Segmentation bidimensionnelle rapide pour l'étude des données Hi-C

Vincent Brault, Julien Chiquet et Céline Lévy-Leduc

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AgroParisTech
INSTITUT DES SCIENCES ET INDUSTRIES DU VIVANT ET DE L'ENVIRONNEMENT
PARIS INSTITUTE OF TECHNOLOGY FOR LIFE, FOOD AND ENVIRONMENTAL SCIENCES

INRA
SCIENCE & IMPACT

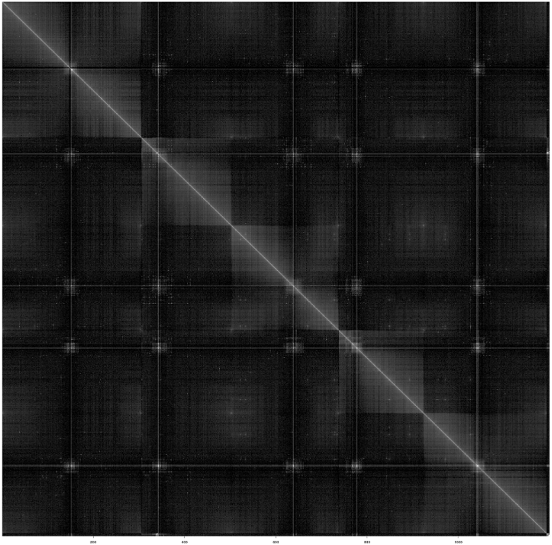
Hi-C data (High Chromosome Contact map)

- To better understand the organisation of a cell (Lieberman-Aiden et al. [2009]).
- To quantify the interaction between two positions of the genome (intra-chromosome and inter-chromosome).
- Each entry (i, j) : Number of interactions between the loci i and j [1].

1. A locus is a particular and invariable location on the chromosome.

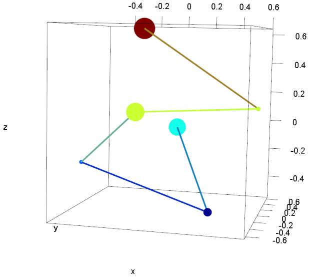
Motivations

Hi-C data of 5 chromosomes of the Arabidopsis Thaliana ; collaboration with M. Benhamed of the *institut de biologie des plantes (UMR 8618)*.



Goal

- To form group without permutations.
- To obtain a grid panel.
- To study matrices 10 000$\times$10 000.



Plan

1. Model
2. Least Absolute Shrinkage eStimatOr
3. Theoretical results
4. Model selection
5. Numerical experiments

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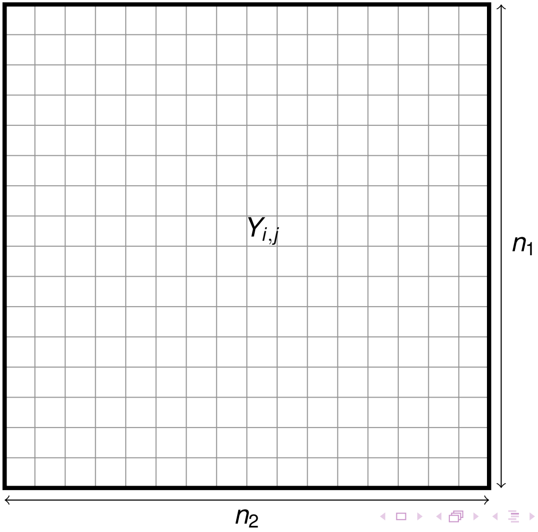
Notations



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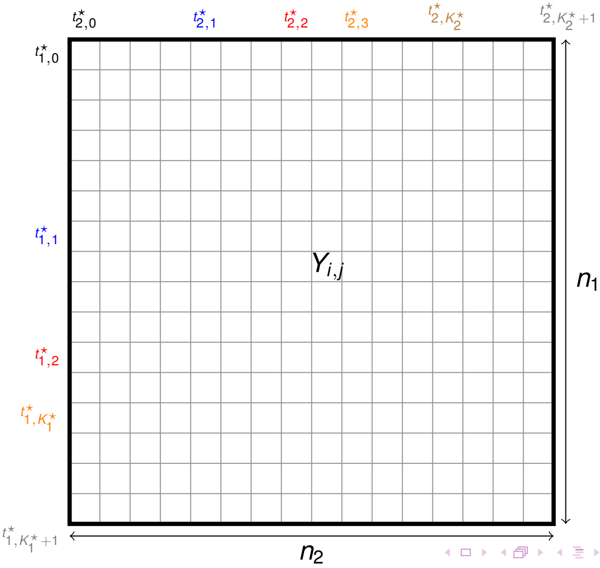
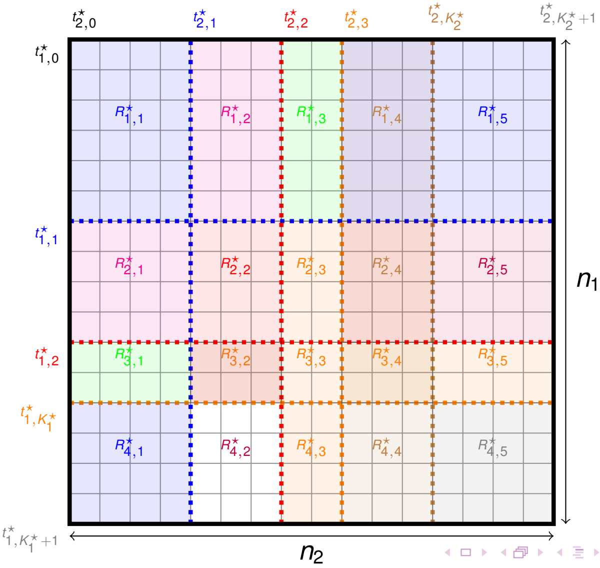

$t^\star_{2,0}$
$t^\star_{2,1}$
$t^\star_{2,2}$
$t^\star_{2,3}$
$t^\star_{2,K_2^\star}$
$t^\star_{2,K_2^\star+1}$
$t^\star_{1,0}$
$t^\star_{1,1}$
$t^\star_{1,2}$
$t^\star_{1,K_1^\star}$
$t^\star_{1,K_1^\star+1}$
$Y_{i,j}$
n_1
n_2

Notations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$t^\star_{1,K^\star_1+1}$
$R^\star_{1,1}$ $R^\star_{1,2}$ $R^\star_{1,3}$ $R^\star_{1,4}$ $R^\star_{1,5}$
$R^\star_{2,1}$ $R^\star_{2,2}$ $R^\star_{2,3}$ $R^\star_{2,4}$ $R^\star_{2,5}$
$R^\star_{3,1}$ $R^\star_{3,2}$ $R^\star_{3,3}$ $R^\star_{3,4}$ $R^\star_{3,5}$
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n_1
n_2

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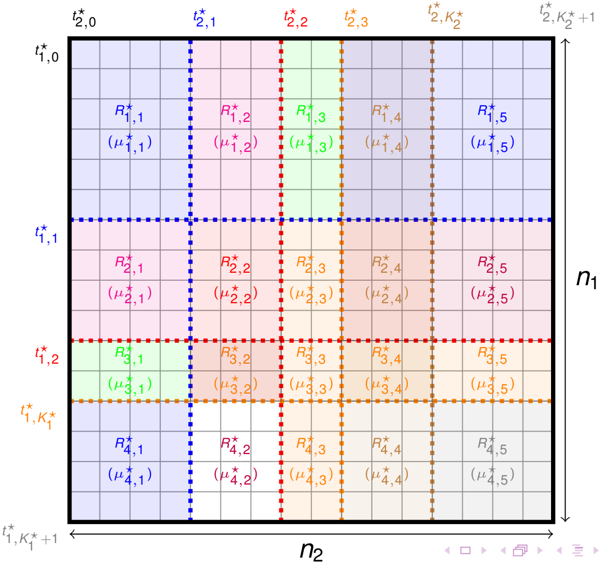
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n_1
n_2

Model

Let $Y = (Y_{i,j})_{1 \leq i,j \leq n}$ be the random matrix defined by

$$\mathbf{Y} = \mathbf{U} + \mathbf{E},$$

where $\mathbf{U} = (U_{i,j})$ is a blockwise constant matrix such that

$$U_{i,j} = \mu^\star_{k,\ell} \quad \text{if } t^\star_{1,k-1} \leq i \leq t^\star_{1,k} - 1 \text{ and } t^\star_{2,\ell-1} \leq j \leq t^\star_{2,\ell} - 1,$$

with the convention $t^\star_{1,0} = t^\star_{2,0} = 1$ and $t^\star_{1,K^\star_1+1} = t^\star_{2,K^\star_2+1} = n + 1$. The entries $E_{i,j}$ of the matrix $E = (E_{i,j})_{1 \leq i,j \leq n}$ are iid zero-mean random variables.

