Some perspectives on separable covariance matrices

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ICS and Related Methods
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Separability

A random vector $\mathbf{x} \in \mathbb{R}^{p_1 p_2}$ is said to be covariance separable if $\mathbf{\Sigma} := \mathrm{Cov}(\mathbf{x})$ satisfies

$$\mathbf{\Sigma} = \mathbf{\Sigma}_2 \otimes \mathbf{\Sigma}_1,$$

for some positive definite $\mathbf{\Sigma}_1 \in \mathbb{R}^{p_1 \times p_1}$, $\mathbf{\Sigma}_2 \in \mathbb{R}^{p_2 \times p_2}$.

- $\otimes$ is the Kronecker product,

$$\mathbf{B} \otimes \mathbf{A} = \begin{pmatrix} b_{11}\mathbf{A} & \cdots & b_{1p_2}\mathbf{A} \\ \vdots & \ddots & \vdots \\ b_{p_2 1}\mathbf{A} & \cdots & b_{p_2 p_2}\mathbf{A} \end{pmatrix}$$

Matrix-valued data

- The vectorization of a matrix

$$\mathbf{X} = (\mathbf{x}_1 \mid \cdots \mid \mathbf{x}_{p_2}) \in \mathbb{R}^{p_1 \times p_2}$$

is the vector

$$\mathrm{vec}(\mathbf{X}) = \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_{p_2} \end{pmatrix} \in \mathbb{R}^{p_1 p_2}.$$

- Separability ensues naturally under vectorized matrix data.

Matrix normal

Matrix normal distribution

If the elements of $\mathbf{Z} \in \mathbb{R}^{p_1 \times p_2}$ are i.i.d. from $\mathcal{N}(0,1)$, then $\mathbf{X} = \boldsymbol{\Sigma}_1^{1/2} \mathbf{Z} \boldsymbol{\Sigma}_2^{1/2}$ is said to have the matrix normal distribution

$$\mathcal{N}_{p_1,p_2}(\mathbf{0}, \boldsymbol{\Sigma}_1, \boldsymbol{\Sigma}_2).$$

- For $\mathbf{X} \sim \mathcal{N}_{p_1,p_2}(\mathbf{0}, \boldsymbol{\Sigma}_1, \boldsymbol{\Sigma}_2)$, we have

$$\mathrm{Cov}\{\mathrm{vec}(\mathbf{X})\} = \boldsymbol{\Sigma}_2 \otimes \boldsymbol{\Sigma}_1.$$

Interpretation of parameters

- The covariance matrix of a column of $\mathbf{X} \sim \mathcal{N}_{p_1,p_2}(\mathbf{0}, \mathbf{\Sigma}_1, \mathbf{\Sigma}_2)$ is

$$\mathrm{Cov}(\mathbf{x}_k) = \sigma_{2kk}\mathbf{\Sigma}_1,$$

and analogously for the rows of $\mathbf{X}$.

Interpretation

$$\mathbf{\Sigma}_1 = \text{ dependencies between the rows of } \mathbf{X},$$
$$\mathbf{\Sigma}_2 = \text{ dependencies between the columns of } \mathbf{X}.$$

Research activity

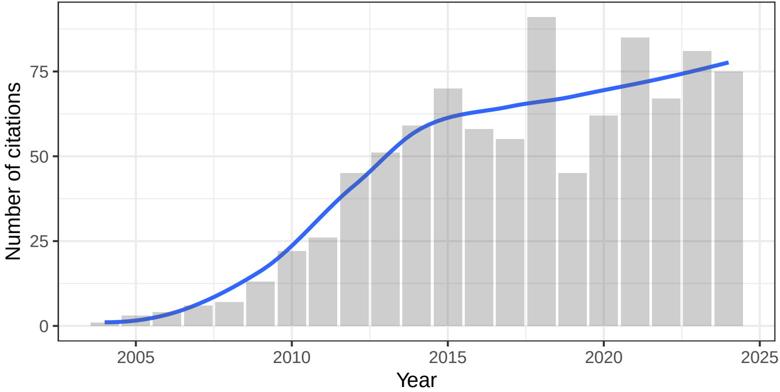

Figure: the aggregated yearly citations to [Dutilleul, 1999, Srivastava et al., 2008, Werner et al., 2008, Wiesel, 2012]

