18th International Joint Conference CFE-CMStatistics
Computational and Methodological Statistics (CMStatistics 2024)
Computational and Financial Econometrics (CFE 2024)
14-16 December 2024, King's College London, UK

BLOCK TESTING IN COVARIANCE AND PRECISION MATRICES FOR FUNCTIONAL DATA ANALYSIS

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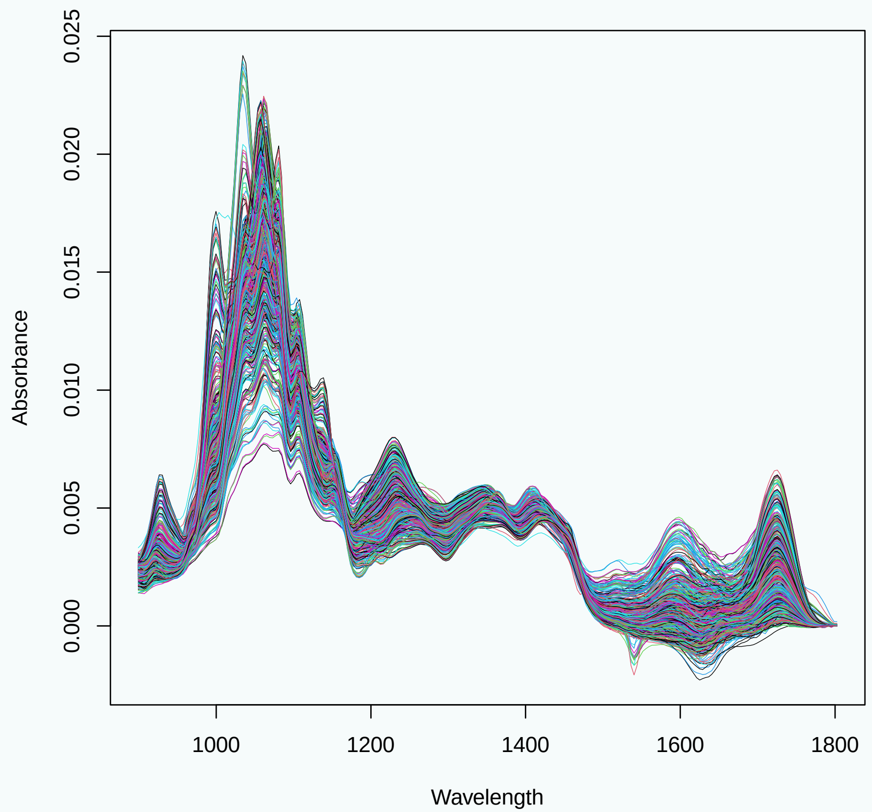
MOTIVATION

- **Infrared spectroscopy**: a technique used to study the composition of a mixture.
- Data are infrared spectra, which can be seen as continuous functions of the wavelength.
- The different parts of the signal are related to the mixture components.
- We are particularly interested in the dependency structure of data along the domain, to understand if the different components are related between each other.