Trick

$$\mathbf{U} = \mathbf{T}\mathbf{B}\mathbf{T}^\top$$

$$\mathbf{T} = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \vdots \\ 1 & 1 & 1 & \dots & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{B} = \begin{array}{c|cccccccccccccccc|c}
 & t^\star_{2,0} & & & & t^\star_{2,1} & & & t^\star_{2,2} & & t^\star_{2,3} & & & t^\star_{2,K_2^\star} & & & & t^\star_{2,K_2^\star+1} \\
\hline
t^\star_{1,0} & B_{1,1} & 0 & 0 & 0 & B_{1,5} & 0 & 0 & B_{1,8} & 0 & B_{1,10} & 0 & 0 & B_{1,13} & 0 & 0 & 0 & \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
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 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
t^\star_{1,1} & B_{7,1} & 0 & 0 & 0 & B_{7,5} & 0 & 0 & B_{7,8} & 0 & B_{7,10} & 0 & 0 & B_{7,13} & 0 & 0 & 0 & \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
t^\star_{1,2} & B_{11,1} & 0 & 0 & 0 & B_{11,5} & 0 & 0 & B_{11,8} & 0 & B_{11,10} & 0 & 0 & B_{11,13} & 0 & 0 & 0 & \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
t^\star_{1,K_1^\star} & B_{13,1} & 0 & 0 & 0 & B_{13,5} & 0 & 0 & B_{13,8} & 0 & B_{13,10} & 0 & 0 & B_{13,13} & 0 & 0 & 0 & \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \\
\hline
t^\star_{1,K_1^\star+1} & & & & & & & & & & & & & & & & &
\end{array}$$

$$\text{with } \mu^\star_{k,\ell} = \sum_{i=1}^{k} \sum_{j=1}^{\ell} B_{t^\star_{1,i},t^\star_{2,j}}.$$

Vectorisation

$$\mathbf{Y} = \mathbf{T}\mathbf{B}\mathbf{T}^\top + \mathbf{E}$$

is equivalent to

$$\mathrm{Vec}(\mathbf{Y}) = \mathrm{Vec}(\mathbf{T}\mathbf{B}\mathbf{T}^\top) + \mathrm{Vec}(\mathbf{E})$$

with

$$\mathrm{Vec}(\mathbf{T}\mathbf{B}\mathbf{T}^\top) = \left(\mathbf{T}^{\top^\top} \otimes \mathbf{T}\right) \mathrm{Vec}(\mathbf{B}) = (\mathbf{T} \otimes \mathbf{T}) \mathrm{Vec}(\mathbf{B})$$

and we obtain

$$\underbrace{\mathcal{Y}}_{n^2 \times 1} = \underbrace{\mathcal{X}}_{n^2 \times n^2} \underbrace{\mathcal{B}}_{n^2 \times 1} + \underbrace{\mathcal{E}}_{n^2 \times 1}.$$

Kronecker product

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Least Absolute Shrinkage eStimatOr (LASSO)

For all $\lambda_n \geq 0$, we define

$$\widehat{\mathcal{B}}(\lambda_n) = \underset{\mathcal{B}\in\mathbb{R}^{n^2}}{\text{Argmin}} \left\{ \|\mathcal{Y} - \mathcal{X}\mathcal{B}\|_2^2 + \lambda_n \|\mathcal{B}\|_1 \right\}$$

and the active set

$$\widehat{\mathcal{A}}(\lambda_n) = \left\{ j \in \{1, \ldots, n^2\} : \widehat{\mathcal{B}}_j(\lambda_n) \neq 0 \right\}$$

A reminder on the norm

Least Absolute Shrinkage eStimatOr (LASSO)

For all $\lambda_n \geq 0$, we define

$$\widehat{\mathcal{B}}(0) = \underset{\mathcal{B} \in \mathbb{R}^{n^2}}{\operatorname{Argmin}} \left\{ \|\mathcal{Y} - \mathcal{X}\mathcal{B}\|_2^2 + \lambda_n \|\mathcal{B}\|_1 \right\}$$

and the active set

$$\widehat{\mathcal{A}}(0) = \left\{ j \in \{1, \ldots, n^2\} : \widehat{\mathcal{B}}_j(\lambda_n) \neq 0 \right\} \approx \{1, \ldots, n^2\}$$

A reminder on the norm

Least Absolute Shrinkage eStimatOr (LASSO)

For all $\lambda_n \geq 0$, we define

$$\widehat{\mathcal{B}}(+\infty) = \underset{\mathcal{B} \in \mathbb{R}^{n^2}}{\operatorname{Argmin}} \left\{ \|\mathcal{Y} - \mathcal{X}\mathcal{B}\|_2^2 + \lambda_n \|\mathcal{B}\|_1 \right\}$$

and the active set

$$\widehat{\mathcal{A}}(+\infty) = \left\{ j \in \{1, \ldots, n^2\} : \widehat{\mathcal{B}}_j(\lambda_n) \neq 0 \right\} = \emptyset$$

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A reminder on the norm

Estimation of break change-point

$$\begin{pmatrix} 1\\2\\3\\4\\5\\6\\7\\8\\9\\10\\11\\12\\13\\14\\15\\16 \end{pmatrix} \Leftrightarrow \begin{array}{cc} & q_a+1 \\ \begin{pmatrix} 1 & 5 & 9 & 13 \\ 2 & 6 & 10 & 14 \\ 3 & 7 & 11 & 15 \\ 4 & 8 & 12 & 16 \end{pmatrix} & r_a+1 \end{array}$$

$\forall a \in \widehat{\mathcal{A}}(\lambda_n)$, we define (q_a, r_a) as the Euclidean division of $(a-1)$ by n, namely $(a-1) = nq_a + r_a$ then

$$\widehat{\mathbf{t}}_1 = (\widehat{t}_{1,k})_{1\leq k\leq |\widehat{\mathcal{A}}_1(\lambda_n)|} \in \widehat{\mathcal{A}}_1(\lambda_n) = \{r_a+1 : a \in \widehat{\mathcal{A}}(\lambda_n)\},$$

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Estimation of break change-point

$$\begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ a \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} \Leftrightarrow \begin{array}{cc} \begin{array}{cccc} & & q_a+1 & \end{array} & \\ \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & a & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} & \begin{array}{c} \\ r_a+1 \\ \\ \\ \end{array} \end{array}$$

For example, a=10

$10 - 1 = 9 = 4 \times 2 + 1$

2+1=3 and 1+1=2

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Standard complexity : [2]

$$\mathcal{O}\left(|\mathcal{A}|\, mp + p\,|\mathcal{A}|^2 + |\mathcal{A}|^3\right).$$

In our case, we have :

$$\mathcal{O}\left(|\mathcal{A}|\, n^4\right).$$

$$\mathcal{X} = \mathbf{T} \otimes \mathbf{T}$$

2. see for example Bach et al. [2011].

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Fast LARS for two-dimensional change-point detection :

Input : data matrix Y, maximal number of active variables s.

// Initialisation

Start with no change-point $\mathcal{A} \leftarrow \emptyset$, $\hat{\mathcal{B}} = \mathbf{0}$

Compute current correlations $\hat{\mathbf{c}} = \mathcal{X}^\top \mathcal{Y}$ $\mathcal{O}(n^2)$

While $\lambda > 0$ or $|\mathcal{A}| < s$

// Update the set of active variables

Determine next change-point(s) by setting $\lambda \leftarrow \|\hat{\mathbf{c}}\|_\infty$ and $\mathcal{A} \leftarrow \left\{j : \hat{\mathbf{c}}_j = \lambda\right\}$

Update the Cholesky factorization of $\mathcal{X}_\mathcal{A}^\top \mathcal{X}_\mathcal{A}$ $\mathcal{O}(|\mathcal{A}|^2)$

// Compute the direction of descent

Get the unormalized direction $\tilde{w}_\mathcal{A} \leftarrow \left(\mathcal{X}_{\cdot\mathcal{A}}^\top \mathcal{X}_{\cdot\mathcal{A}}\right)^{-1} \mathrm{sign}(\hat{c}_\mathcal{A})$ $\mathcal{O}(|\mathcal{A}|^2)$

Normalize $w_\mathcal{A} \leftarrow \alpha \tilde{w}_\mathcal{A}$ with $\alpha \leftarrow 1/\sqrt{\tilde{w}_\mathcal{A}^\top \mathrm{sign}(\hat{c}_\mathcal{A})}$

Compute the equiangular vector $u_\mathcal{A} = \mathcal{X}_\mathcal{A} w_\mathcal{A}$ and $\mathbf{a} = \mathcal{X}^\top u_\mathcal{A}$ $\mathcal{O}(n^2)$

// Compute the direction step

Find the maximal step preserving equicorrelation $\gamma_{\mathrm{in}} \leftarrow \min^+_{j\in\mathcal{A}^c} \left\{ \frac{\lambda - \mathbf{c}_j}{\alpha - a_j}, \frac{\lambda + \mathbf{c}_j}{\alpha + a_j} \right\}$

Find the maximal step preserving the signs $\gamma_{\mathrm{out}} \leftarrow \min^+_{j\in\mathcal{A}} \left\{-\hat{\mathcal{B}}_\mathcal{A}/w_\mathcal{A}\right\}$

The direction step that preserves both is $\hat{\gamma} \leftarrow \min(\gamma_{\mathrm{in}}, \gamma_{\mathrm{out}})$

Update the correlations $\hat{\mathbf{c}} \leftarrow \hat{\mathbf{c}} - \hat{\gamma}\mathbf{a}$ and $\hat{\mathcal{B}}_\mathcal{A} \leftarrow \hat{\mathcal{B}}_\mathcal{A} + \hat{\gamma} w_\mathcal{A}$ accordingly $\mathcal{O}(n)$

// Drop variable crossing the zero line

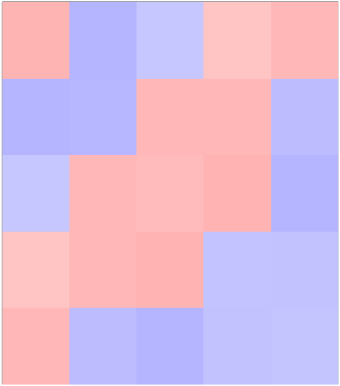
If $\gamma_{\mathrm{out}} < \gamma_{\mathrm{in}}$

Remove existing change-point(s) $\mathcal{A} \leftarrow \mathcal{A} \setminus \left\{j \in \mathcal{A} : \hat{\mathcal{B}}_j = 0\right\}$

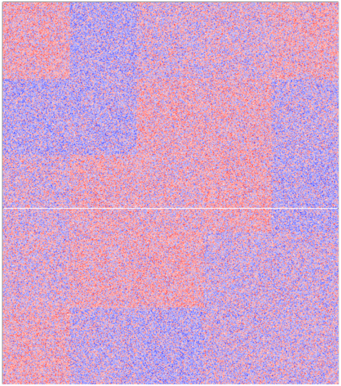
Downdate the Cholesky factorization of $\mathcal{X}_\mathcal{A}^\top \mathcal{X}_\mathcal{A}$ $\mathcal{O}(|\mathcal{A}|)$

Output : Sequence of triplet $(\mathcal{A}, \lambda, \hat{\mathcal{B}})$ recorded at each iteration.