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Non-identifiability of scale

- From $\mathbf{X} = \mathbf{\Sigma}_1^{1/2}\mathbf{Z}\mathbf{\Sigma}_2^{1/2}$ we see that the choices

$$(\mathbf{\Sigma}_1, \mathbf{\Sigma}_2) \qquad \text{and} \qquad (\lambda\mathbf{\Sigma}_1, \lambda^{-1}\mathbf{\Sigma}_2)$$

  yield the same distribution for $\mathbf{X}$.
- The parameters $\mathbf{\Sigma}_1, \mathbf{\Sigma}_2$ are identifiable only up to scale.

Estimator I

- The moment estimators

$$\mathrm{E}(\mathbf{X}\mathbf{X}') = \mathrm{tr}(\boldsymbol{\Sigma}_2)\boldsymbol{\Sigma}_1$$
$$\mathrm{E}(\mathbf{X}'\mathbf{X}) = \mathrm{tr}(\boldsymbol{\Sigma}_1)\boldsymbol{\Sigma}_2$$

are used in numerous works
  - [Zhang and Zhou, 2005]
  - [Li et al., 2010]
  - [Ding and Cook, 2015]
  - [Virta et al., 2017]
  - [Radojičić et al., 2025]
  - . . .

Estimator I - properties

- Their sample versions

$$\mathbf{C}_1 := \frac{1}{n}\sum_{i=1}^{n}\mathbf{X}_i\mathbf{X}_i' \quad \text{and} \quad \mathbf{C}_2 := \frac{1}{n}\sum_{i=1}^{n}\mathbf{X}_i'\mathbf{X}_i$$

  are

  - conceptually simple,
  - fast to compute,
  - consistent and asymptotically normal,
  - orthogonally equivariant, i.e., for orthogonal $\mathbf{U}, \mathbf{V}$,

$$\mathbf{X}_i \mapsto \mathbf{U}\mathbf{X}_i\mathbf{V}' \quad \text{induces} \quad (\mathbf{C}_1, \mathbf{C}_2) \mapsto (\mathbf{U}\mathbf{C}_1\mathbf{U}', \mathbf{V}\mathbf{C}_2\mathbf{V}')$$

Affine equivariance?

Conjecture in [Virta et al., 2017]

No estimator $\mathbf{S}_1(\mathbf{X}_i)$ exists for which

$$\mathbf{S}_1(\mathbf{A}\mathbf{X}_i\mathbf{B}') \propto \mathbf{A}\mathbf{S}_1(\mathbf{X}_i)\mathbf{A}',$$

for all non-singular $\mathbf{A}, \mathbf{B}$.

Affine equivariance?

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for all non-singular $\mathbf{A}, \mathbf{B}$.

Not true!

Estimator II

MLE of $(\mathbf{\Sigma}_1, \mathbf{\Sigma_2})$ under matrix normal

The maximum likelihood estimator $(\mathbf{S}_1, \mathbf{S}_2)$ of $(\mathbf{\Sigma}_1, \mathbf{\Sigma_2})$ is any solution to

$$\begin{cases} \mathbf{S}_1 & = \frac{1}{np_2} \sum_{i=1}^n \mathbf{X}_i \mathbf{S}_2^{-1} \mathbf{X}_i', \\ \mathbf{S}_2 & = \frac{1}{np_1} \sum_{i=1}^n \mathbf{X}_i' \mathbf{S}_1^{-1} \mathbf{X}_i. \end{cases}$$

Estimator II - properties

- The sample MLE is
  - affine equivariant (up to scale),
  - a.s. unique for continuous $\mathbf{X}$ when $n > \frac{p_1}{p_2} + \frac{p_2}{p_1} + 1$,
  - a solution to g-convex problem.
- Moreover, under normality
  - the MLE is strictly more efficient than the moment estimator when $\mathbf{\Sigma}_2 \otimes \mathbf{\Sigma}_1 \not\propto \mathbf{I}_{p_1 p_2}$,
  - The scaled estimators

