

Adaptive shrinkage of singular values of a low-rank mean matrix when a covariance matrix is unknown

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- 1 The reconstruction of a low-rank matrix from its noisy observation is useful in many applications. This problem is reformulated into a constrained nuclear norm minimization problem (regularized problem).
- 2 An important ingredient of this problem is how to choose a regularization parameter based on data. Usually the data is independently and identically distributed with unknown variance.
- 3 (1) The discrepancy principle approach, (2) Stein's Unbiased risk estimator(SURE) approach.
- 4 Inspired by approach(2) we consider the problem of estimating a low-rank matrix mean in MANOVA(Multivariate Analysis of Variance) setting ¹when a positive-definite covariance matrix of error is unknown.

¹We have data for unknown covariance matrix. The distribution of this data is mean-zero.

MANOVA model and its canonical model

Let $m, n, p \in \mathbb{N}$ such that $\min(m, p) \geq p$. Consider a multivariate regression model

$$\underbrace{\mathbf{W}}_{(m+n) \times p} = \underbrace{\mathbf{A}}_{(m+n) \times m} \underbrace{\mathbf{B}}_{m \times p} + \underbrace{\mathbf{Err}}_{(m+n) \times p},$$

where \mathbf{A} is a **known** design matrix of full rank, \mathbf{B} is an **unknown** regression matrix of rank $r (< \min(m, p)$ and r is **unknown**), and \mathbf{Err} is an unobservable error matrix. Here rows of \mathbf{Err} are independently and identically distributed as $\mathbf{N}_p(\mathbf{0}_p, \Sigma)$ where Σ is a $p \times p$ positive-definite **unknown** matrix.

Notation

1

$$\mathbf{Err} = \begin{bmatrix} \mathbf{e}_1^\top \\ \mathbf{e}_2^\top \\ \vdots \\ \mathbf{e}_{m+n}^\top \end{bmatrix} : (m+n) \times p, \quad \text{vec}(\mathbf{Err}) := \begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \vdots \\ \mathbf{e}_{m+n} \end{bmatrix}$$

where \mathbf{e}_j 's are independently and identically distributed as $\mathbf{N}_p(\mathbf{0}_p, \Sigma)$ ($j = 1, 2, \dots, (m+n)$).

2 Write

$$\begin{aligned} \text{COV}(\mathbf{Err}) &= \mathbb{E} \left[\left\{ \text{vec}(\mathbf{Err} - \mathbb{E}[\mathbf{Err}]) \right\} \left\{ \text{vec}(\mathbf{Err} - \mathbb{E}[\mathbf{Err}]) \right\}^\top \right] \\ &= \mathbf{I}_{m+n} \otimes \Sigma, \\ \mathbf{Err} &\sim \mathbf{N}_{(m+n) \times p}(\mathbf{0}_{(m+n) \times p}, \mathbf{I}_{m+n} \otimes \Sigma). \end{aligned}$$

1 Let

$$P = (A^T A)^{-1/2} A^T : m \times (m + n)$$

and take $P^\perp : n \times (m + n)$ s.t.

$$P(P^\perp)^T = \mathbf{0}_{m \times n} \quad \text{and} \quad P^\perp(P^\perp)^T = I_n,$$

Note that

$$\begin{bmatrix} P \\ P^\perp \end{bmatrix} [P^T, (P^\perp)^T] = I_{m+n}.$$

2 Put $\Xi := (A^T A)^{1/2} B$ and

$$\begin{bmatrix} X \\ Y \end{bmatrix} := \begin{bmatrix} P \\ P^\perp \end{bmatrix} W \sim N_{(m+n) \times p} \left(\begin{bmatrix} \Xi \\ \mathbf{0}_{n \times p} \end{bmatrix}, I_{m+n} \otimes \Sigma \right).$$

Problem set-up

Assume that $\min\{m, n\} \geq p$ and that

$$\begin{matrix} m \\ n \end{matrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \Xi \\ \mathbf{0} \end{pmatrix} + E; \quad E = \begin{pmatrix} \overset{p}{\longleftrightarrow} \\ \longleftrightarrow \\ \vdots \\ \longleftrightarrow \\ \longleftrightarrow \end{pmatrix}$$

where $\begin{bmatrix} X \\ Y \end{bmatrix}$ is observation and Ξ is an $m \times p$ non-random matrix (unknown) of rank $r < p$, E is an $(m+n) \times p$ error matrix (unobservable) whose rows are identically distributed as $N_p(\mathbf{0}, \Sigma)$. Here Σ is a $p \times p$ positive-definite and unknown matrix.