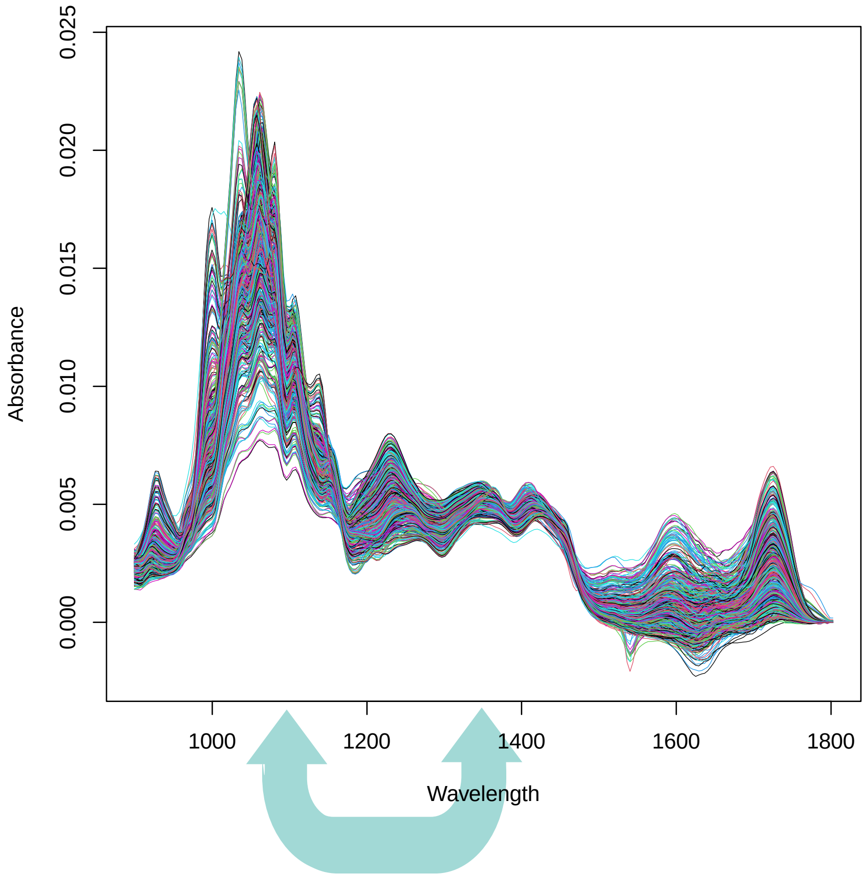
Example: fruit purees spectra



MOTIVATION

- **Aim**: to test (conditional) independence between different parts of the functions' domain.

Example: fruit purees spectra



MOTIVATION

- **Aim**: to test (conditional) independence between different parts of the functions' domain.
- Assumption 1: the domain can be partitioned into regions of interest.

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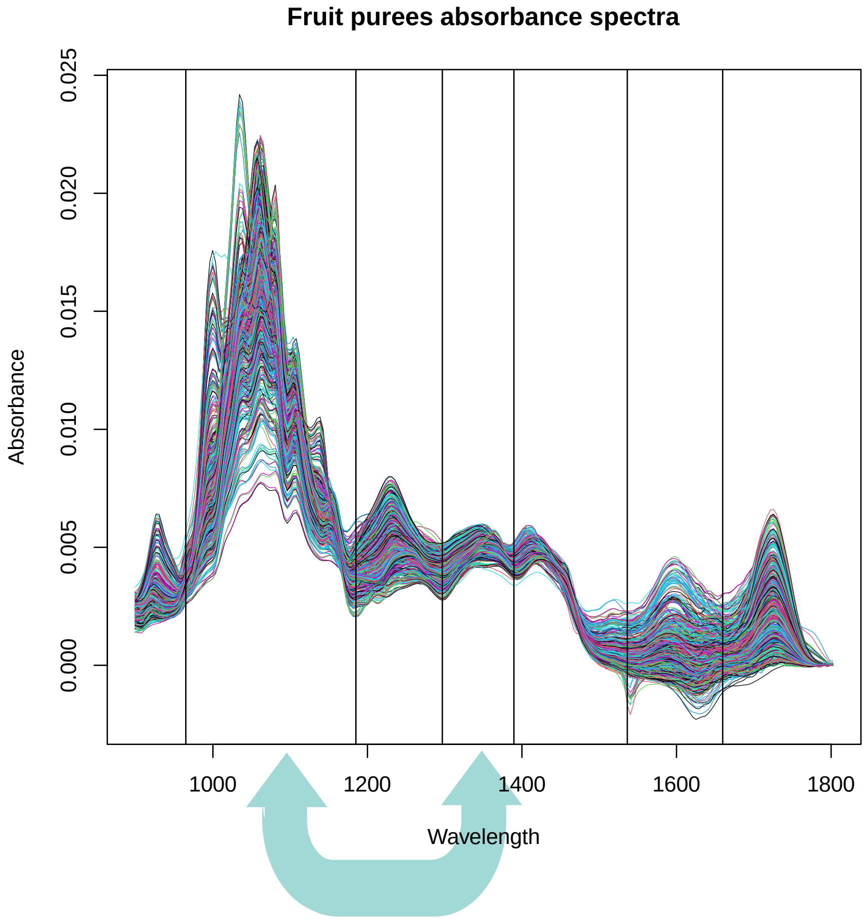
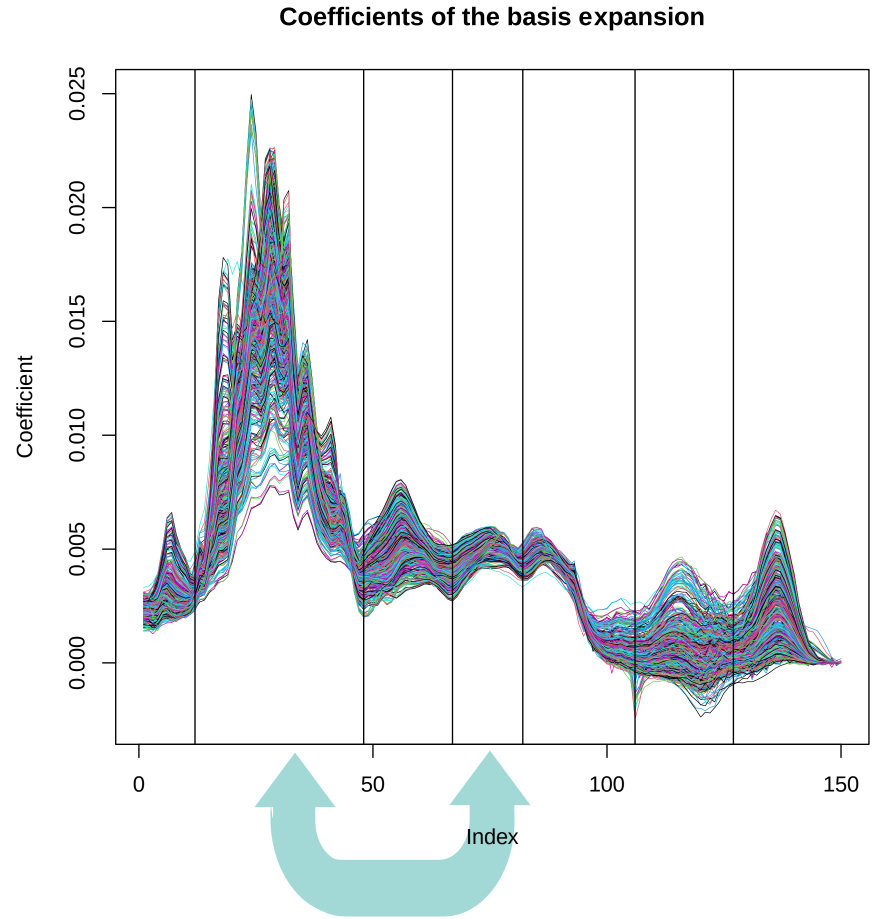
Example: fruit purees spectra