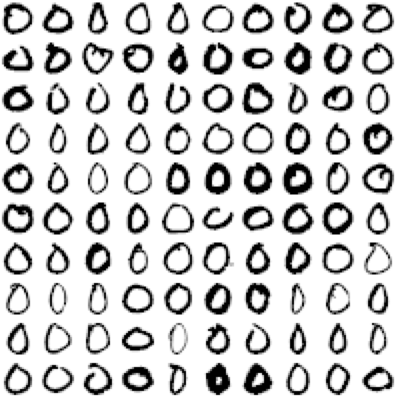
$$\frac{\mathbf{S}_1}{|\mathbf{S}_1|^{1/p_1}} \quad \text{and} \quad \frac{\mathbf{S}_2}{|\mathbf{S}_2|^{1/p_2}}$$

    are asymptotically independent.

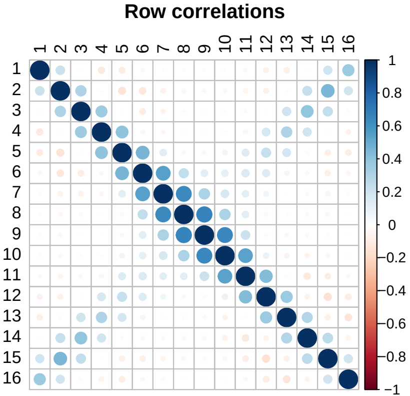
[Wiesel, 2012, Soloveychik and Trushin, 2016, Drton et al., 2021, McCormack and Hoff, 2023]

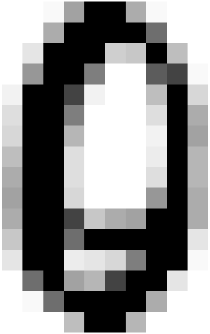
Example data

$\mathbf{X}_i \in [0,1]^{p_1 \times p_2}$ with $n = 1194$, $p_1 = p_2 = 16$.

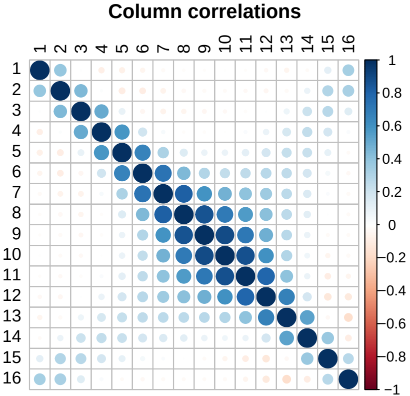


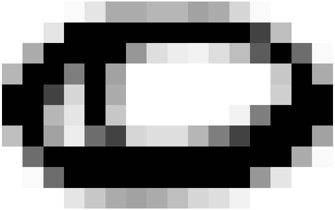
MLE $\mathbf{S}_1$ for the digits





MLE $\mathbf{S}_2$ for the digits





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Motivation

- Under $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_2 \otimes \boldsymbol{\Sigma}_1$, the number of parameters is reduced from $\mathcal{O}(p_1^2 p_2^2)$ to $\mathcal{O}(p_1^2 + p_2^2)$.
- Separability testing typically uses Gaussian LRT:
  - [Lu and Zimmerman, 2005]
  - [Mitchell et al., 2005]
  - [Roy and Khattree, 2005]
  - [Simpson, 2010]
  - [Filipiak et al., 2016]
  - $\cdots$

A wider model

Matrix elliptical distributions

We assume

$$\mathbf{X} = \mathbf{\Sigma}_1^{1/2}\mathbf{Z}\mathbf{\Sigma}_2^{1/2},$$

where $\mathbf{Z}$ is matrix spherical, i.e., $\mathbf{Z} \sim \mathbf{UZV}'$ for all orthogonal $\mathbf{U}, \mathbf{V}$.