We consider the problem of estimating Ξ under a low-rank mean matrix condition, i.e.,

$$\text{rank } \Xi = r < p; \quad r \text{ is unknown}$$

under a loss function and its risk

$$L_{\Sigma}(\widehat{\Xi}, \Xi) = \text{tr} \{ (\widehat{\Xi} - \Xi) \Sigma^{-1} (\widehat{\Xi} - \Xi)^{\top} \} =: \|\widehat{\Xi} - \Xi\|_{F, \Sigma}^2$$

and

$$R_{\Sigma}(\widehat{\Xi}, \Xi) = \mathbb{E}[L_{\Sigma}(\widehat{\Xi}, \Xi)]$$

where $\widehat{\Xi}$ is an estimator based on (\mathbf{X}, \mathbf{S}) . Here $\mathbf{S} = \mathbf{Y}^{\top} \mathbf{Y} \sim W_p(\Sigma, \mathbf{n})$, which is the Wishart distribution with the degree of freedom \mathbf{n} and the scale matrix Σ .

Mean matrix estimation when a covariance is known

- Assume that m , p are positive integers s.t. $m \geq p$.
- Let

$$Z = \begin{pmatrix} \mathbf{z}_1^T \\ \mathbf{z}_2^T \\ \vdots \\ \mathbf{z}_m^T \end{pmatrix}$$

be an $m \times p$ data matrix whose row vectors are independently distributed as

$$\mathbf{z}_i : p \times 1 \sim N(\tilde{\xi}_i, \sigma^2 I_p), \quad (i = 1, 2, \dots, m)$$

Here $\tilde{\Xi}^T := (\tilde{\xi}_1, \dots, \tilde{\xi}_m)$ is unknown but $\sigma > 0$ are known.

- We assume that **low-rank mean matrix condition**, i.e.,

$$\text{rank}(\tilde{\Xi}) = r < p; \quad r \text{ is unknown.}$$

- Consider the problem of estimating $\tilde{\Xi}$ under a loss function and its risk

$$L_1(\hat{\Xi}, \tilde{\Xi}) = \text{tr} \{ (\hat{\Xi} - \tilde{\Xi})(\hat{\Xi} - \tilde{\Xi})^T \} =: \|\hat{\Xi} - \tilde{\Xi}\|_F^2$$

and

$$R_1(\hat{\Xi}, \tilde{\Xi}) = \mathbb{E}[L_1(\hat{\Xi}, \tilde{\Xi})].$$

- Here $\hat{\Xi}$ is an estimator based on \mathbf{Z} .
- $\text{tr} \mathbf{A}$ and \mathbf{A}^T stand for the trace and the transpose of a matrix \mathbf{A} , respectively.
- $\|\mathbf{A}\|_F := \sqrt{\text{tr}(\mathbf{A}^T \mathbf{A})}$, the Frobenius norm of a matrix \mathbf{A} .

Eckart-Young approximation theorem

- Singular Value Decomposition: We can assume that $m \geq p$ without loss of generality. Decompose \mathbf{Z} as

$$\mathbf{Z} = \mathbf{U}\mathbf{L}\mathbf{V}^T; \quad \mathbf{U} = (\mathbf{u}_1, \dots, \mathbf{u}_p), \quad \mathbf{V} = (\mathbf{v}_1, \dots, \mathbf{v}_p)$$

$$\mathbf{L} = \text{diag}(\ell_1, \ell_2, \dots, \ell_p) \quad \text{with } \ell_1 \geq \ell_2 \geq \dots \geq \ell_p \geq 0$$

where $\mathbf{u}_i \in \mathbb{R}^m$, $\mathbf{v}_i \in \mathbb{R}^p$ ($i = 1, \dots, p$) s.t.

$$\mathbf{U}^T \underbrace{\mathbf{U}}_{m \times p} = \mathbf{V}^T \mathbf{V} = \mathbf{I}_p.$$