MOTIVATION

- **Aim**: to test (conditional) independence between different parts of the functions' domain.
- Assumption 1: the domain can be partitioned into regions of interest.
- Assumption 2: data can be described with a B-splines basis expansion.
  - Coefficients are directly related to the parts of the domain.
  - A significant dependence between basis coefficients translates into a significant dependence between parts of the domain.

Example: fruit purees spectra



MOTIVATION

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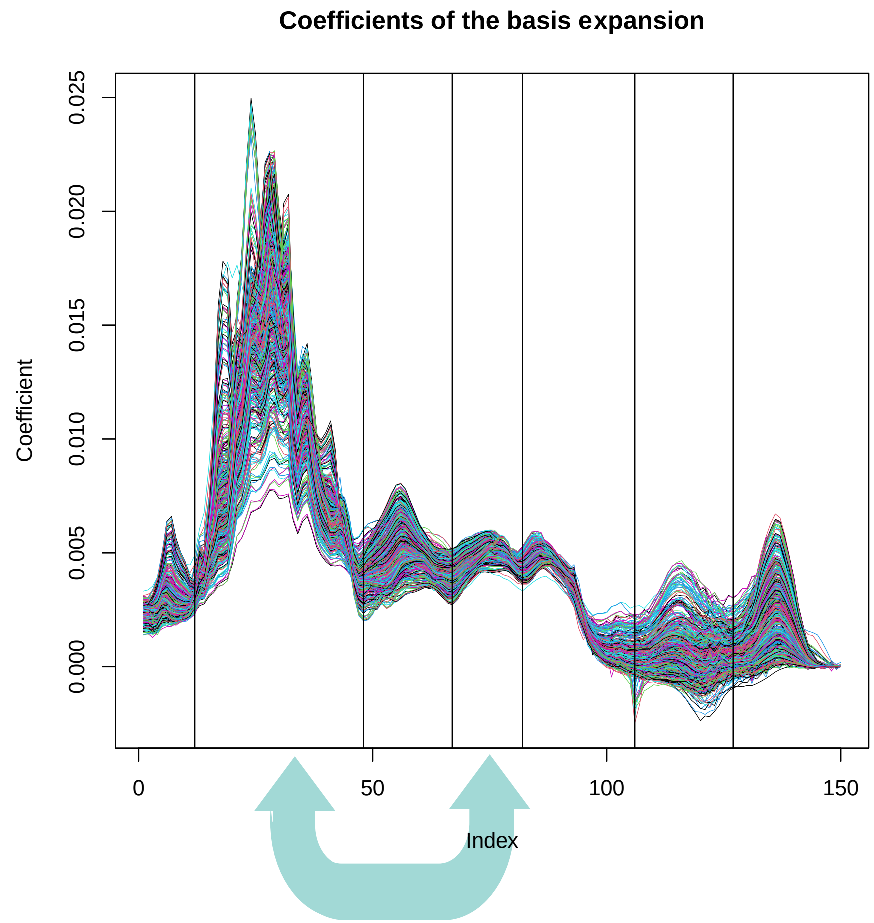
- Assumption 1: the domain can be partitioned into regions of interest.
- Assumption 2: data can be described with a B-splines basis expansion.
  - Coefficients are directly related to the parts of the domain.
  - A significant dependence between basis coefficients translates into a significant dependence between parts of the domain.
- We look at the block structure of the covariance matrix (precision matrix) of the basis coefficients.