Mu matrix



Orignal matrix



Gray version

Plan

1. Model
2. Least Absolute Shrinkage eStimatOr
3. Theoretical results
4. Model selection
5. Numerical experiments

Proposition

Let $(Y_{i,j})_{\substack{1\leq i\leq n_1\\ 1\leq j\leq n_2}}$ a data matrix and $\widehat{t}_{1,k}$, $\widehat{t}_{2,k}$ the estimators obtained by the LASSO.
Under some assumptions and assume that $|\widehat{\mathcal{A}}_1(\lambda_n)| = K_1^\star$ and that $|\widehat{\mathcal{A}}_2(\lambda_n)| = K_2^\star$ then for all $a \in \{1, \ldots, n^2\}$,

$$\mathbb{P}\left(\left\{\max_{1\leq k\leq K_1^\star}\left|\widehat{t}_{1,k} - t_{1,k}^\star\right| \leq n_1\delta_{n_1,n_2}\right\} \cap \left\{\max_{1\leq k\leq K_2^\star}\left|\widehat{t}_{2,k} - t_{2,k}^\star\right| \leq n_2\delta_{n_1,n_2}\right\}\right) \underset{n\to\infty}{\longrightarrow} 1.$$

$$\frac{n_1}{\log n_2} \underset{n_1,n_2\to+\infty}{\longrightarrow} +\infty$$

Key of proof

Proposition

Let $(Y_{i,j})_{\substack{1 \le i \le n_1 \\ 1 \le j \le n_2}}$ a data matrix and $\widehat{t}_{1,k}$, $\widehat{t}_{2,k}$ the estimators obtained by the LASSO.
Under some assumptions and assume that $|\widehat{\mathcal{A}}_1(\lambda_n)| = K_1^\star$ and that $|\widehat{\mathcal{A}}_2(\lambda_n)| = K_2^\star$ then for all $a \in \{1, \dots, n^2\}$,

$$\mathbb{P}\left(\left\{\max_{1 \le k \le K_1^\star} \left|\widehat{t}_{1,k} - t_{1,k}^\star\right| \le n_1 \delta_{n_1,n_2}\right\} \cap \left\{\max_{1 \le k \le K_2^\star} \left|\widehat{t}_{2,k} - t_{2,k}^\star\right| \le n_2 \delta_{n_1,n_2}\right\}\right) \underset{n \to \infty}{\longrightarrow} 1.$$

$$\frac{n_1}{\log n_2} \underset{n_1, n_2 \to +\infty}{\longrightarrow} +\infty$$

Key of proof

Plan

1. Model
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Stability selection

Stability selection :

Input : data vector $\mathcal{Y} \in \mathcal{M}_{n^2 \times 1}$, an integer $M \in \mathbb{N}^\star$, a pair of numbers $(K_1^\star, K_2^\star) \in \{1, \ldots, n\}^2$.

For $\underline{iter \in \{1, \ldots, M\}}$

Chose randomly $ind^{(iter)} = \{i_1, \ldots, i_{n^2/2}\} \subset \{1, \ldots, n^2\}$.

Use the procedure with $(K_1^\star, K_2^\star)$ change-points on the data $\mathcal{Y}_{ind^{(iter)}}$ to obtain $\left(\widehat{\mathbf{t}}_1^{(iter)}, \widehat{\mathbf{t}}_2^{(iter)}\right)$.

Output : Sequence of couples $\left(\widehat{\mathbf{t}}_1^{(iter)}, \widehat{\mathbf{t}}_2^{(iter)}\right)$ recorded at each iteration or only the couple of change-points appearing a number of times larger than a given threshold.

Adaptation

$$\begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \end{pmatrix} \Leftrightarrow \begin{pmatrix} 1 & 5 & 9 & 13 \\ 2 & 6 & 10 & 14 \\ 3 & 7 & 11 & 15 \\ 4 & 8 & 12 & 16 \end{pmatrix}$$

Adaptation

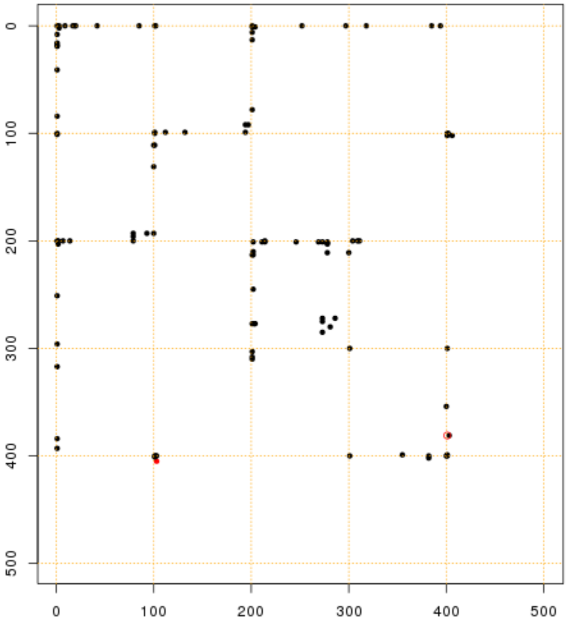
$$\begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ . \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \end{pmatrix} \Leftrightarrow \begin{pmatrix} 1 & 5 & 9 & 13 \\ 2 & 6 & . & 14 \\ 3 & 7 & 11 & 15 \\ 4 & 8 & 12 & 16 \end{pmatrix}$$

Adaptation

$$\begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ 13 \\ 14 \\ 15 \\ 16 \end{pmatrix} \Leftrightarrow \begin{pmatrix} 1 & 5 & \cdot & 13 \\ 2 & 6 & \cdot & 14 \\ 3 & 7 & \cdot & 15 \\ 4 & 8 & \cdot & 16 \end{pmatrix}$$

Adaptation

$$\begin{pmatrix} 1 \\ 2 \\ . \\ 4 \\ 5 \\ 6 \\ . \\ 8 \\ . \\ . \\ . \\ . \\ 13 \\ 14 \\ . \\ 16 \end{pmatrix} \Leftrightarrow \begin{pmatrix} 1 & 5 & . & 13 \\ 2 & 6 & . & 14 \\ . & . & . & . \\ 4 & 8 & . & 16 \end{pmatrix}$$


0
100
200
300
400
500
0
100
200
300
400
500

Adaptation stability selection

Stability selection :

Input : data matrix $Y \in \mathcal{M}_{n\times n}$, an integer $M \in \mathbb{N}^\star$, a pair of numbers $(K_1^\star, K_2^\star) \in \{1, \dots, n\}^2$.

For $\underline{iter \in \{1, \dots, M\}}$

Choose randomly $ind_1^{(iter)} = \left\{i_1^{(1)}, \dots, i_{n/2}^{(1)}\right\} \subset \{1, \dots, n\}$ and $ind_2^{(iter)} = \left\{i_1^{(2)}, \dots, i_{n/2}^{(2)}\right\} \subset \{1, \dots, n\}$.

Use the procedure with $(K_1^\star, K_2^\star)$ change-points on the data $Y_{ind_1^{(iter)}, ind_2^{(iter)}}$ to obtain $\left(N_1^{(iter)}, N_2^{(iter)}\right)$ the number of times that each change-point of $\{1, \dots, n\}^2$ was selected.

Output : Sequence of couple of numbers $\left(N_1^{(iter)}, N_2^{(iter)}\right)$ recorded at each iteration.

Plan

1 Model

2 Least Absolute Shrinkage eStimatOr

3 Theoretical results

4 Model selection

5 Numerical experiments

Experimental design

- $K_1^\star = K_2^\star = 4$.
- $\left(\mu_{k,\ell}^\star\right)_{k\in\{1,\ldots K_1^\star+1\},\ell\in\{1,\ldots K_2^\star+1\}} = \begin{pmatrix} 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \end{pmatrix}$.
- $(t_{1,k}^\star)_{1\leq k\leq K_1^\star} = ([nk/(K_1^\star + 1)] + 1)_{1\leq k\leq K_1^\star}$ and $(t_{2,k}^\star)_{1\leq k\leq K_2^\star} = ([nk/(K_2^\star + 1)] + 1)_{1\leq k\leq K_2^\star}$.
- $E_{i,j} \sim \mathcal{N}\left(0, \sigma^2\right)$.
- 1000 matrices simulated for each case.

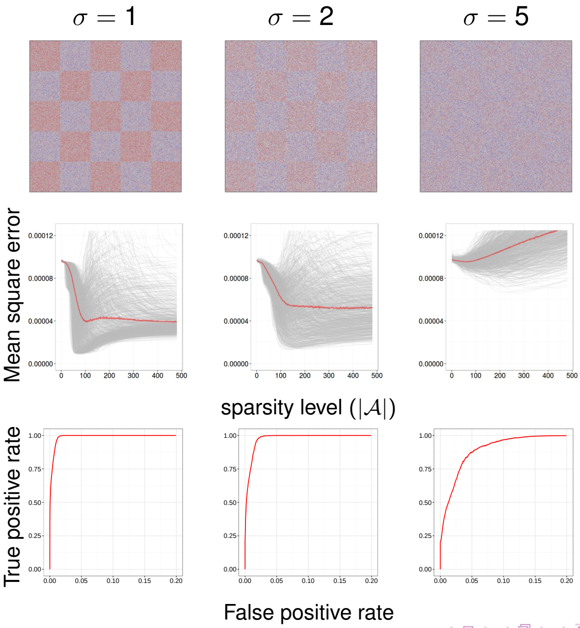
Statistical performances

Parameters :

- $n = 500$.
- $\sigma \in \{1, 2, 5\}$.