- The total least squares (TLS) pseudo estimator is given by

$$\hat{\Xi}_{TLS} = \sum_{i=1}^r \ell_i \mathbf{u}_i \mathbf{v}_i^T. \quad \Leftrightarrow \quad \hat{\Xi}_{TLS} \in \underset{\Xi: \text{rank}(\Xi) \leq r}{\text{argmin}} \|\Xi - \mathbf{Z}\|_F^2.$$

Notation $\sigma_j(\mathbf{A}) > 0$ ($j = 1, 2, \dots, r$) are non-zero singular values of a matrix \mathbf{A} with $r = \text{rank}(\mathbf{A})$.

Regularization approach

- We consider an estimator which minimizes the penalized least squares criterion

$$\text{Mat}(\mathbf{m}, \mathbf{p}; \mathbb{R}) \ni \Xi \mapsto \frac{1}{2} \|\mathbf{Z} - \Xi\|_F^2 + \text{pen}_\lambda(\Xi) \in [0, \infty)$$

where $\text{pen}_\lambda(\cdot) (\geq 0)$ is a penalty function of Ξ and $\lambda (\geq 0)$ is a tuning parameter.

- Examples of penalties: For a positive $\lambda > 0$,

- ★ $\text{pen}_\lambda(\Xi) = \lambda \text{rank}(\Xi)$

\Rightarrow a hard-thresholding rule, i.e., $\text{SVHT}_\lambda(\mathbf{Z}) = \sum_{j=1}^p \ell_j \mathbb{1}\{\ell_j \geq \lambda\} \mathbf{u}_j \mathbf{v}_j^\top$,

where $\mathbb{1}\{\text{event}\} = \begin{cases} 1 & \text{if event is true,} \\ 0 & \text{otherwise} \end{cases}$.

- ★ $\text{pen}_\lambda(\Xi) = \lambda \|\Xi\|_1 := \lambda \sum_{j=1}^p |\sigma(\Xi)_j|$ ($\sigma(\Xi)_j$: SV's of Ξ)

where $\{(\sigma(\Xi)_j, \mathbf{u}_j, \mathbf{v}_j)\}_{j=1}^{\min(m,p)}$ is a system of singular values of Ξ

\Rightarrow a soft-thresholding rule, i.e.,

$$\text{SVST}_\lambda(\mathbf{Z}) = \sum_{i=1}^p (\ell_i - \lambda) \mathbb{1}\{\ell_i \geq \lambda\} \mathbf{u}_i \mathbf{v}_i^\top.$$

A hard-shreshholding rule

- Assume that σ^2 is **known**.
- Solve

$$\mathbf{SVHT}_\lambda(\mathbf{Z}) = \underset{\Xi}{\operatorname{argmin}} \left[\frac{1}{2} \|\Xi - \mathbf{Z}\|_F^2 + \lambda \operatorname{rank}(\Xi) \right]$$

where $\lambda > \mathbf{0}$ is a tuning scalar parameter.

- Then the solution is given by

$$\mathbf{SVHT}_\lambda(\mathbf{Z}) = \sum_{j=1}^p \ell_j \mathbb{1}\{\ell_j \geq \lambda\} \mathbf{u}_j \mathbf{v}_j^T; \quad \mathbb{1}\{\ell_j \geq \lambda\} = \begin{cases} 1 & \ell_j \geq \lambda \\ 0 & \text{otherwise} \end{cases}$$

- The optimal shreshholding is $\frac{4}{\sqrt{3}} \sqrt{p} \sigma$ when $p = m$.

(See Donoho and Garvish (2017, IEEE, Trans. Inform Theory).

Steps to obtain an adaptive thresholding estimator

- 1 Solve regularized minimization problem

$$\hat{\Xi}_\lambda \in \arg \min_{\Xi \in \text{Mat}(m, p; \mathbb{R})} \left\{ \|Z - \Xi\|_F^2 + \text{pen}_\lambda(\Xi) \right\}.$$

- 2 Calculate SURE if possible (a closed form of $\hat{\Xi}_\lambda$):

$$R_1(\hat{\Xi}_\lambda, \Xi) = \mathbb{E} \left[\text{SURE}(\hat{\Xi}_\lambda) \right]$$

Note that $\text{SURE}(\hat{\Xi}_\lambda)$ is a function of λ and observable data.