Example: fruit purees spectra

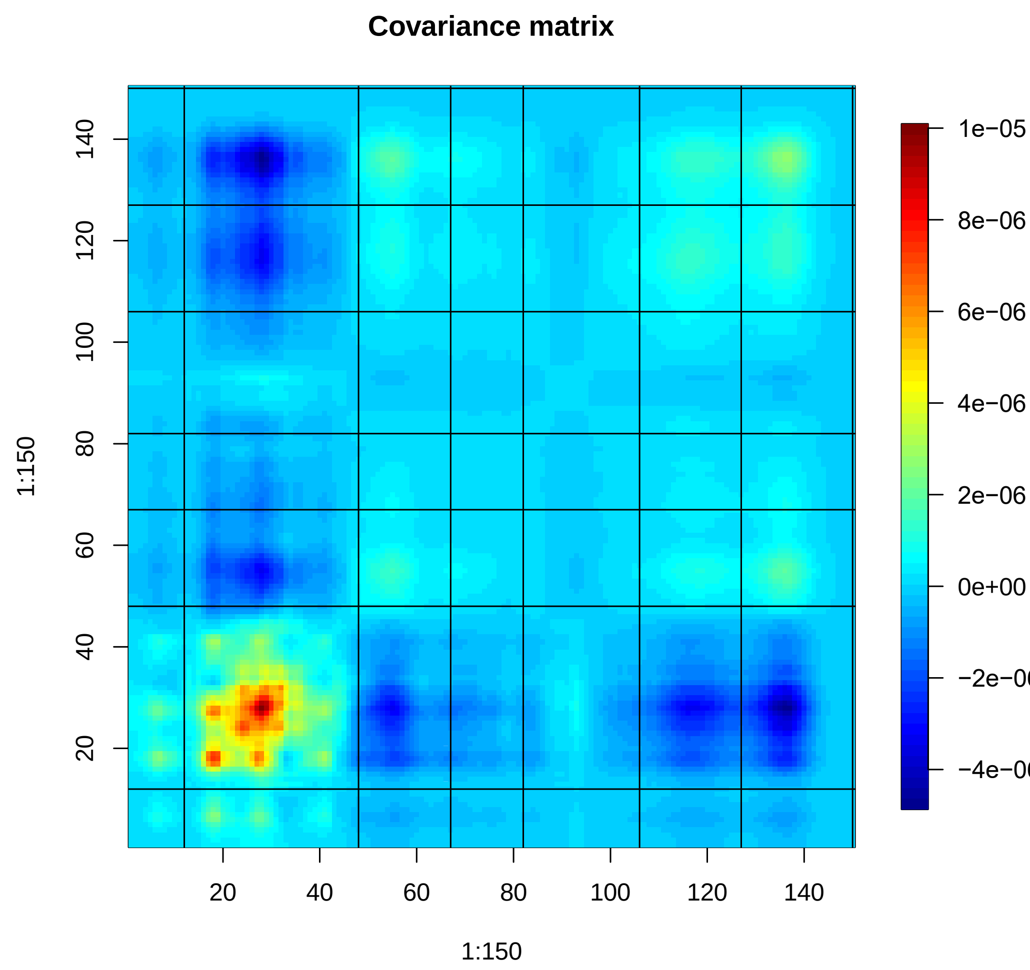


INTUITION

Linear dependence between two RoI

⇕

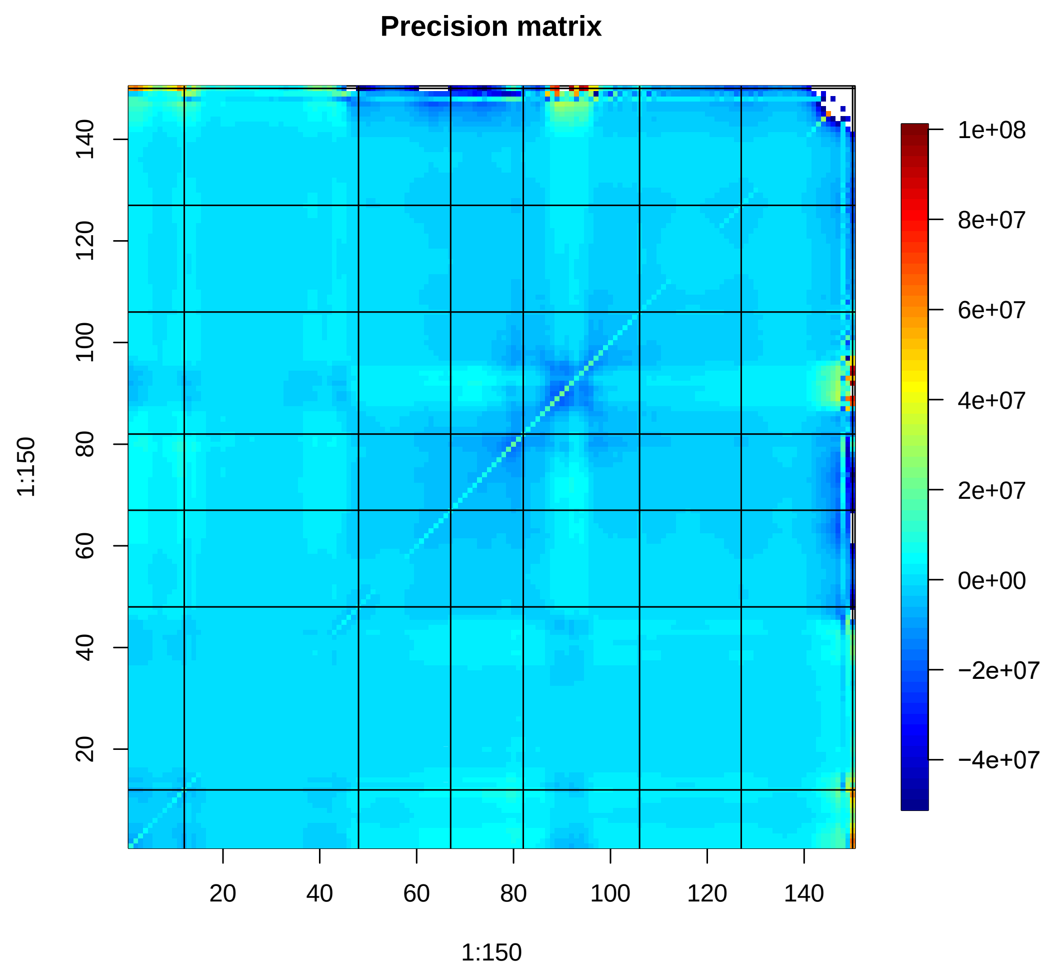
Block of the covariance matrix ≠ 0



INTUITION

Conditional linear dependence between two RoI

Block of the precision matrix ≠ 0



Estimator proposed by Xia et al. (2018)

THE MODEL

Functional data. We assume to observe functional data in $L^2(D)$ with $D \subset \mathbb{R}$

$$\mathbf{X}_1(t), \ldots, \mathbf{X}_n(t) \qquad t \in D, \mathbf{X}_i \in L^2(D)$$

Basis expansion.

$$\mathbf{X}_i(t) = \sum_{j=1}^{p} \phi_j(t) C_{ij} \qquad (\mathbf{X}_1, \ldots, \mathbf{X}_n) \Rightarrow (\mathbf{C}_1, \ldots, \mathbf{C}_n)$$

Blocks. The coefficients $\{C_{ij}\}$ are partitioned into M blocks, associated to different RoI:

$$\mathcal{J}_1, \ldots \mathcal{J}_M \subset \{1, \ldots, p\}$$

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Blocks. The coefficients $\{C_{ij}\}$ are partitioned into M blocks, associated to different RoI:

$$\mathcal{J}_1, \dots \mathcal{J}_M \subset \{1, \dots, p\}$$

1. Test for a single block of the covariance (precision) matrix
2. Adjustment for taking into account block multiplicity

TEST ON A BLOCK OF THE COVARIANCE MATRIX

Permutation test of linear independence between coefficients in blocks $\mathcal{J}_m$ and $\mathcal{J}_{m'}$:

$$H_{0,m,m'} : \mathbf{C}_{\mathcal{J}_m'}, \mathbf{C}_{\mathcal{J}_m'} \text{ are independent} \qquad H_{1,m,m'} : \Sigma_{\mathcal{J}_m \times \mathcal{J}_m'} \neq 0$$

TEST ON A BLOCK OF THE COVARIANCE MATRIX

Permutation test of linear independence between coefficients in blocks $\mathcal{J}_m$ and $\mathcal{J}_{m'}$:

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- **Test statistic:**

$$T_{mm'} = \sum_{j \in \mathcal{J}_m, j' \in \mathcal{J}_{m'}} \left(\frac{\widehat{\Sigma}_{jj'}}{\sqrt{\widehat{\Sigma}_{jj} \widehat{\Sigma}_{j'j'}}} \right)^2$$

