### M-estimators of scatter with eigenvalue shrinkage

### Esa Ollila

Department of Signal Processing and Acoustics Aalto University, Finland

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### Joint work with



Daniel P. Palomar



Frédéric Pascal

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### 1 Introduction

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## **Covariance estimation problem**

- **x** : *p*-variate (centered) random vector.
- $\mathbf{x}_1, \ldots, \mathbf{x}_n$  i.i.d. realizations of  $\mathbf{x}$  and assume n > p.
- The unknown covariance matrix  $\mathbb{E}[\mathbf{x}\mathbf{x}^{\top}] \in \mathbb{S}_{++}^{p \times p}$  is commonly esimated using the sample covariance matrix (SCM)

$$\mathbf{S} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^\top.$$

- When p = O(n), then S is very inaccurate estimator.
- Regularization: regularized (shrinkage) SCM (RSCM)

$$\mathbf{S}_{\beta} = \beta \mathbf{S} + (1 - \beta) \frac{\operatorname{tr}(\mathbf{S})}{p} \mathbf{I}, \quad \beta \in (0, 1]$$

shrinks the eigenvalues towards the grand mean of the eigenvalues.

### Non-gaussian data and outliers

- (R)SCM is sensitive to outliers and non-Gaussianity of the data.
- M-estimators of scatter [Mar76] provides a robust alternative:

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{n} \sum_{i=1}^{n} u(\mathbf{x}_{i}^{\top} \hat{\boldsymbol{\Sigma}}^{-1} \mathbf{x}_{i}) \mathbf{x}_{i} \mathbf{x}_{i}^{\top},$$

where  $u:[0,\infty)\to [0,\infty)$  is a non-increasing weight function.

We study the natural alternative to the RSCM

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⇒ we propose simple and data-adaptive computation of the optimal MMSE parameter  $\beta$  for  $\hat{\Sigma}_{\beta}$  for any weight function u.

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### Shrinkage M-estimators of scatter

$$\hat{\boldsymbol{\Sigma}}_{\beta} = \beta \hat{\boldsymbol{\Sigma}} + (1 - \beta) \frac{\operatorname{tr}(\hat{\boldsymbol{\Sigma}})}{p} \mathbf{I}, \quad \beta \in (0, 1].$$

 $\bullet$  An M-estimator  $\hat{\Sigma}$  is consistent to underlying population parameter, defined as a solution to

$$\boldsymbol{\Sigma}_0 = \mathbb{E} \big[ u(\mathbf{x}^\top \boldsymbol{\Sigma}_0^{-1} \mathbf{x}) \mathbf{x} \mathbf{x}^\top \big].$$

Ideally, we would like to find

$$\beta_o = \arg\min_{\beta} \left\{ \text{MSE}(\hat{\boldsymbol{\Sigma}}_{\beta}) = \mathbb{E} \left[ \| \hat{\boldsymbol{\Sigma}}_{\beta} - \boldsymbol{\Sigma}_0 \|_{\text{F}}^2 \right] \right\},\$$

but the problem is not tractable due to implicit form of M-estimators.

### Surrogate for the M-estimator

 $\bullet$  An M-estimator  $\hat{\Sigma}$  can be computed by iterating

$$\hat{\boldsymbol{\Sigma}}_{k+1} = \frac{1}{n} \sum_{i=1}^{n} u(\mathbf{x}_i^{\top} \hat{\boldsymbol{\Sigma}}_k^{-1} \mathbf{x}_i) \mathbf{x}_i \mathbf{x}_i^{\top}, \quad k = 0, 1, \dots$$

• Consider a 1-step M-estimator that starts from true parameter  $\Sigma_0$ :

$$\mathbf{C} = \frac{1}{n} \sum_{i=1}^{n} u(\mathbf{x}_{i}^{\top} \boldsymbol{\Sigma}_{0}^{-1} \mathbf{x}_{i}) \mathbf{x}_{i} \mathbf{x}_{i}^{\top}.$$

Then use a 1-step M-estimator

$$\mathbf{C}_{\beta} = \beta \mathbf{C} + (1 - \beta) [\operatorname{tr}(\mathbf{C})/p] \mathbf{I}$$

as a proxy for  $\hat{\Sigma}_{\beta}$ .