- 3 Solve minimization problem

$$\hat{\lambda} \in \text{SURE}(\hat{\Xi}_\lambda) \implies \hat{\Xi}_{\hat{\lambda}}.$$

Remarks

- 1 This method works for the soft-thresholding rule. See Cándes *et al.* (2013).
- 2 **SURE** does not work for the hard-thresholding rule since Stein's identity, integration-by-parts formula with respect to multivariate normal distribution, fails for the hard-thresholding rule because of discontinuity of estimator.

A soft-thresholding rule

- Cèdes et al. define an adaptive soft-thresholding rule based on SURE:

$$\mathbf{SVST}_\lambda(\mathbf{Z}) = \sum_{j=1}^p (\ell_j - \lambda) \mathbb{1}\{\ell_j \geq \lambda\} \mathbf{u}_j \mathbf{v}_j^\top =: \sum_{j=1}^p (\ell_j - \lambda)_+ \mathbf{u}_j \mathbf{v}_j^\top \quad (1)$$

which is obtained from

$$\min_{\mathbf{Y}} \left\{ \frac{1}{2} \|\mathbf{Z} - \mathbf{Y}\|_F^2 + \lambda \sum_{j=1}^p \lambda_j \right\} \quad \mathbf{Y} = \mathbf{SVST}_\lambda(\mathbf{Z}).$$

- The parameter λ in (1) is selected by minimizing SURE, Stein's unbiased risk estimate for (1).

- Gaussian integration-by-parts (=Stein's identity) and a bit of algebraic calculation lead to

$$R_1(\mathbf{SVST}_\lambda, \Xi) = \mathbb{E}[\mathbf{SURE}(\mathbf{SVST}_\lambda)(\mathbf{Z})],$$

$$\begin{aligned} \mathbf{SURE}(\mathbf{SVST}_\lambda)(\mathbf{Z}) &= -mp\sigma^2 + \sum_{j=1}^p \min\{\ell_j^2, \lambda^2\} \\ &\quad + 2\sigma^2 \operatorname{div}(\mathbf{SVST}_\lambda(\mathbf{X})), \end{aligned}$$

$$\begin{aligned} \operatorname{div}(\mathbf{SVST}_\lambda(\mathbf{Z})) &= (m-p) \sum_{j=1}^p \left(1 - \frac{\lambda}{\ell_j}\right)_+ + \sum_{j=1}^p \mathbb{1}\{\ell_j > \lambda\} \\ &\quad + 2 \sum_{j=1}^p \sum_{k \neq j}^p \frac{\ell_j(\ell_j - \lambda)_+}{\ell_j^2 - \ell_k^2} \end{aligned}$$

whenever $\ell_1 > \ell_2 > \dots > \ell_p \geq 0$.

- An adaptive estimator is given by

$$\mathbf{SVST}_{\hat{\lambda}}(\mathbf{Z}) = \sum_{j=1}^p (\ell_j - \hat{\lambda})_+ \mathbf{u}_j \mathbf{v}_j^T, \quad (2)$$

$$\hat{\lambda} \in \arg \min_{\lambda \geq 0} \left[\sum_{i=1}^p \min\{\ell_i^2, \lambda^2\} + 2\sigma^2 \text{div}(\mathbf{SVST}_{\lambda}(\mathbf{Z})) \right].$$

- Numerical evaluation of the risk of (2) was carried out by Candés et. al.
- But it is not clear if $\mathbf{R}_1(\mathbf{SVST}_{\hat{\lambda}}(\mathbf{Z}), \tilde{\Xi})$ is close to $\mathbf{R}_1(\tilde{\Xi}_{\text{TLS}}(\mathbf{Z}), \tilde{\Xi})$ for $\forall \tilde{\Xi}$ s.t. $\text{rank}(\tilde{\Xi}) \leq r < \min(m, p)$.