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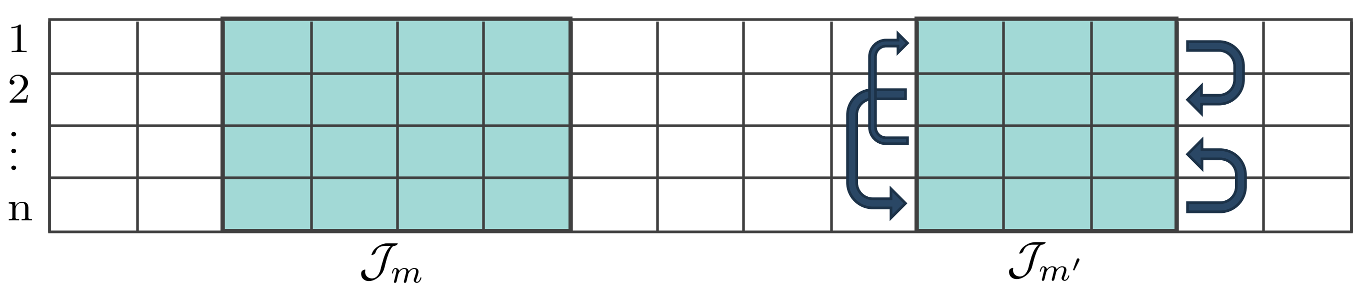
- **Permutations:** $n!$ permutations of the coefficients C_{ij} $j \in \mathcal{J}_m$ keeping C_{ij} $j \in \mathcal{J}_{m'}$ fixed, (or vice-versa).



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- **Permutations:** $n!$ permutations of the coefficients C_{ij} $j \in \mathcal{J}_m$ keeping C_{ij} $j \in \mathcal{J}_{m'}$ fixed, (or vice-versa).

- **p-value:**

$$p_{m,m'} = \frac{\#\{T^*_{mm'} \geq T_{mm'}\}}{n!}$$

Test statistic evaluated on original data

Test statistic evaluated on permuted data

THEORETICAL PROPERTIES: TEST ON COVARIANCE MATRIX

- *The test of linear independence is* ***exact****, but it might be* ***not consistent under general alternatives*** *(e.g., when the dependence is not linear):*

$$\mathbb{P}_{H_{0,m,m'}}[p_{m,m'} \leq \alpha] = \alpha$$
$$\lim_{n\to\infty} \mathbb{P}_{H_{1,m,m'}}[p_{m,m'} \leq \alpha] = 1$$
$$\lim_{n\to\infty} \mathbb{P}_{H^C_{0,m,m'}}[p_{m,m'} \leq \alpha] \leq 1$$

- *For Gaussian data: the test of linear independence is a test for independence. It is* ***exact*** *for any sample size and* ***consistent*** *under every alternative.*

$$\mathbb{P}_{H_{0,m,m'}}[p_{m,m'} \leq \alpha] = \alpha$$
$$\lim_{n\to\infty} \mathbb{P}_{H_{1,m,m'}}[p_{m,m'} \leq \alpha] = 1$$
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TEST ON A BLOCK OF THE PRECISION MATRIX

Permutation test of conditional linear independence between coefficients in blocks $\mathcal{J}_m$ and $\mathcal{J}_{m'}$:

$$H_{0,m,m'} : \begin{cases} \mathbf{C}_{\mathcal{J}_m} = \mathbf{C}_{\{1,\dots,p\}\setminus(\mathcal{J}_m \cup \mathcal{J}_{m'})}\mathbf{A} + \boldsymbol{\varepsilon}_{\mathcal{J}_m} \\ \mathbf{C}_{\mathcal{J}_{m'}} = \mathbf{C}_{\{1,\dots,p\}\setminus(\mathcal{J}_m \cup \mathcal{J}_{m'})}\mathbf{A}' + \boldsymbol{\varepsilon}_{\mathcal{J}_{m'}} \\ \boldsymbol{\varepsilon}_{\mathcal{J}_m}, \boldsymbol{\varepsilon}_{\mathcal{J}_{m'}} \quad \text{independent} \end{cases} \qquad H_{1,m,m'} = \boldsymbol{\Omega}_{\mathcal{J}_m \times \mathcal{J}_{m'}} \neq 0$$

TEST ON A BLOCK OF THE PRECISION MATRIX

Permutation test of conditional linear independence between coefficients in blocks $\mathcal{J}_m$ and $\mathcal{J}_{m'}$:

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- **Test statistic:**

$$T_{mm'} = \sum_{j \in \mathcal{J}_m, j' \in \mathcal{J}_{m'}} \left(\widehat{\boldsymbol{\Omega}}_{jj'}\right)^2$$

- Xia Y., Cai T., Cai T.T. Multiple testing of submatrices of a precision matrix with applications to identification of between pathway interactions J. Am Stat. Assoc., 113(521), 328–339 (2018).

TEST ON A BLOCK OF THE PRECISION MATRIX

Permutation test of conditional linear independence between coefficients in blocks $\mathcal{J}_m$ and $\mathcal{J}_{m'}$:

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- **Test statistic:**

$$T_{mm'} = \sum_{j \in \mathcal{J}_m, j' \in \mathcal{J}_{m'}} \left(\widehat{\boldsymbol{\Omega}}_{jj'}\right)^2$$

- **Permutations**~~: $n!$ permutations of the coefficients C_{ij} $j \in \mathcal{J}_m$ keeping C_{ij} $j \in \mathcal{J}_{m'}$ fixed, (or vice-versa).~~

Data are no longer independent under H_0!