- All matrix elliptical distributions are separable.
- The family contains matrix normal, matrix-t, ... [Gupta and Nagar, 2018]

Separability test

Test statistic

For the sample covariance matrix $\mathbf{S}$ of the $\mathrm{vec}(\mathbf{X}_i)$, we let

$$\hat{t} := \left\| \left(\frac{\mathbf{S}}{|\mathbf{S}|^{\frac{1}{p_1 p_2}}} \right)^{-1/2} \left(\frac{\mathbf{S}_2}{|\mathbf{S}_2|^{\frac{1}{p_2}}} \otimes \frac{\mathbf{S}_1}{|\mathbf{S}_1|^{\frac{1}{p_1}}} \right) \left(\frac{\mathbf{S}}{|\mathbf{S}|^{\frac{1}{p_1 p_2}}} \right)^{-1/2} - \mathbf{I}_{p_1 p_2} \right\|_F^2 .$$

$\mathrm{Cov}\{\mathrm{vec}(\mathbf{Z}) \otimes \mathrm{vec}(\mathbf{Z})\}$ when $p_1 = p_2 = 2$

$$
\left(\begin{array}{cccc|cccc|cccc|cccc}
* & 0 & 0 & 0 & 0 & * & 0 & 0 & 0 & 0 & * & 0 & 0 & 0 & 0 & * \\
0 & * & 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & * & 0 & 0 & * & 0 \\
0 & 0 & * & 0 & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 & * & 0 & 0 \\
0 & 0 & 0 & * & 0 & 0 & * & 0 & 0 & * & 0 & 0 & * & 0 & 0 & 0 \\
\hline
0 & * & 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & * & 0 & 0 & * & 0 \\
* & 0 & 0 & 0 & 0 & * & 0 & 0 & 0 & 0 & * & 0 & 0 & 0 & 0 & * \\
0 & 0 & 0 & * & 0 & 0 & * & 0 & 0 & * & 0 & 0 & * & 0 & 0 & 0 \\
0 & 0 & * & 0 & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 & * & 0 & 0 \\
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0 & 0 & * & 0 & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 & * & 0 & 0 \\
0 & 0 & 0 & * & 0 & 0 & * & 0 & 0 & * & 0 & 0 & * & 0 & 0 & 0 \\
* & 0 & 0 & 0 & 0 & * & 0 & 0 & 0 & 0 & * & 0 & 0 & 0 & 0 & * \\
0 & * & 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & * & 0 & 0 & * & 0 \\
\hline
0 & 0 & 0 & * & 0 & 0 & * & 0 & 0 & * & 0 & 0 & * & 0 & 0 & 0 \\
0 & 0 & * & 0 & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 & * & 0 & 0 \\
0 & * & 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & * & 0 & 0 & * & 0 \\
* & 0 & 0 & 0 & 0 & * & 0 & 0 & 0 & 0 & * & 0 & 0 & 0 & 0 & *
\end{array}\right)
$$

The starred elements are parametrized by a total of three values.

Null distribution

Limiting distribution of $\hat{t}$ [Virta and Matsuda, 2025]

Under the matrix elliptical, $\hat{t}$ satisfies

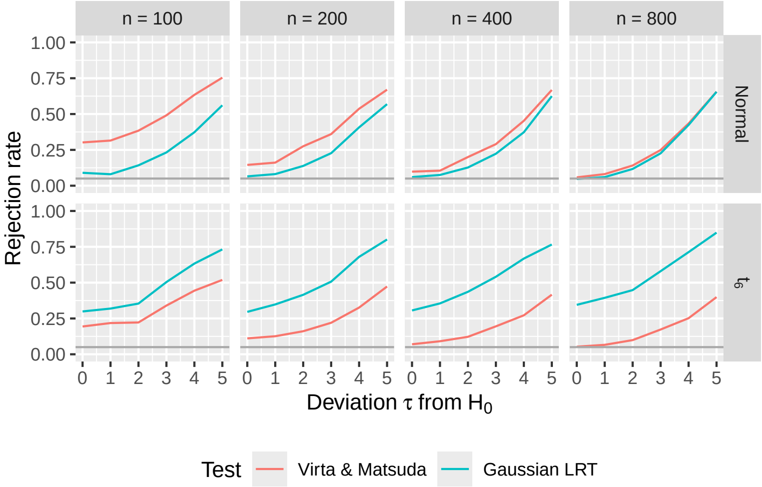
$$n\hat{t} \rightsquigarrow \beta_1 \chi^2_{\frac{1}{4}(p_1+2)(p_1-1)(p_2+2)(p_2-1)} + \beta_2 \chi^2_{\frac{1}{4}p_1 p_2 (p_1-1)(p_2-1)},$$

where $\beta_1, \beta_2 > 0$ are certain fourth moments of $\mathbf{Z}$.