Mean matrix estimation when a covariance matrix is unknown

- Assume that $\min\{m, n\} \geq p$ and that

$$\begin{matrix} m \\ n \end{matrix} \begin{matrix} p \\ \\ \end{matrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \Xi \\ \mathbf{0} \end{pmatrix} + E; \quad E = \begin{pmatrix} \overleftrightarrow{} \\ \overleftrightarrow{} \\ \vdots \\ \overleftrightarrow{} \\ \overleftrightarrow{} \end{pmatrix}$$

- The $m \times p$ mean matrix Ξ is of rank $r < p$
- The error E is an $(m + n) \times p$ error matrix (unobservable) whose rows are identically distributed as $N_p(\mathbf{0}, \Sigma)$.
- The covariance matrix Σ is a $p \times p$ positive-definite and **unknown**.

- We consider the problem of estimating Ξ under low-rank mean matrix condition, i.e.,

$$\text{rank } \Xi = r < \min(m, p); \quad r \text{ is unknown.}$$

- A loss function and its risk are given by

$$L_{\Sigma}(\widehat{\Xi}, \Xi) = \text{tr} \{ (\widehat{\Xi} - \Xi) \Sigma^{-1} (\widehat{\Xi} - \Xi)^{\top} \} =: \|\widehat{\Xi} - \Xi\|_{F, \Sigma}^2$$

and

$$R_{\Sigma}(\widehat{\Xi}, \Xi) = \mathbb{E}[L_{\Sigma}(\widehat{\Xi}, \Xi)]$$

where $\widehat{\Xi}$ is an estimator based on (\mathbf{X}, \mathbf{S}) .

- $\mathbf{S} = \mathbf{Y}^{\top} \mathbf{Y} \sim W_p(\Sigma, n)$, which is the Wishart distribution with the degree of freedom n and the scale matrix Σ .

- To derive a class of estimators, first assume that Σ is known.
- Then we have

$$X\Sigma^{-1/2} \sim N_{m \times p}(\tilde{\Xi}, I_m \otimes I_p), \quad \tilde{\Xi} = \Xi\Sigma^{-1/2}$$

which leads to an estimator of $\tilde{\Xi}$ given by

$$\hat{\tilde{\Xi}}_{TLS} \in \arg \min_{\text{rank } \Xi \leq r} \|X\Sigma^{-1/2} - \Xi\|_F^2 \implies \hat{\Xi} = \hat{\tilde{\Xi}}_{TLS}\Sigma^{1/2}.$$

- Hence we consider a class of estimators of the form

$$\hat{\Xi}_H = \left(\sum_{i=1}^p h_i(\ell_i) u_i v_i^T \right) S^{1/2}; \quad XS^{-1/2} = ULV^T$$

where $L = \text{diag}(\ell_1, \dots, \ell_p)$, $H = \text{diag}(h_1, \dots, h_p)$,

$U = (u_1, \dots, u_p)$ and $V = (v_1, \dots, v_p)$ s.t.

$$U^T U = V^T V = I_p.$$

Regularized minimization problem

- Known Σ case: For $\lambda \geq 0$,

$$\text{Mat}(m, p; \mathbb{R}) \ni \Xi \Sigma^{-1/2}$$

$$\mapsto \|X \Sigma^{-1/2} - \Xi \Sigma^{-1/2}\|_F^2 + 2\lambda \|\Xi \Sigma^{-1/2}\|_1$$

- Unknown Σ case: For $\lambda \geq 0$, find a minimizer $\hat{\Xi}$ of a regularized minimization problem

$$\text{Mat}(m, p; \mathbb{R}) \ni \Xi$$

$$\mapsto \|X S^{-1/2} - \Xi\|_F^2 + 2\lambda \|\Xi\|_1$$

and

$$\hat{\Xi} = \hat{\Xi} S^{1/2} = \left(\sum_{j=1} \ell_j (\ell_j - \lambda)_+ u_j v_j^T \right) S^{1/2}$$

where $\{(\ell_j, u_j, v_j)\}$ is a system of singular values of $X S^{-1/2}$

- If

$$h_j(\ell_j) = \ell_j - \frac{c}{\ell_j} \quad (j = 1, 2, \dots, p);$$

c is a known positive constant,

then it results in the Efron-Morris estimator which is given by

$$\begin{aligned} \widehat{\Xi}_H &= \mathbf{X}\mathbf{S}^{-1/2} \left[\mathbf{I}_p - c \{ (\mathbf{X}\mathbf{S}^{-1/2})^\top (\mathbf{X}\mathbf{S}^{-1/2}) \}^{-1} \right] \mathbf{S}^{1/2} \\ &= \mathbf{X} - c \mathbf{X} \{ \mathbf{X}^\top \mathbf{X} \}^{-1} \mathbf{S}. \end{aligned}$$