Evaluation :

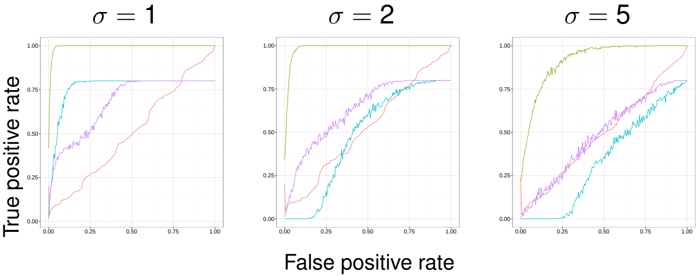
- Mean square error $n^{-2}\|\mathcal{B} - \widehat{\mathcal{B}}\|_2^2$ as a function of the number of nonzero elements in $\widehat{\mathcal{B}}$ for each scenario.
- ROC curves for the estimated change-points in rows.



$\sigma = 1$
$\sigma = 2$
$\sigma = 5$
Mean square error
0.00012
0.00008
0.00004
0.00000
0 100 200 300 400 500
sparsity level ($|\mathcal{A}|$)
True positive rate
1.00
0.75
0.50
0.25
0.00
0.00 0.05 0.10 0.15 0.20
False positive rate

- Green : Our method.
- Blue : One-dimensional LASSO[3] with at least in one row.
- Purple : One-dimensional LASSO[3] with at least in $([n/2]+1)$ rows.
- Red : Extension of CART.

$n = 250$ with 100 matricies



3. Using the procedure of Harchaoui and Lévy-Leduc [2010]

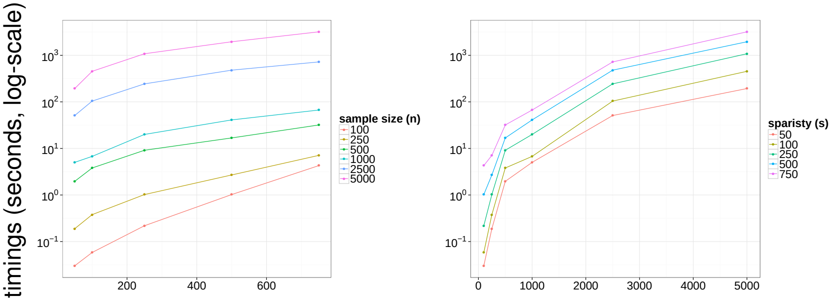
Statistical performances

Parameters :

- $n \in \{100, 250, 500, 1000, 2500, 5000\}$.
- $|\mathcal{A}| \in \{50, 100, 250, 500, 750\}$.
- $\sigma = 10$.
- Linux workstation with Intel Xeon 2.4 GHz processor and 8 GB of memory

Evaluation :

- The median runtimes.



sparsity level ($|\mathcal{A}|$) sample size (n)

1 000 $\times$ 1 000 $=$ 1 000 000 less than 2 minutes.

Model selection

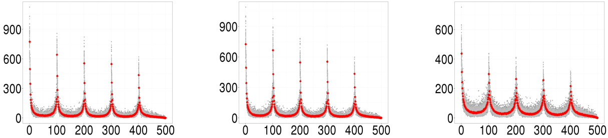
Parameters :

- $n = 500$.
- $\sigma \in \{1, 2, 5\}$.
- $M = 100$.

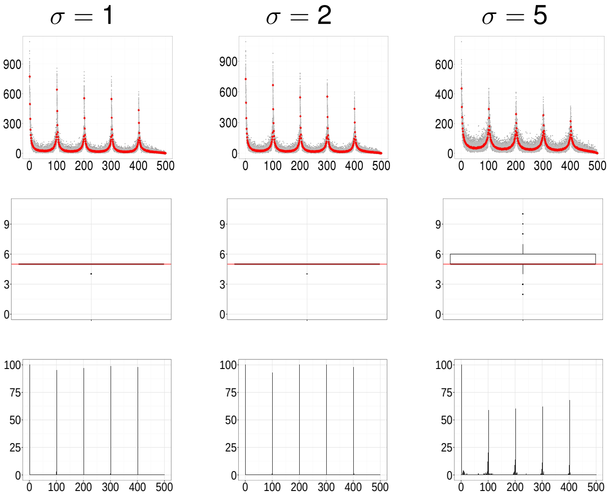
Evaluation :

- Boxplots of the estimation of $K_1^\star$.
- Histograms of the estimated change-points in rows.

$\sigma = 1$ $\sigma = 2$ $\sigma = 5$



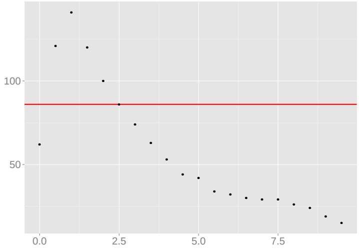
Colour Film Gray Film

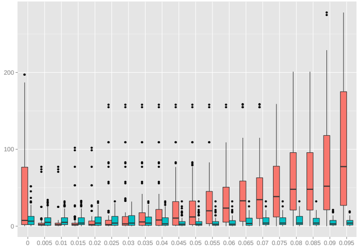


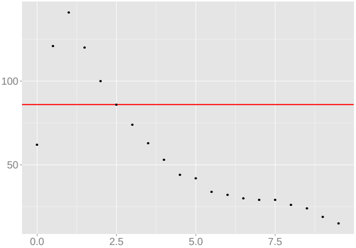
σ = 1
σ = 2
σ = 5
900
600
300
0
0
100
200
300
400
500
400
200
9
6
3
100
75
50
25

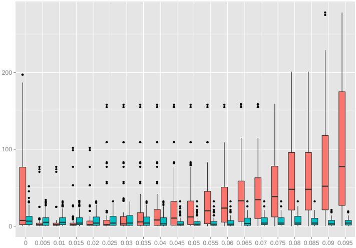
Real data

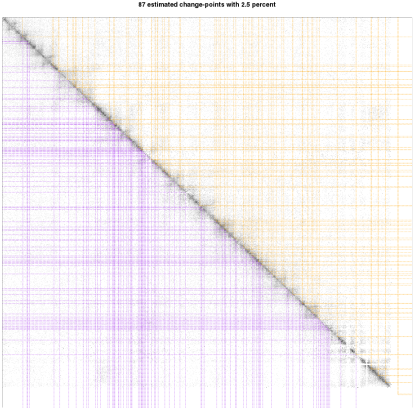
- Chromosome 19 of the mouse cortex at a resolution 40 kb.
- Comparison with Dixon et al. [2012].

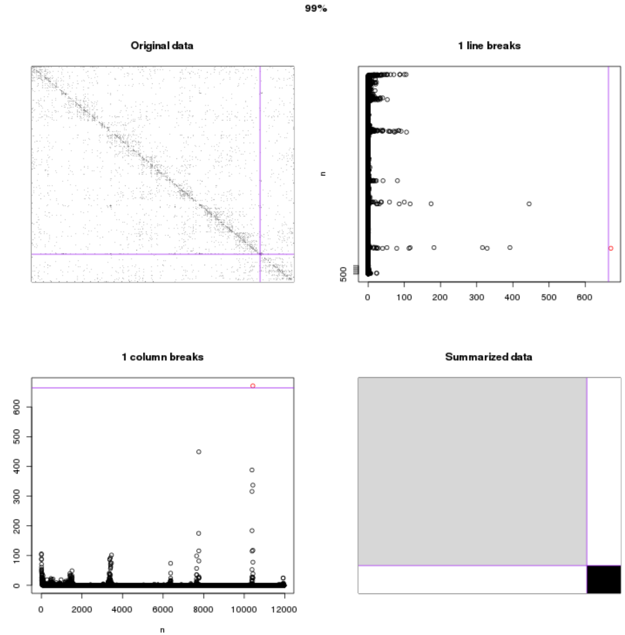

100
50
0.0
2.5
5.0
7.5


200
100
0
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035
0.04
0.045
0.05
0.055
0.06
0.065
0.07
0.075
0.08
0.085
0.09
0.095

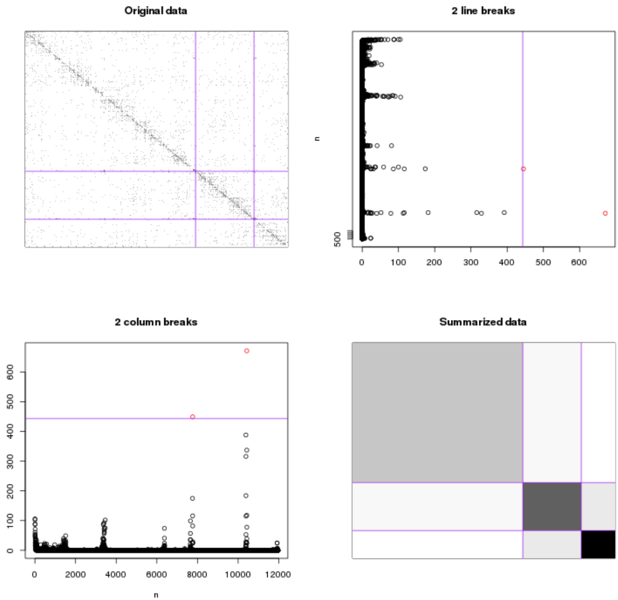

100
50
0.0
2.5
5.0
7.5


200
100
0
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035
0.04
0.045
0.05
0.055
0.06
0.065
0.07
0.075
0.08
0.085
0.09
0.095

