}$	0.99	0.97	0.96	0.78	0.24	0.71	0.63	0.33	0.46	0.70	0.23	0.68	
$\widehat{\mathbf{\Sigma}}_2^\mathcal{T}$	0.95	0.98	1.00	0.74	0.35	0.80	0.61	0.34	0.51	0.66	0.31	0.72	
					n = 1	100, p =	= 200						
		Norma	t_3			Pareto			Log-normal				
	2	\max	F	2	\max	F	2	\max	F	2	\max	F	
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}}$	1.00	0.96	0.99	0.79	0.23	0.78	0.63	0.46	0.57	0.53	0.21	0.47	
$\widehat{\mathbf{\Sigma}}_3^{\mathcal{H}}$	0.98	0.98	0.97	0.79	0.24	0.79	0.69	0.48	0.58	0.57	0.22	0.48	
$\widehat{\mathbf{\Sigma}}_1^\mathcal{T}$	1.00	1.00	0.99	0.78	0.21	0.77	0.65	0.45	0.57	0.55	0.23	0.50	
$egin{array}{c} \widehat{oldsymbol{\Sigma}}_1^{\mathcal{H}} \ \widehat{oldsymbol{\Sigma}}_3^{\mathcal{H}} \ \widehat{oldsymbol{\Sigma}}_1^{\mathcal{T}} \ \widehat{oldsymbol{\Sigma}}_2^{\mathcal{T}} \ \widehat{oldsymbol{\Sigma}}_2^{\mathcal{T}} \end{array}$	0.97	1.02	1.03	0.73	0.32	0.83	0.62	0.54	0.61	0.50	0.29	0.55	

Table 2: RME under equal correlation structure.

=

Table 3: RME under power decay structure.

Table 5: KME under power decay structure.													
$n = 50, \ p = 100$													
		Normal	l	t_3			Pareto			Log-normal			
	2	max	F	2	\max	F	2	max	F	2	max	F	
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{3}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{3}^{\mathcal{T}}$	0.98	0.95	0.98	0.58	0.30	0.71	0.48	0.29	0.57	0.69	0.39	0.79	
$\widehat{\mathbf{\Sigma}}_3^{\mathcal{H}}$	0.95	0.95	0.93	0.58	0.28	0.72	0.48	0.26	0.58	0.70	0.39	0.78	
$\widehat{\mathbf{\Sigma}}_1^\mathcal{T}$	0.97	0.98	0.96	0.59	0.30	0.71	0.49	0.26	0.57	0.72	0.39	0.77	
$\widehat{\mathbf{\Sigma}}_2^\mathcal{T}$	0.98	0.98	0.99	0.52	0.33	0.77	0.47	0.31	0.60	0.66	0.45	0.81	
n = 50, p = 200													
	Normal				t_3			Pareto			Log-normal		
	2	max	F	2	max	F	2	max	F	2	max	F	
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}}$	0.98	0.95	0.97	0.58	0.30	0.71	0.48	0.29	0.57	0.69	0.39	0.79	
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{3}^{\mathcal{H}}$	0.96	0.93	0.95	0.56	0.29	0.66	0.49	0.26	0.55	0.72	0.38	0.77	
$\hat{\mathbf{\Sigma}}_{1}^{\mathcal{T}} \ \hat{\mathbf{\Sigma}}_{2}^{\mathcal{T}}$	0.98	0.97	0.97	0.59	0.27	0.71	0.48	0.26	0.58	0.70	0.36	0.80	
$\widehat{\mathbf{\Sigma}}_2^\mathcal{T}$	0.98	0.98	1.01	0.54	0.24	0.76	0.41	0.31	0.60	0.68	0.42	0.82	
					n = 1	100, p	= 200						
Normal					t_3			Pareto			Log-normal		
	2	max	F	2	max	F	2	max	F	2	max	F	
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}}$	0.99	0.98	1.00	0.45	0.25	0.66	0.42	0.31	0.54	0.48	0.35	0.62	
$\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{3}^{\mathcal{H}} \ \widehat{\mathbf{\Sigma}}_{1}^{\mathcal{H}}$	0.98	0.98	0.99	0.47	0.26	0.68	0.41	0.30	0.53	0.47	0.34	0.61	
$\widehat{\mathbf{\Sigma}}_1^{\mathcal{T}}$	1.00	0.99	1.00	0.50	0.30	0.68	0.41	0.34	0.56	0.49	0.38	0.64	
$\widehat{\mathbf{\Sigma}}_2^{\mathcal{T}}$	0.99	1.04	1.01	0.41	0.31	0.70	0.40	0.39	0.59	0.43	0.43	0.69	