- On the other hand, Tsukuma and Kubokawa (2015) considered estimators of the form

$$\widehat{\Xi}_T = \mathbf{X} - \mathbf{U}\mathbf{T}\mathbf{U}^\top \mathbf{X}$$

where $\mathbf{T} = \text{diag}(t_1(\ell_1^2), \dots, t_p(\ell_p^2))$ and $\mathbf{X}\mathbf{S}^{-1/2} = \mathbf{U}\mathbf{L}\mathbf{V}^\top$ with $m \times \min(m, p)$ matrix \mathbf{U} s.t. $\mathbf{U}^\top \mathbf{U} = \mathbf{I}_{\min(m, p)}$.

- Recall that

$$XS^{-1/2} = ULV^T \iff L^{-1}U^T X = V^T S^{1/2}.$$

From a simple calculation we get

$$\widehat{\Xi}_H = UHV^T S^{1/2} = UHL^{-1}U^T X = UL^{-1}HX.$$

- If we set $I_p - T = L^{-1}H(t_j(x) = h_j(\sqrt{x}))$, then we have

$$\widehat{\Xi}_H = \widehat{\Xi}_T.$$

- From this we can see that

$$L_{\Sigma}(\widehat{\Xi}_H, \Xi) = L_{\Sigma}(\widehat{\Xi}_T, \Xi).$$

- Furthermore, using the result due to Tsukuma and Kubokawa (2015), we have

$$\mathbf{R}_{\Sigma}(\widehat{\Xi}_T, \Xi) = \mathbb{E}[\mathbf{SURE}(T)];$$

$$\mathbf{SURE}(T) = \sum_{j=1}^p \left[m + a\ell_j^2 t_j^2 - 2bt_j - 4\ell_j^2 t_j \tilde{t}_j - 4\ell_j^2 \tilde{t}_j \right. \\ \left. - 2 \sum_{k \neq j}^p \frac{\ell_j^4 t_j^2 - \ell_k^4 t_k^2}{\ell_j^2 - \ell_k^2} - 4 \sum_{k \neq j}^p \frac{\ell_j^2 t_j - \ell_k^2 t_k}{\ell_j^2 - \ell_k^2} \right];$$

$$t_j = 1 - \frac{h_j(\ell_j)}{\ell_j}; \quad t'_j = -\frac{1}{2\ell_j^2} \left(\tilde{h}'_j(\ell_j) + \frac{h(\ell_j)}{\ell_j} \right),$$

a, b : known positive constants.

- Then we have an adaptive soft-thresholding rule

$$\widehat{\Xi}_{\widehat{\lambda}} = \mathbf{S} \mathbf{V} \mathbf{S}^{\mathbf{T}} \widehat{\mathbf{T}}_{\widehat{\lambda}} (\mathbf{X} \mathbf{S}^{-1/2}) \mathbf{S}^{1/2} = \left(\sum_{j=1}^p (\ell_j - \widehat{\lambda})_+ \mathbf{u}_j \mathbf{v}_j^{\mathbf{T}} \right) \mathbf{S}^{1/2}$$

where $\widehat{\lambda} = \operatorname{argmin}_{\lambda \geq 0} \operatorname{SURE}(\mathbf{S} \mathbf{V} \mathbf{S}^{\mathbf{T}} \mathbf{T}_{\lambda}) (\mathbf{X} \mathbf{S}^{-1/2})$;

$$\operatorname{SURE}(\mathbf{S} \mathbf{V} \mathbf{S}^{\mathbf{T}} \mathbf{T}_{\lambda}) (\mathbf{X} \mathbf{S}^{-1/2}) = \sum_{j=1}^p \left[m + a \ell_j^2 t_j^2 - 2 b t_j - 4 \ell_j^2 t_j \widetilde{t}_j - 4 \ell_j^2 \widetilde{t}_j - 2 \sum_{k \neq j}^p \frac{\ell_j^4 t_j^2 - \ell_k^4 t_k^2}{\ell_j^2 - \ell_k^2} - 4 \sum_{j \neq i} \frac{\ell_i^2 t_i - \ell_j^2 t_j}{\ell_i^2 - \ell_j^2} \right];$$