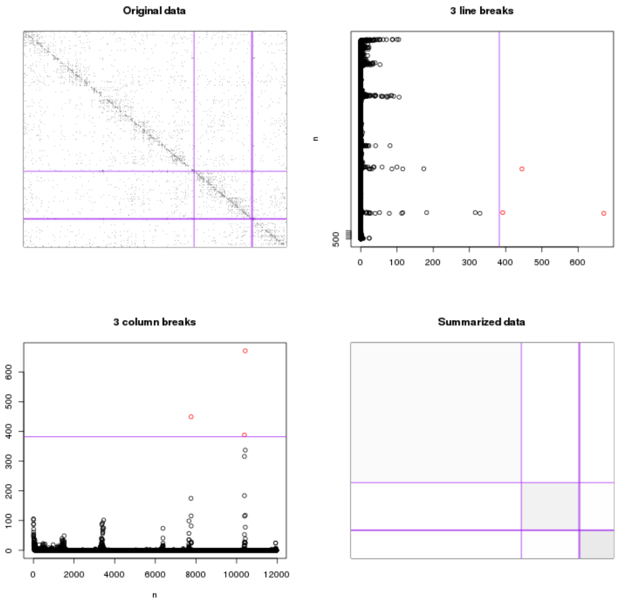

87 estimated change-points with 2.5 percent

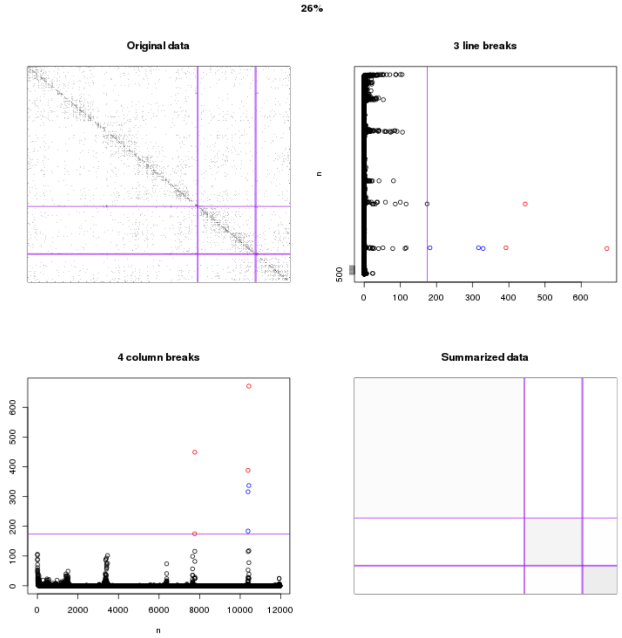

99%
Original data
1 line breaks
n
500
0
100
200
300
400
500
600
1 column breaks
600
500
400
300
200
100
0
2000
4000
6000
8000
10000
12000
n
Summarized data

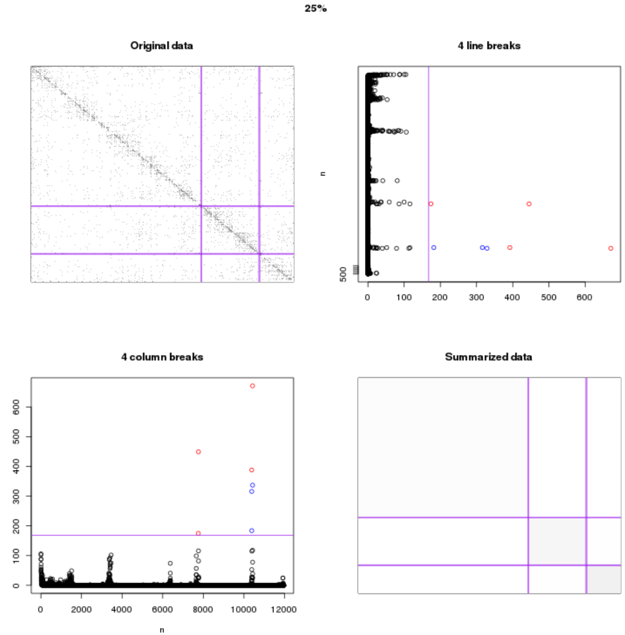
66%


Original data
2 line breaks
n
500
0 100 200 300 400 500 600
2 column breaks
0 100 200 300 400 500 600
0 2000 4000 6000 8000 10000 12000
n
Summarized data

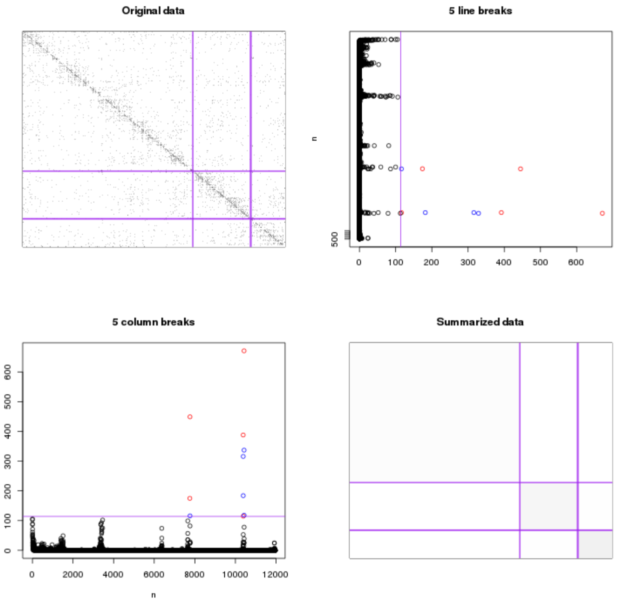
57%

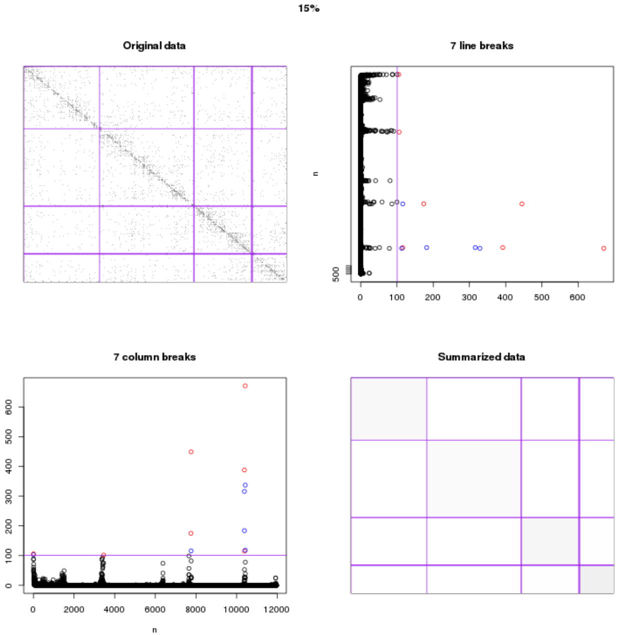

Original data
3 line breaks
n
500
0
100
200
300
400
500
600
3 column breaks
0
100
200
300
400
500
600
0
2000
4000
6000
8000
10000
12000
n
Summarized data


26%
Original data
3 line breaks
n
500
0 100 200 300 400 500 600
4 column breaks
0 100 200 300 400 500 600
0 2000 4000 6000 8000 10000 12000
n
Summarized data

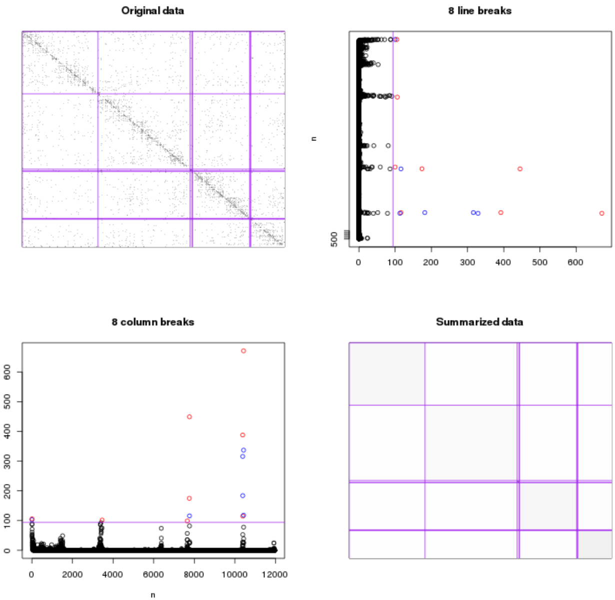

25%
Original data
4 line breaks
n
500
0
100
200
300
400
500
600
4 column breaks
0
100
200
300
400
500
600
0
2000
4000
6000
8000
10000
12000
n
Summarized data

17%


Original data
5 line breaks
n
500
0
100
200
300
400
500
600
5 column breaks
0
100
200
300
400
500
600
0
2000
4000
6000
8000
10000
12000
n
Summarized data

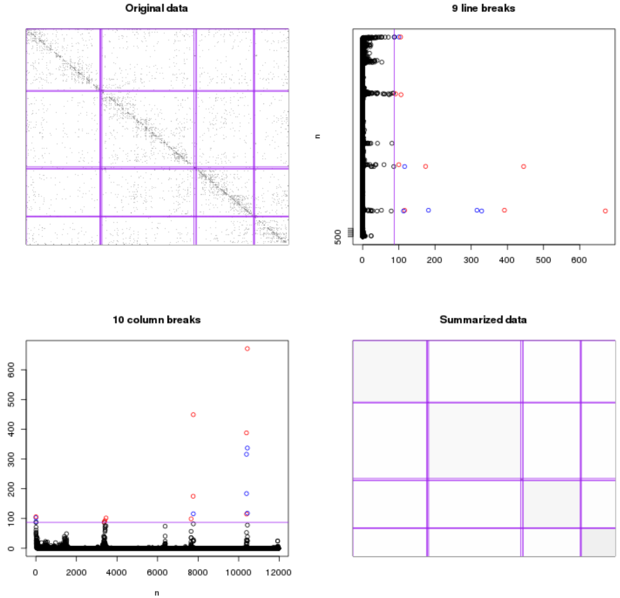

15%
Original data
7 line breaks
n
500
0 100 200 300 400 500 600
7 column breaks
600 500 400 300 200 100 0
0 2000 4000 6000 8000 10000 12000
n
Summarized data