• Naturally,  $\mathbf{C}_{eta}$  is fictional, as the initial value  $\mathbf{\Sigma}_0$  is unknown.

# Approximation of the optimum shrinkage

• We use

$$\beta_o^{\mathrm{app}} = \operatorname*{arg\,min}_{\beta} \, \Big\{ \mathrm{MSE}(\mathbf{C}_{\beta}) = \mathbb{E} \Big[ \big\| \mathbf{C}_{\beta} - \boldsymbol{\Sigma}_0 \big\|_{\mathrm{F}}^2 \Big] \Big\}.$$

as approximation for  $\beta_o$ . Similar approach was used in [CWH11]. Theorem 1. Given  $\mathbb{P}[\mu(C)]$  is so one has that

$$\beta_o^{\text{app}} = \frac{p(\gamma - 1)\eta_o^2}{\mathbb{E}[\text{tr}(\mathbf{C}^2)] - p^{-1}\mathbb{E}[\text{tr}(\mathbf{C})^2]}$$

where  $\eta_o=rac{ ext{tr}(\Sigma_0)}{v}$  is a scale and  $\gamma$  is a **sphericity measure**,

$$\gamma = rac{p \operatorname{tr}(\boldsymbol{\Sigma}_0^2)}{\operatorname{tr}(\boldsymbol{\Sigma}_0)^2}.$$

 The expression for β<sub>o</sub><sup>app</sup> can be simplified assuming that samples are from elliptically symmetric distribution.

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# Elliptically symmetric (ES) distributions

 $\mathbf{x} \sim \mathcal{E}_p(\mathbf{0}, \mathbf{\Sigma}, g)$  when its pdf is [FKN90, OTKP12]

$$f(\mathbf{x}) \propto |\mathbf{\Sigma}|^{-1/2} g(\mathbf{x}^{\top} \mathbf{\Sigma}^{-1} \mathbf{x}),$$

where

- $\Sigma \in \mathbb{S}_{++}^{p imes p}$  is the unknown scatter matrix parameter
- $g:[0,\infty) \to [0,\infty)$  is density generator
- Multivariate normal (MVN) :  $g(t) = \exp(-t/2)$
- Multivariate t (MVT) with  $\nu$  d.o.f :  $g(t) = (1 + t/\nu)^{-\frac{p+\nu}{2}}$ .
- $\mathbb{E}[\mathbf{x}\mathbf{x}^{\top}] \propto \mathbf{\Sigma}$

## Shrinkage parameter

• The relationship between  $\Sigma$  and the population M-estimator  $\Sigma_0$ :

$$\Sigma_0 = \sigma \Sigma,$$

where  $\sigma > 0$  is a solution to an equation

$$\mathbb{E}\left[\psi\left(\frac{\mathbf{x}^{\top}\boldsymbol{\Sigma}^{-1}\mathbf{x}}{\sigma}\right)\right] = p,$$

where  $\psi(t) = u(t)t$  and u(t) is the weight fnc of the M-estimator. • Define a constant

$$\psi_1 = \frac{1}{p(p+2)} \mathbb{E} \left[ \psi \left( \frac{\mathbf{x}^\top \boldsymbol{\Sigma}^{-1} \mathbf{x}}{\sigma} \right)^2 \right]$$

• Theorem 2. For  $\{\mathbf{x}_i\} \stackrel{iid}{\sim} \mathcal{E}_p(\mathbf{0}, \mathbf{\Sigma}, g)$ 

$$\beta_o^{\text{app}} = \frac{\gamma - 1}{(\gamma - 1)(1 - 1/n) + \psi_1(1 - 1/p)(2\gamma + p)/n}$$

where  $\gamma$  is the sphericity measure.