$$t_j = 1 - \frac{(\ell_j - \lambda)_+}{\ell_j} \quad (j = 1, \dots, p);$$

$$\widetilde{t}_j = -(2\ell_j)^{-2} \left(\mathbb{1}\{\ell_j > \lambda\} + \frac{(\ell_j - \lambda)_+}{\ell_j} \right).$$

Special case

- $\Sigma = \sigma^2 I_p$ where σ is positive but unknown.
- Let $\mathbf{s}^2 = \text{tr}(\mathbf{Y}^\top \mathbf{Y})/p$.
- Then an adaptive soft-thresholding rule for this case is given by $\hat{\Xi}_{\hat{\lambda}} = \sum_{j=1}^p (\ell_j - \hat{\lambda} \mathbf{s}^2) \mathbf{u}_j \mathbf{v}_j^\top$; $\mathbf{X} = \mathbf{U} \mathbf{L} \mathbf{V}^\top$, with $\hat{\lambda} = \underset{\lambda \geq 0}{\text{argmin}} \text{SURE}(\mathbf{S} \mathbf{V} \mathbf{S}^\top T_\lambda)(\mathbf{X})$ and

$$\begin{aligned} \text{SURE}(\mathbf{S} \mathbf{V} \mathbf{S}^\top T_\lambda)(\mathbf{X}) &= \sum_{j=1}^p \left[m \mathbf{s}^2 + a \ell_j^2 t_j^2 - 4 \ell_j \tilde{t}_j - 2 \sum_{k \neq j}^p \frac{\ell_j^4 t_j^2 - \ell_k^4 t_k^2}{\ell_j^2 - \ell_k^2} \right. \\ &\quad \left. + \mathbf{s}^2 \left(a \ell_j^2 t_j^2 - 4 \ell_j^2 t_j \tilde{t}_j - 4 \sum_{k \neq j}^p \frac{\ell_j^2 t_j - \ell_k t_k}{\ell_j^2 - \ell_k^2} \right) \right] \end{aligned}$$

where

$$t_j = 1 - \frac{(\ell_j - \lambda s^2)_+}{\ell_j}; \quad \tilde{t}_j = -\frac{1}{\ell_j^2} \left(\mathbb{1}\{\ell_j > \lambda s^2\} + \frac{(\ell_j - \lambda s^2)_+}{\ell_j} \right).$$

Concluding remarks

1 Derivation of an adaptive thresholding rule:

- For $\lambda \geq 0$, solve a regularized minimization problem (random one)

$$\hat{\Xi} \in \arg \min_{\Xi \in \text{Mat}(m, p; \mathbb{R})} \left\{ \frac{1}{2} \|\mathbf{X}\mathbf{S}^{-1/2} - \Xi\|_F^2 + \lambda \|\Xi\|_1 \right\}.$$

- We have $\hat{\Xi}_\lambda = \hat{\Xi} \mathbf{S}^{1/2} = \left(\sum_{j=1}^m \ell_j (\ell_j - \lambda)_+ \mathbf{u}_j \mathbf{v}_j^\top \right) \mathbf{S}^{1/2}$.

where $\{(\ell_j, \mathbf{u}_j, \mathbf{v}_j)\}_{j=1,2,\dots,m}$ is a system of singular values of $\mathbf{X}\mathbf{S}^{-1/2}$.

- Obtain SURE $\mathbf{R}_\Sigma(\hat{\Xi}_\lambda, \Xi) = \mathbb{E}[\text{SURE}(\hat{\Xi}_\lambda)]$

- Solve the minimization problem

$$\hat{\lambda} \in \arg \min_{\lambda \geq 0} \text{SURE}(\hat{\Xi}_\lambda) \implies \hat{\Xi}_{\hat{\lambda}}.$$

- ### 2 It is routine to convert this result to case for complex normal distribution.

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