- For matrix normal, $\beta_1 = \beta_2 = 2$, giving just a χ^2-distribution.
- The total degrees of freedom is equal to the difference between the numbers of parameters in $\boldsymbol{\Sigma}$ and $\boldsymbol{\Sigma}_2 \otimes \boldsymbol{\Sigma}_1$.

Power comparison

- Average rejection rates under local alternatives of the form "$\tau/\sqrt{n}$" when $n = 500$



Bootstrapped null distribution

- If data are unlikely to obey an elliptical distribution, we can simulate the null distribution of $\hat{t}$ as follows:
  1. Whiten the data using $\mathbf{S}^{-1/2}$.
  2. Draw a bootstrap sample.
  3. Backtransform via $(\mathbf{S}_2 \otimes \mathbf{S}_1)^{1/2}$.
  4. Compute $\hat{t}$.

Example

- For the digit data we get $p < 10^{-4}$ regardless of the null distribution (asymptotic or bootstrap).
- We conclude that the distribution is not separable.

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Kronecker covariance

Kronecker covariance

For a random matrix $\mathbf{X} \in \mathbb{R}^{p_1 \times p_2}$ with arbitrary $\mathrm{Cov}\{\mathrm{vec}(\mathbf{X})\}$, [Hoff et al., 2023] define the Kronecker covariance of $\mathbf{X}$ to be

$$k(\mathbf{X}) := \mathbf{\Psi}_2 \otimes \mathbf{\Psi}_1,$$

where $(\mathbf{\Psi}_1, \mathbf{\Psi}_2)$ is the Gaussian MLE evaluated at $\mathbf{X}$.

Kronecker covariance properties

- The Kronecker covariance $k(\mathbf{X})$
  - is equal to $\mathbf{\Sigma}_2 \otimes \mathbf{\Sigma}_1$ when $\mathbf{X}$ is covariance separable,
  - is a.s. unique under mild conditions,
  - is a solution to g-convex problem,
  - is affine equivariant in the sense that

$$k(\mathbf{AXB}') = (\mathbf{A} \otimes \mathbf{B}) k(\mathbf{X}) (\mathbf{A}' \otimes \mathbf{B}').$$

Core covariance

Core covariance

The core covariance of $\mathbf{X}$ is defined as

$$c(\mathbf{X}) = k(\mathbf{X})^{-1/2}\mathrm{Cov}\{\mathrm{vec}(\mathbf{X})\}k(\mathbf{X})^{-1/2}.$$

- The core covariance $c(\mathbf{X})$ is
  - equal to $\mathbf{I}_{p_1 p_2}$ when $\mathbf{X}$ is covariance separable,
  - affine invariant in the sense that

$$c(\mathbf{AXB}') = (\mathbf{U} \otimes \mathbf{V})c(\mathbf{X})(\mathbf{U}' \otimes \mathbf{V}'),$$

for some orthogonal $\mathbf{U}, \mathbf{V}$.