14%

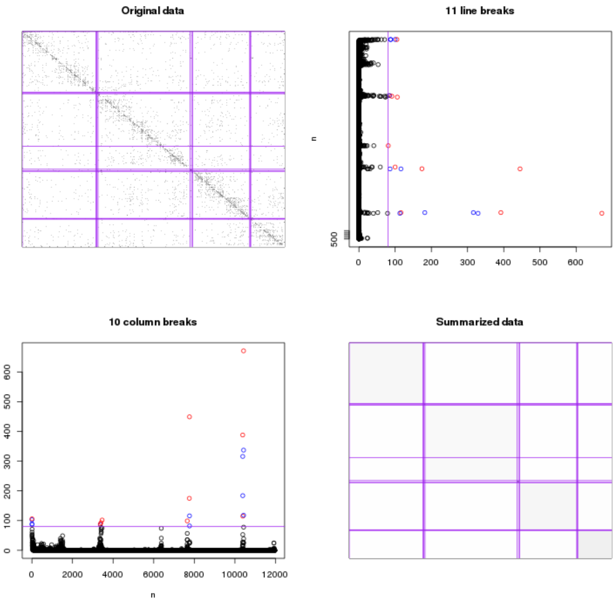


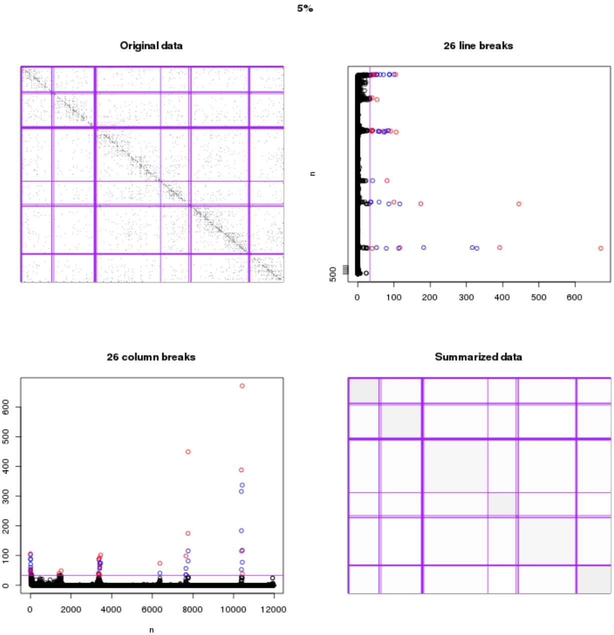
Original data
8 line breaks
n
500
0
100
200
300
400
500
600
8 column breaks
0
100
200
300
400
500
600
0
2000
4000
6000
8000
10000
12000
n
Summarized data

13%

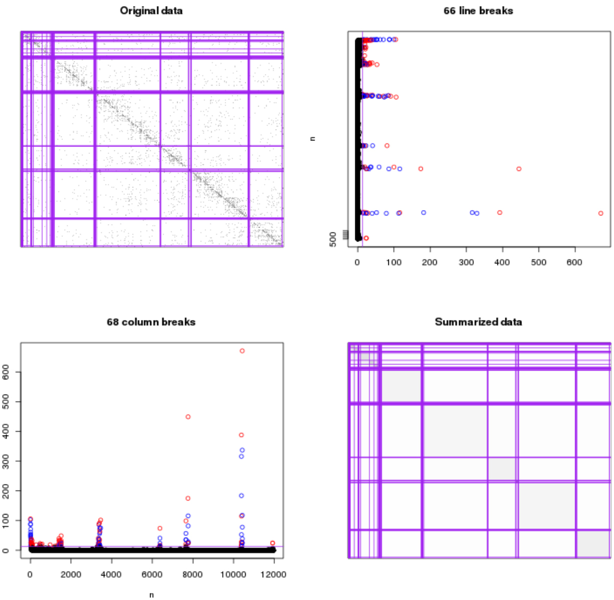

Original data
9 line breaks
n
500
0
100
200
300
400
500
600
10 column breaks
0
100
200
300
400
500
600
0
2000
4000
6000
8000
10000
12000
n
Summarized data

12%


Original data
11 line breaks
n
500
0
100
200
300
400
500
600
10 column breaks
0
100
200
300
400
500
600
0
2000
4000
6000
8000
10000
12000
n
Summarized data


5%
Original data
26 line breaks
n
500
0
100
200
300
400
500
600
26 column breaks
0
100
200
300
400
500
600
0
2000
4000
6000
8000
10000
12000
n
Summarized data

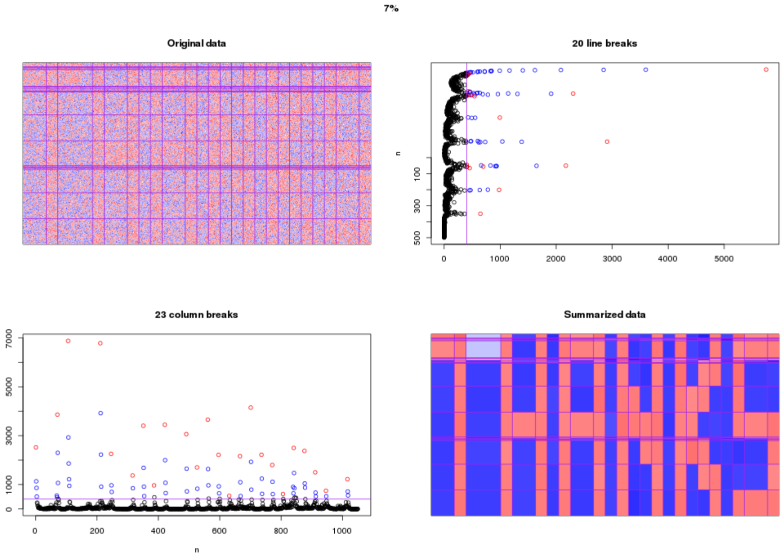
2%


Original data
66 line breaks
n
500
0
100
200
300
400
500
600
68 column breaks
0
2000
4000
6000
8000
10000
12000
n
Summarized data

Perspectives

- Theoretical result for model selection.
- Improvement of our package : *Blockseg*.
- Improvement 3D representation.
- Adaptation to symmetric matrices.
- More real datas.

Thank you for your attention



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Plan

6 Usual notations

7 Gray film

8 Optimization of the algorithm

9 Proof

Let $\mathbf{A} \in \mathcal{M}_{n\times m}(\mathbb{R})$ and $\mathbf{B} \in \mathcal{M}_{p\times q}(\mathbb{R})$ two matrices, the kronecker product of $\mathbf{A}$ and $\mathbf{B}$ is a matrix $(np) \times (mq)$ satisfying :

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} & \cdots & a_{2m}\mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1}\mathbf{B} & a_{n2}\mathbf{B} & \cdots & a_{nm}\mathbf{B} \end{pmatrix}$$

$$= \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & \cdots & a_{11}b_{1q} & a_{12}b_{11} & \cdots & \cdots & a_{1m}b_{11} & \cdots & a_{1m}b_{1q} \\ a_{11}b_{21} & a_{11}b_{22} & \cdots & a_{11}b_{2q} & a_{12}b_{21} & \cdots & \cdots & a_{1m}b_{21} & \cdots & a_{1m}b_{2q} \\ \vdots & \vdots & \ddots & \vdots & \vdots & & & \vdots & \ddots & \vdots \\ a_{11}b_{p1} & a_{11}b_{p2} & \cdots & a_{11}b_{pq} & a_{12}b_{p1} & \cdots & \cdots & a_{1m}b_{p1} & \cdots & a_{1m}b_{pq} \\ \vdots & \vdots & & \vdots & \vdots & \ddots & & \vdots & & \vdots \\ \vdots & \vdots & & \vdots & \vdots & & \ddots & \vdots & & \vdots \\ a_{n1}b_{11} & a_{n1}b_{12} & \cdots & a_{n1}b_{1q} & a_{n2}b_{11} & \cdots & \cdots & a_{nm}b_{11} & \cdots & a_{nm}b_{1q} \\ \vdots & \vdots & \ddots & \vdots & \vdots & & & \vdots & \ddots & \vdots \\ a_{n1}b_{p1} & a_{n1}b_{p2} & \cdots & a_{n1}b_{pq} & a_{n2}b_{p1} & \cdots & \cdots & a_{nm}b_{p1} & \cdots & a_{nm}b_{pq} \end{pmatrix}.$$

Return vectorisation

$$
\begin{aligned}
\mathcal{X} &= \mathbf{T} \otimes \mathbf{T} \\
&= \begin{pmatrix}
\mathbf{T} & 0 & 0 & \cdots & 0 \\
\mathbf{T} & \mathbf{T} & 0 & \cdots & 0 \\
\vdots & & \ddots & \ddots & \vdots \\
\vdots & & & \ddots & 0 \\
\mathbf{T} & \cdots & \cdots & & \mathbf{T}
\end{pmatrix}
\end{aligned}
$$