## Shrinkage parameter estimation

- $\beta_o^{\mathrm{app}}$  depends on
  - sphericity measure  $\gamma = \frac{p \operatorname{tr}(\boldsymbol{\Sigma}_0^2)}{\operatorname{tr}(\boldsymbol{\Sigma}_0)^2}$
  - $\Rightarrow$  we use the same estimator as in [ZW16, OR19]:

$$\hat{\gamma}^{\mathsf{EII1}} = \frac{n}{n-1} \left( \frac{p}{n} \sum_{i=1}^{n} \frac{\mathbf{x}_i \mathbf{x}_i^{\top}}{\|\mathbf{x}_i\|^2} - \frac{p}{n} \right)$$

• Constant depending on the weight function *u*:

$$\psi_1 = \frac{1}{p(p+2)} \mathbb{E} \left[ \psi \left( \frac{\mathbf{x}^\top \boldsymbol{\Sigma}^{-1} \mathbf{x}}{\sigma} \right)^2 \right]$$

 $\begin{array}{l} \text{where } \psi(t) = u(t)t. \\ \Rightarrow \ \hat{\psi}_1 \text{ is discussed next for different M-estimators.} \\ \bullet \ \text{Compute } \hat{\Sigma}_{\beta} \text{, where } \beta = \beta_o^{\mathrm{app}}(\hat{\gamma}^{\mathsf{EII1}}, \hat{\psi}_1). \end{array} \end{array}$ 

# Regularized SCM (RSCM) M-estimator

• Choose  $u(t) \equiv 1$  for all t

 $\Rightarrow \hat{\Sigma} = \mathbf{S}$  and  $\mathbf{C}_{\beta} = \mathbf{S}_{\beta}$  and hence  $\beta_o = \beta_o^{\mathrm{app}}$  (approximation is exact)

• The constant  $\psi_1$  is

$$\psi_1 = \frac{\mathbb{E}[(\mathbf{x}^\top \boldsymbol{\Sigma}^{-1} \mathbf{x})^2]}{p(p+2)} = 1 + \kappa$$

where 
$$\kappa = \frac{1}{3} \operatorname{kurt}(x_i)$$
  
 $\Rightarrow \hat{\psi}_1 = 1 + \hat{\kappa}.$   
•  $\mathbf{S}_{\beta} = \beta \mathbf{S} + (1 - \beta) \frac{\operatorname{tr}(\mathbf{S})}{p} \mathbf{I}$ , where  $\beta = \beta_o^{\operatorname{app}}(\hat{\gamma}^{\mathsf{EII}}, \hat{\psi}_1)$ 

# Regularized Huber's (RHub) M-estimator

Huber's weight function

$$u_{\rm H}(t;c) = \begin{cases} 1/b, & \text{ for } t \leqslant c^2 \\ c^2/(tb), & \text{ for } t > c^2 \end{cases}$$

where c > 0 is a user defined *tuning constant* and b is a scaling factor. • Define a winsorized observation w:

$$\mathbf{w} = \mathsf{wins}(\mathbf{x}) = \frac{1}{\sqrt{b}} \times \begin{cases} \mathbf{x}, & \|\mathbf{\Sigma}^{-1/2}\mathbf{x}\|^2 \leqslant c^2\\ c\frac{\mathbf{x}}{\|\mathbf{\Sigma}^{-1/2}\mathbf{x}\|}, & \|\mathbf{\Sigma}^{-1/2}\mathbf{x}\|^2 > c^2 \end{cases}$$

• Constant  $\psi_1$  is then

$$\psi_1 = 1 + \kappa_{\mathbf{w}}$$

where  $\kappa_{\mathbf{w}} = (1/3) \operatorname{kurt}(w_i) \Rightarrow \hat{\psi}_1 = 1 + \hat{\kappa}_{\mathbf{w}}.$ 

# Regularized MVT (RMVT) estimator

- Suppose the data follows MVT distribution with  $\nu$  d.o.f..
- The ML-weight function is

$$u_{\mathsf{T}}(t;\nu) = \frac{p+\nu}{\nu+t}$$

• The constant  $\psi_1$  is then

$$\psi_1 = \frac{p+\nu}{2+p+\nu}$$

RMVT estimator:

- Compute estimate  $\hat{\nu}$  of  $\nu$  based on the data.
- Compute the M-estimator  $\hat{\Sigma}$  using  $u_{\mathrm{T}}(t;\hat{\nu})$ .
- Compute  $\hat{\psi}_1$  using  $\hat{\nu}$ .
- Compute  $\hat{\Sigma}_{\beta}$ , where  $\beta = \beta_o^{\text{app}}(\hat{\gamma}^{\text{EII}}, \hat{\psi}_1)$ .