Kronecker-core decomposition

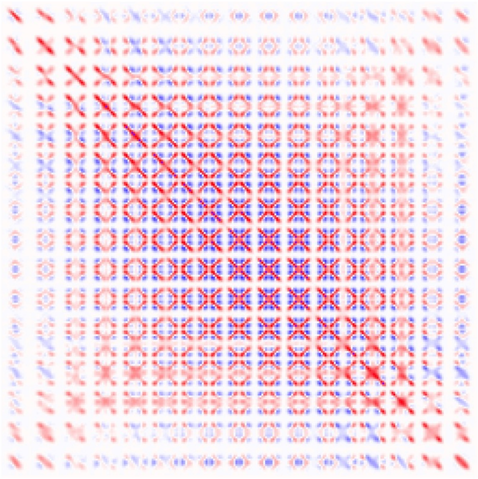
- The Kronecker-core decomposition (KCD) is

$$\mathrm{Cov}\{\mathrm{vec}(\mathbf{X})\} = k(\mathbf{X})^{1/2} c(\mathbf{X}) k(\mathbf{X})^{1/2}.$$

Interpretation

$$\begin{aligned} k(\mathbf{X}) &= \text{ row-column variation / “main effects”}, \\ c(\mathbf{X}) &= \text{ residual variation / “interactions”}. \end{aligned}$$

$\mathrm{Cov}\{\mathrm{vec}(\mathbf{X})\}$ for the digits



K and **C** for the digits

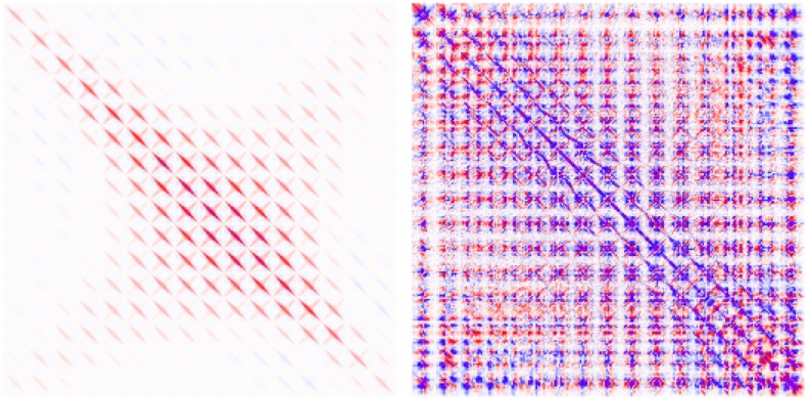
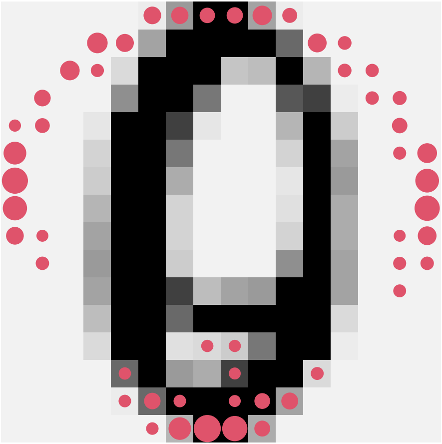


Figure: **K** (left) and **C** (right)

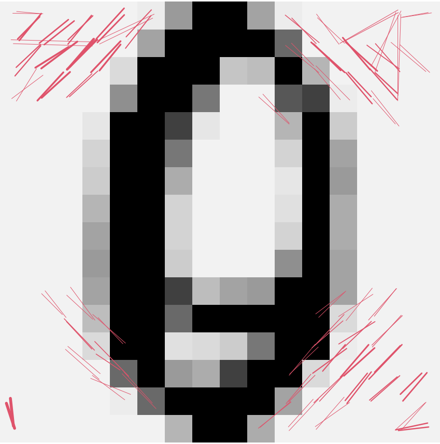
Violations 1

- Pixels whose variances most violate separability



Violations 2

- Pixel pairs whose positive correlations most violate separability



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List of R-packages

- Gaussian MLE / hypothesis testing
  - `MixMatrix`
  - `tensr`
  - `MN`
  - `sEparaTe`
- Non-Gaussian matrix-variate distributions
  - `MixMatrix`
- Kronecker-core decomposition
  - `covKCD`
- General operations for matrix/tensor data
  - `tensorBSS`
  - `tensr`

Future prospects

- General theory of scatter matrices for matrix data
- Matrix ICS
- M-estimators of scatter for matrix data
- Robust analysis of matrix data
- ...

Thank you for your attention!

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Work under progress.

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