spectrum-wise truncation techniques to robustify the sample covariance matrix. The robustness, referred to as the *tail robustness*, is demonstrated by finite-sample deviation analysis in the presence of heavy-tailed data: the proposed estimators achieve exponential-type deviation bounds under mild moment conditions. We emphasize that the tail robustness is different from the classical notion of robustness that is often characterized by the breakdown point (Hampel, 1971). Nevertheless, it does not provide any information on the convergence properties of an estimator, such as consistency and efficiency. Tail robustness is a concept that combines robustness, consistency, and finite-sample error bounds.

We discussed three types of procedures in Section 3: truncation-based methods, their *M*-estimation counterparts and the median-of-means method. Truncated estimators have closed-form expressions and therefore are easy to implement in practice. The corresponding *M*-estimators achieve comparable sub-Gaussian-type error bounds, which are of the order $\sqrt{\log(d/\delta)/n}$ under the max norm and of order $\sqrt{r(\Sigma) \log(d/\delta)/n}$ under the spectral norm, but with sharper moment-dependent constants. Computationally, *M*-estimators can be efficiently evaluated via gradient descent method or iteratively reweighted least squares algorithm. Both truncated and M-estimators involve robustification parameters that need to be calibrated to fit the noise level of the problem. Adaptation and tuning of these parameters are discussed in Section 4. The MOM estimator proposed in Section 3.4 is tuning-free because the number of blocks depends neither on noise level nor on confidence level. Following the terminology proposed by Devroye et al. (2016), truncation-based estimators are δ -dependent estimators as they depend on the confidence level $1 - \delta$ at which one aims to control, while the MOM estimator achieves sub-Gaussian error bounds simultaneously at all confidence levels in a certain range but requires slightly stronger assumptions, namely, the existence of sixth moments instead of fourth.

Three examples discussed in Section 5 illustrate that both element-wise and spectrum-wise truncated covariance estimators can serve as building blocks for a variety of estimation problems in high dimensions. A natural question is whether one can construct a single robust estimator that achieves exponentially fast concentration both element-wise and spectrum-wise, that is, satisfies the results in Theorems 3.1 and 3.2 simultaneously. Here we discuss a theoretical solution to this question. In fact, one can arbitrarily pick one element, denoted as $\hat{\Sigma}^{\mathcal{T}}$, from the collection of matrices

$$\mathcal{H} = \left\{ \mathbf{S} \in \mathbb{R}^{d \times d} : \ \mathbf{S} = \mathbf{S}^{\mathsf{T}}, \ \|\widehat{\mathbf{\Sigma}}_{2}^{\mathcal{T}} - \mathbf{S}\|_{2} \le 2v\sqrt{\frac{\log(2d) + \log\delta^{-1}}{m}} \right.$$

and $\|\widehat{\mathbf{\Sigma}}_{1}^{\mathcal{T}} - \mathbf{S}\|_{\max} \le 2\|\mathbf{V}\|_{\max}\sqrt{\frac{2\log d + \log\delta^{-1}}{m}} \right\}.$

Due to Theorems 3.1 and 3.2, with probability at least $1-3\delta$, the set \mathcal{H} is non-empty since it contains the true covariance matrix Σ . Therefore, it follows from the the

triangle inequality that the inequalities

$$\|\widehat{\boldsymbol{\Sigma}}^{\mathcal{T}} - \boldsymbol{\Sigma}\|_{2} \leq 4v \sqrt{\frac{\log(2d) + \log \delta^{-1}}{m}},$$

and $\|\widehat{\boldsymbol{\Sigma}}^{\mathcal{T}} - \boldsymbol{\Sigma}\|_{\max} \leq 4\|\mathbf{V}\|_{\max} \sqrt{\frac{2\log d + \log \delta^{-1}}{m}}.$

hold simultaneously with probability at least $1 - 3\delta$.

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