Return vectorisation

$\|u\|_2^2$ is defined for a vector u in $\mathbb{R}^N$ by

$$\|u\|_2^2 = \sum_{i=1}^{N} u_i^2$$

and $\|u\|_1$ is defined for a vector u in $\mathbb{R}^N$ by

$$\|u\|_1 = \sum_{i=1}^{N} |u_i|.$$

Return LASSO

Plan

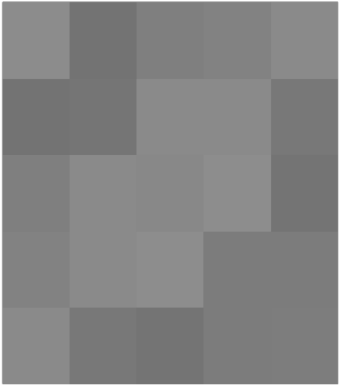
6 Usual notations

7 Gray film

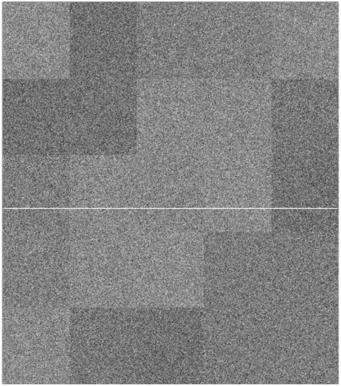
8 Optimization of the algorithm

9 Proof

Mu matrix



Orignal matrix



Colour version

Plan

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8 Optimization of the algorithm

9 Proof

By the form of $\mathcal{X}$, we have for all $\mathcal{V} \in \mathbb{R}^{n^2}$ with $\mathbf{v}$ the associated matrix

$$\mathcal{X}\mathcal{V} = \mathrm{Vec}\left[\left(\sum_{i'=1}^{i}\sum_{j'=1}^{j} v_{i',j'}\right)_{1\leq i,j\leq n}\right]$$

$$= \mathrm{Vec}\left[\begin{pmatrix} v_{1,1} & v_{1,1}+v_{1,2} & \cdots & \sum_{j=1}^{n} v_{1,j} \\ v_{1,1}+v_{2,1} & v_{1,1}+v_{2,1}+v_{1,2} & & \sum_{j=1}^{n} v_{1,j}+\sum_{j=1}^{n} v_{2,j} \\ \vdots & & \ddots & \vdots \\ \sum_{i=1}^{n} v_{i,1} & \sum_{i=1}^{n} v_{i,1}+\sum_{i=1}^{n} v_{i,2} & \cdots & \sum_{i=1}^{n}\sum_{j=1}^{n} v_{i,j} \end{pmatrix}\right]$$

Lemma :

For any vector $\mathcal{V} \in \mathbb{R}^{n^2}$, computing $\mathcal{X}\mathcal{V}$ and $\mathcal{X}^\top\mathcal{V}$ requires at worse $2n^2$ operations.

Return algo

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Return algo

Lemma :

Let $\mathcal{A} = \{a_1, \ldots, a_K\}$ and for each a in $\mathcal{A}$ let us consider the Euclidean division of $a - 1$ by n given by $a - 1 = nq_a + r_a$, then

$$\left((\mathcal{X}^\top \mathcal{X})_{\mathcal{A},\mathcal{A}}\right)_{1\leq k,\ell\leq K} = ((n - (q_{a_k} \vee q_{a_\ell})) \times (n - (r_{a_k} \vee r_{a_\ell})))_{1\leq k,\ell\leq K} .$$

Moreover, for any non empty subset $\mathcal{A}$ of distinct indices in $\{1, \ldots, n^2\}$, the matrix $\mathcal{X}_\mathcal{A}^\top \mathcal{X}_\mathcal{A}$ is invertible.

In some cases, we have the explicit form of $\left(\mathcal{X}_\mathcal{A}^\top \mathcal{X}_\mathcal{A}\right)^{-1}$.

Return algo

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In some cases, we have the explicit form of $\left(\mathcal{X}_{\mathcal{A}}^\top \mathcal{X}_{\mathcal{A}}\right)^{-1}$.

Return algo

Lemma :

Assume that we have at our disposal the Cholesky factorization of $\mathcal{X}_{\mathcal{A}}^{\top}\mathcal{X}_{\mathcal{A}}$.
The updated factorization on the extended set $\mathcal{A} \cup \{j\}$ only requires solving a $|\mathcal{A}|$-size triangular system, with complexity $\mathcal{O}(|\mathcal{A}|^2)$.
Moreover, the downdated factorization on the restricted set $\mathcal{A} \setminus \{j\}$ requires a rotation with negligible cost to preserve the triangular form of the Cholesky factorization after a column deletion.

Cholesky factorization Return algo

Cholesky factorization

Every positive-definite matrix $\mathbf{A} \in \mathcal{M}_{n\times n}(\mathbb{R})$ can be decompose in the product

$$\mathbf{A} = \mathbf{L}\mathbf{L}^\top$$

with $\mathbf{L}$ is a lower triangular matrix.

Return lemma

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Notations

$$I^\star_{\min} = \min_{0\leq k\leq K_1^\star} |t^\star_{1,k+1} - t^\star_{1,k}| \wedge \min_{0\leq k\leq K_2^\star} |t^\star_{2,k+1} - t^\star_{2,k}|,$$
$$J^\star_{\min} = \min_{1\leq k\leq K_1^\star, 1\leq \ell\leq K_2^\star+1} |\mu^\star_{k+1,\ell} - \mu^\star_{k,\ell}| \wedge \min_{1\leq k\leq K_1^\star+1, 1\leq \ell\leq K_2^\star} |\mu^\star_{k,\ell+1} - \mu^\star_{k,\ell}|,$$

which corresponds to the smallest length between two consecutive change-points and to the smallest jump size between two consecutive blocks, respectively.

Return theorem

Assumption

(A1) The random variables $(E_{i,j})_{\substack{1\leq i\leq n_1 \\ 1\leq j\leq n_2}}$ are iid zero mean random variables such that there exists a positive constant β such that for all ν in $\mathbb{R}$, $\mathbb{E}[\exp(\nu E_{1,1})] \leq \exp(\beta\nu^2)$.

(A2) The sequence (δ_{n_1,n_2}) is a non increasing and positive sequence tending to zero such that $n_1\delta_{n_1,n_2}{J^\star_{\min}}^2/\log(n_2) \to \infty$ and $n_2\delta_{n_1,n_2}{J^\star_{\min}}^2/\log(n_1) \to \infty$, as n_1 and n_2 tends to infinity.

(A3) The sequence (λ_{n_1,n_2}) is such that $(n_1\delta_{n_1,n_2}J^\star_{\min})^{-1}\lambda_{n_1,n_2} \to 0$ and $(n_2\delta_{n_1,n_2}J^\star_{\min})^{-1}\lambda_{n_1,n_2} \to 0$, as n_1 and n_2 tends to infinity.

(A4) $I^\star_{\min} \geq n_1\delta_{n_1,n_2}$ and $I^\star_{\min} \geq n_2\delta_{n_1,n_2}$.

Return theorem

Lemma

Let $(Y_{i,j})_{\substack{1\leq i\leq n_1\\1\leq j\leq n_2}}$ the data matrix. Then, $\widehat{\mathcal{U}} = \mathcal{X}\widehat{\mathcal{B}}$ is such that

$$\sum_{k=r_a+1}^{n_1}\sum_{\ell=q_a+1}^{n_2} Y_{k,\ell} - \sum_{k=r_a+1}^{n_1}\sum_{\ell=q_a+1}^{n_2} \widehat{\mathcal{U}}_{k,\ell} = \frac{\lambda_{n_1,n_2}}{2}\mathrm{sign}(\widehat{\mathcal{B}}_a), \text{ if } \widehat{\mathcal{B}}_a \neq 0,$$

$$\left|\sum_{k=r_a+1}^{n_1}\sum_{\ell=q_a+1}^{n_2} Y_{k,\ell} - \sum_{k=r_a+1}^{n_1}\sum_{\ell=q_a+1}^{n_2} \widehat{\mathcal{U}}_{k,\ell}\right| \leq \frac{\lambda_{n_1,n_2}}{2}, \text{ if } \widehat{\mathcal{B}}_a = 0,$$

where $(a-1) = nq_a + r_a$.

Return theorem

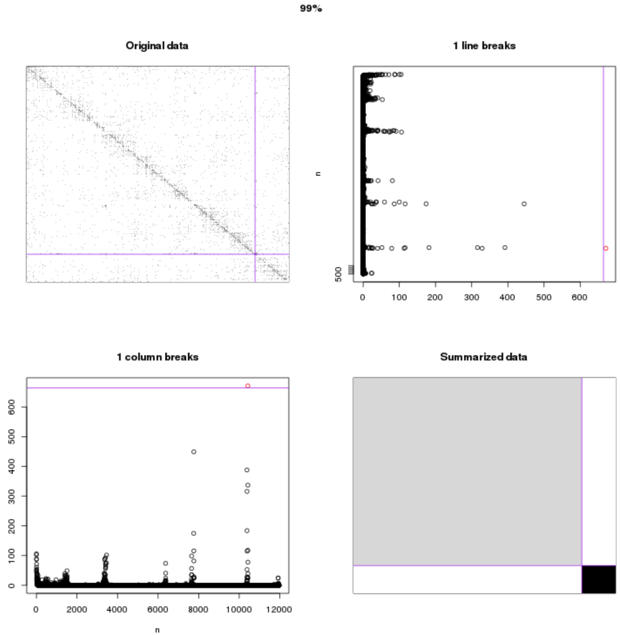
Lemma

Let $(E_{i,j})_{\substack{1\le i\le n_1\\1\le j\le n_2}}$ be random variables satisfying (A1). Let also (v_{n_1,n_2}) and (x_{n_1,n_2}) be two positive sequences such that $v_{n_1,n_2}x^2_{n_1,n_2}/\log(n_2)\to\infty$, then

$$\mathbb{P}\left(\max_{\substack{1\le r_{n_1,n_2}<s_{n_1,n_2}\le n_2\\|r_{n_1,n_2}-s_{n_1,n_2}|\ge v_{n_1,n_2}}}\left|(s_{n_1,n_2}-r_{n_1,n_2})^{-1}\sum_{j=r_n}^{s_n-1}E_{n,j}\right|\ge x_{n_1,n_2}\right)\underset{n_1,n_2\to\infty}{\longrightarrow}0,$$

the result remaining valid if $E_{n,j}$ is replaced by $E_{j,n}$.