TEST ON A BLOCK OF THE PRECISION MATRIX

Permutation test of conditional linear independence between coefficients in blocks $\mathcal{J}_m$ and $\mathcal{J}_{m'}$:

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- **Test statistic:**

$$T_{mm'} = \sum_{j \in \mathcal{J}_m, j' \in \mathcal{J}_{m'}} \left(\widehat{\boldsymbol{\Omega}}_{jj'}\right)^2$$

Under the null hypothesis the errors of those two linear models are exchangeable:

$$\mathbf{C}_{\mathcal{J}_m} = \mathbf{C}_{\{1,\dots,p\}\setminus(\mathcal{J}_m \cup \mathcal{J}_{m'})}\mathbf{A} + \boldsymbol{\varepsilon}_{\mathcal{J}_m}$$
$$\mathbf{C}_{\mathcal{J}_{m'}} = \mathbf{C}_{\{1,\dots,p\}\setminus(\mathcal{J}_m \cup \mathcal{J}_{m'})}\mathbf{A}' + \boldsymbol{\varepsilon}_{\mathcal{J}_{m'}}$$

- **Permutations:** $n!$ permutations of the residuals $\widehat{\boldsymbol{\varepsilon}}_{ij}$ $j \in \mathcal{J}_m$ keeping $\widehat{\boldsymbol{\varepsilon}}_{ij}$ $j \in \mathcal{J}_{m'}$ fixed, (or vice-versa).

TEST ON A BLOCK OF THE PRECISION MATRIX

Permutation test of conditional linear independence between coefficients in blocks $\mathcal{J}_m$ and $\mathcal{J}_{m'}$:

$$H_{0,m,m'}: \begin{cases} \mathbf{C}_{\mathcal{J}_m} = \mathbf{C}_{\{1,\dots,p\}\setminus(\mathcal{J}_m \cup \mathcal{J}_{m'})}\mathbf{A} + \boldsymbol{\varepsilon}_{\mathcal{J}_m} \\ \mathbf{C}_{\mathcal{J}_{m'}} = \mathbf{C}_{\{1,\dots,p\}\setminus(\mathcal{J}_m \cup \mathcal{J}_{m'})}\mathbf{A}' + \boldsymbol{\varepsilon}_{\mathcal{J}_{m'}} \\ \boldsymbol{\varepsilon}_{\mathcal{J}_m}, \boldsymbol{\varepsilon}_{\mathcal{J}_{m'}} \quad \text{independent} \end{cases} \qquad H_{1,m,m'} = \boldsymbol{\Omega}_{\mathcal{J}_m \times \mathcal{J}_{m'}} \neq 0$$

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- **Permutations:** $n!$ permutations of the residuals $\widehat{\boldsymbol{\varepsilon}}_{ij}$ $j \in \mathcal{J}_m$ keeping $\widehat{\boldsymbol{\varepsilon}}_{ij}$ $j \in \mathcal{J}_{m'}$ fixed, (or vice-versa).

- **p-value:**

$$p = \frac{\#\{T^*_{mm'} \geq T_{mm'}\}}{n!}$$

THEORETICAL PROPERTIES: TEST ON PRECISION MATRIX

- *The test of conditional linear independence is* ***asymptotically exact*** *and* ***consistent****. However, only linear conditional independence is tested (which can not be generalized to conditional independence).*

$$\lim_{n\to\infty} \mathbb{P}_{H_{0,m,m'}}[p_{m,m'} \leq \alpha] = \alpha$$
$$\lim_{n\to\infty} \mathbb{P}_{H_{1,m,m'}}[p_{m,m'} \leq \alpha] = 1$$

- *For Gaussian data: the test of conditional linear independence is a test for conditional independence. It is* ***asymptotically exact*** *and* ***consistent*** *under every alternative.*

MULTIPLE TESTING OF SUBMATRICES

The total number of tests is **M(M-1)/2**. So, we need to adjust p-values.

Available methods include Bonferroni adjustment (Holm, 1976), Closed Testing Procedure (Marcus et al, 1976), or methods specifically designed for the precision matrix (Xia et al. 2018):

generally very conservative;

do not exploit the proximity structure between blocks.

Instead, we generalize the interval-wise testing procedure (Pini and Vantini, 2016, 2017), a method to adjust for multiplicity controlling the FWER over closed sub-intervals of the domain.