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### Simulation studies

Set-up:

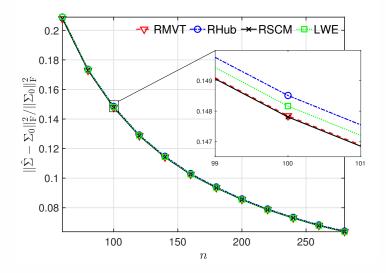
- i.i.d. data from  $\mathcal{E}_p(\mathbf{0}, \mathbf{\Sigma}, g)$
- $\Sigma$  has an AR(1) structure,  $(\Sigma)_{ij} = 10 \varrho^{|i-j|}$ , where  $\varrho = 0.6$ .
- p = 40 and n varies from 60 to 280.
- We compute the normalized MSE (NMSE)

$$\|\hat{\mathbf{\Sigma}}_eta - \mathbf{\Sigma}_0\|_{ ext{F}}^2 / \|\mathbf{\Sigma}_0\|_{ ext{F}}^2$$

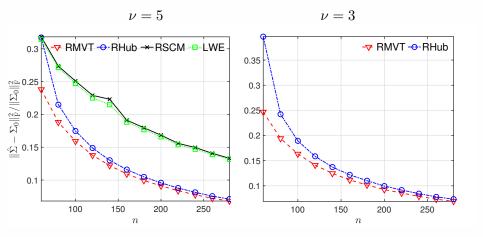
averaged over 2000 MC trials.

• We compare with the Ledoit-Wolf estimator [LW04].

# MVN (Gaussian) data

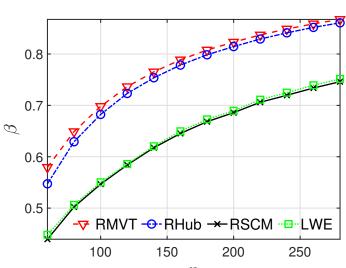


## MVT (*t*-distributed) data



### Estimate of shrinkage parameter

MVT data with  $\nu = 5$  d.o.f.



# What's cooking

A journal extension is currently being finalized ... It includes

- Extension to complex-valued data
- Principled approaches for estimating parameter  $\nu$  of the MVT distribution.
- Tyler's M-estimator is also considered.
- Advanced approaches for estimating the shrinkage parameter for each specific M-estimator (Huber, Gaussian, Tyler, MVT).
- Application to portfolio optimization: investigation using both synthetic and real stock returns data.
- Journal extension will be sent to ArXiv with Matlab and R codes made publicly available.

## References

- Yilun Chen, Ami Wiesel, and Alfred O. Hero, *Robust shrinkage estimation of high-dimensional covariance matrices*, IEEE Trans. Signal Process. **59** (2011), no. 9, 4097 4107.
- Kai-Tai Fang, Samuel Kotz, and Kai-Wang Ng, *Symmetric multivariate and related distributions*, Chapman and hall, London, 1990.
- Olivier Ledoit and Michael Wolf, *A well-conditioned estimator for large-dimensional covariance matrices*, Journal of multivariate analysis **88** (2004), no. 2, 365–411.
- Ricardo A. Maronna, Robust M-estimators of multivariate location and scatter, Ann. Stat. 5 (1976), no. 1, 51–67.
- Esa Ollila and Elias Raninen, Optimal shrinkage covariance matrix estimation under random sampling from elliptical distributions, IEEE Transactions on Signal Processing 67 (2019), no. 10, 2707–2719.
- Esa Ollila, David E. Tyler, Visa Koivunen, and H. Vincent Poor, Complex elliptically symmetric distributions: survey, new results and applications, IEEE Trans. Signal Process. 60 (2012), no. 11, 5597–5625.