Return theorem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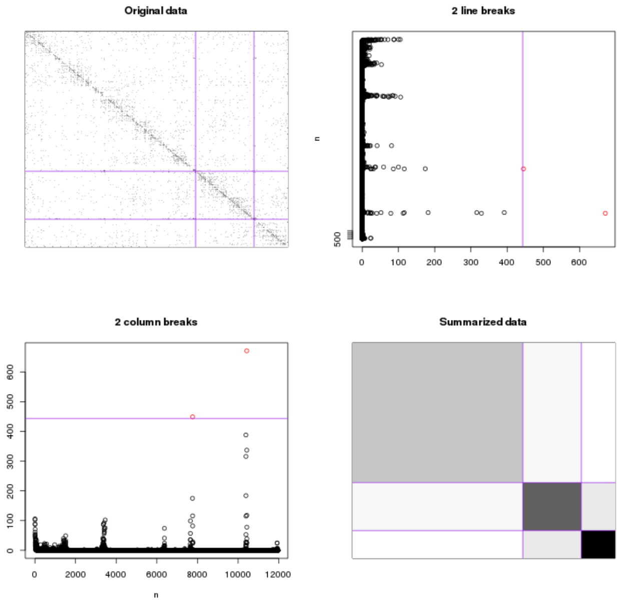
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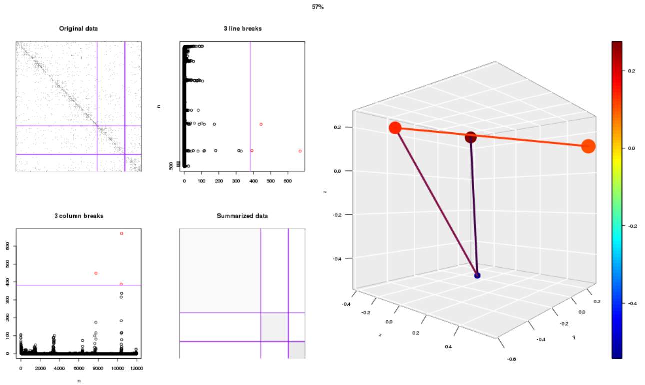
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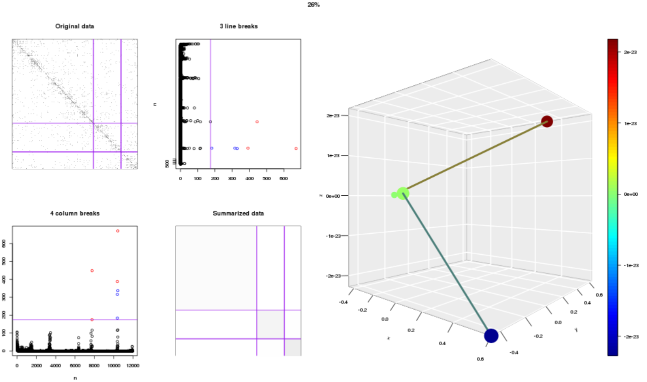
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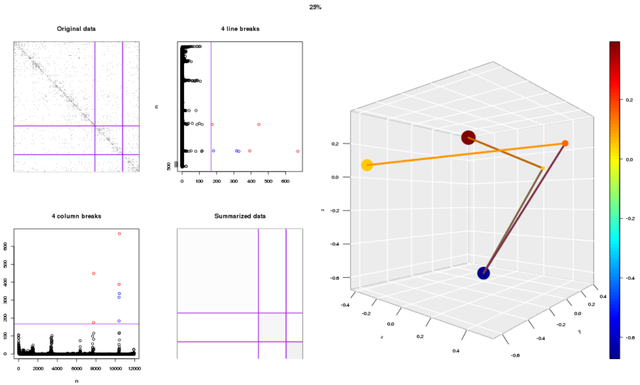
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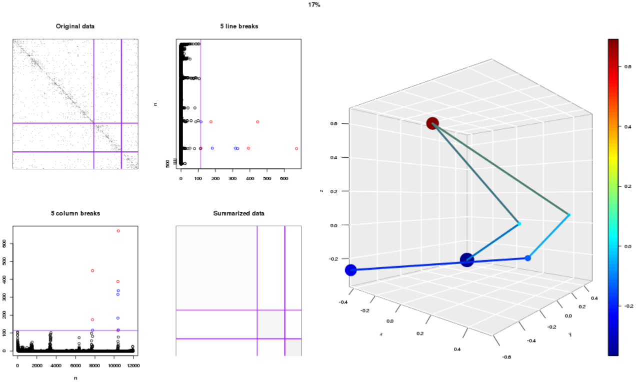
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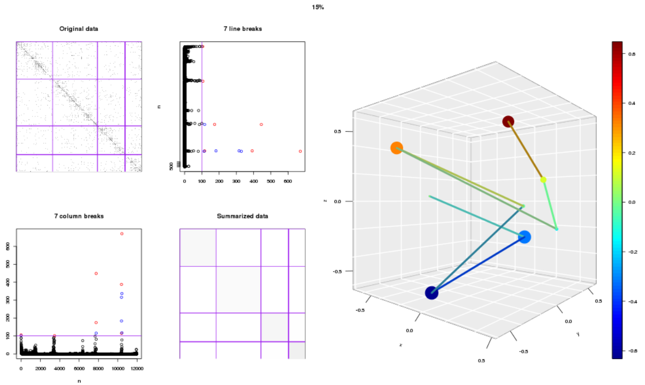
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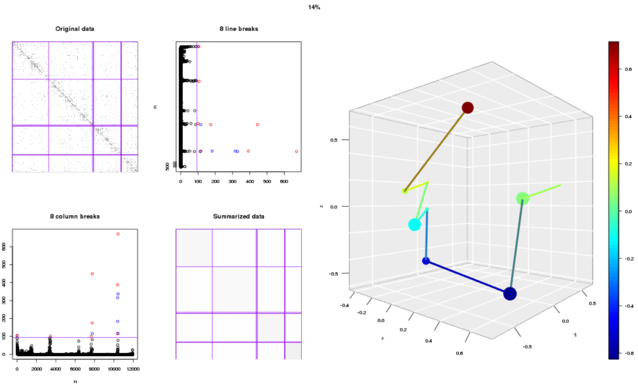
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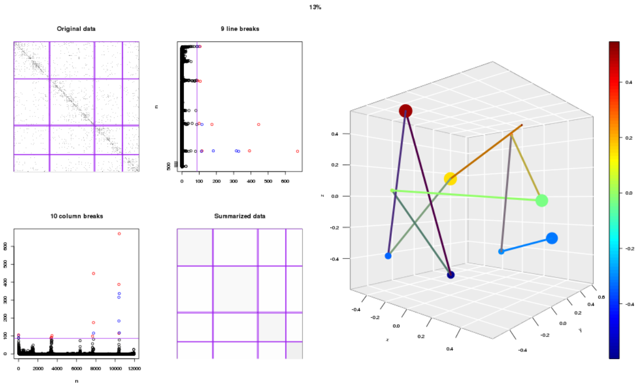
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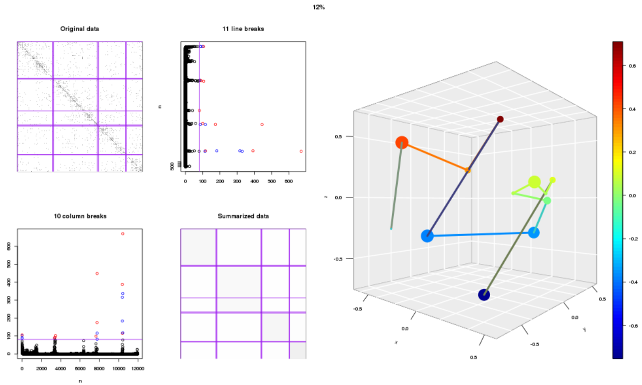
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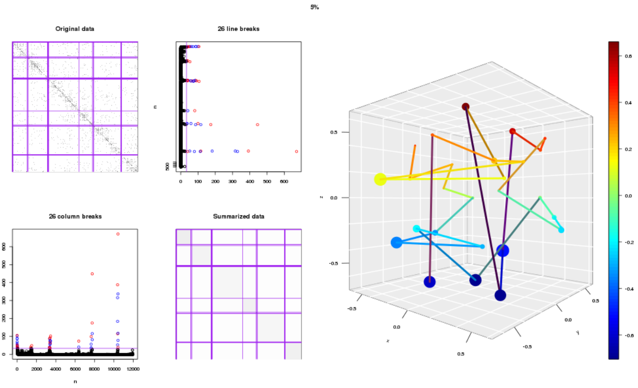
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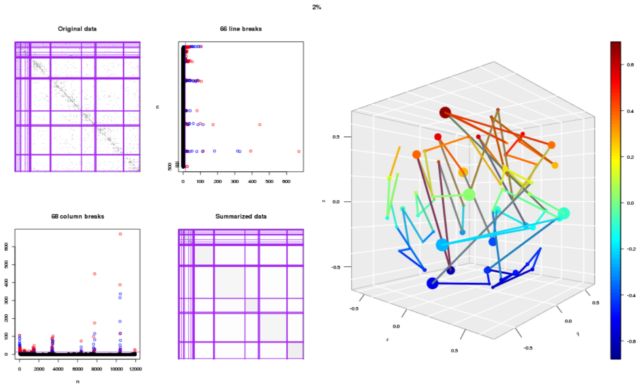
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