- Holm, S.: A simple sequentially rejective multiple test procedure Scand. J. Stat., 6(2), 65–70 (1979)
- Marcus, R., Eric, P., & Gabriel, K. R. On closed testing procedures with special reference to ordered analysis of variance. *Biometrika*, *63*(3), 655-660 (1976).
- Pini, A. and Vantini, S. The interval testing procedure: a general framework for inference in functional data analysis Biometrics 72(3) 835–845 (2016).
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MULTIPLE TESTING OF SUBMATRICES

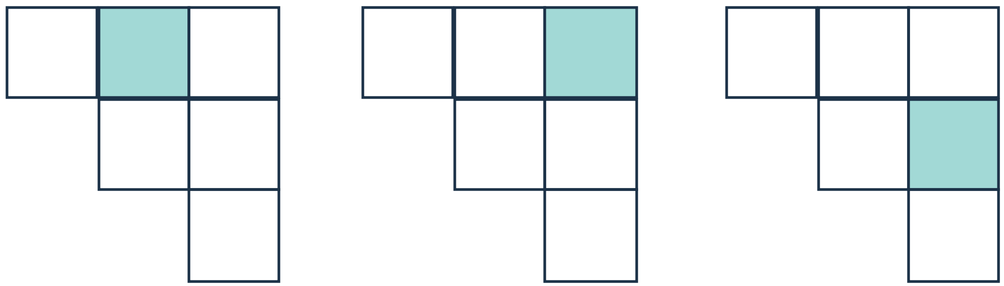
1. Perform a test on each couple of blocks.
2. Perform a tests on each couple of non-overlapping intervals of blocks.
3. For each couple of blocks $\mathcal{J}_m$ and $\mathcal{J}_{m'}$, compute the adjusted p-value as the maximum between all p-values of tests of intervals of blocks including $\mathcal{J}_m$ and $\mathcal{J}_{m'}$ (including blocks $\mathcal{J}_m$ and $\mathcal{J}_{m'}$ themselves).

$$\tilde{p}_{m,m'} = \max_{\substack{\mathcal{I}:m\in\mathcal{I} \\ \mathcal{I}':m'\in\mathcal{I}'}} p_{\mathcal{I},\mathcal{I}'}$$

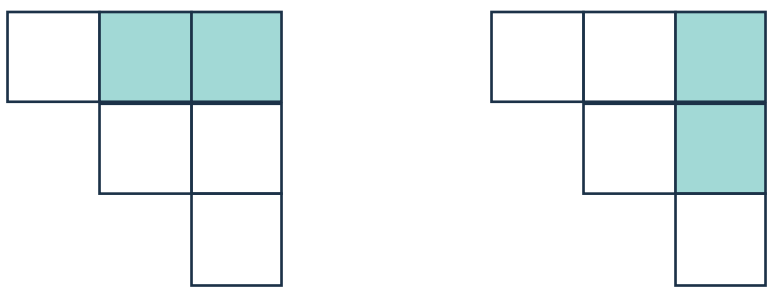
MULTIPLE TESTING OF SUBMATRICES

Example: three RoI

- Performed tests:



$H_{0_{1,2}}$ $H_{1_{1,2}}$ $H_{0_{1,3}}$ $H_{1_{1,3}}$ $H_{0_{2,3}}$ $H_{1_{2,3}}$



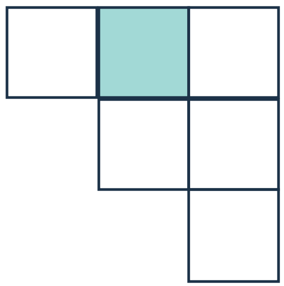
$H_{0_{1,(2,3)}}$ $H_{1_{1,(2,3)}}$ $H_{0_{(1,2),3}}$ $H_{1_{(1,2),3}}$

All tests can be performed with the same procedure described earlier

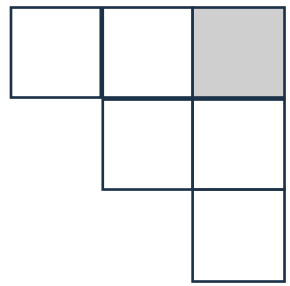
MULTIPLE TESTING OF SUBMATRICES

Example: three RoI

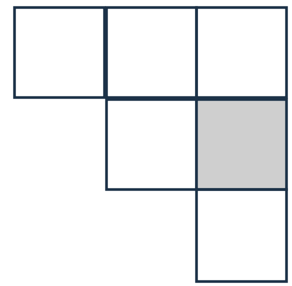
- Performed tests
- Adjusted p-value for couple (1,2):



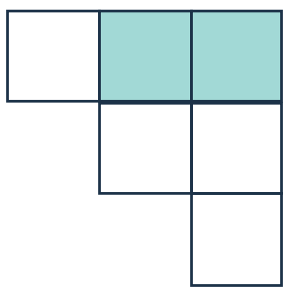
$H_{0_{1,2}}$ $H_{1_{1,2}}$



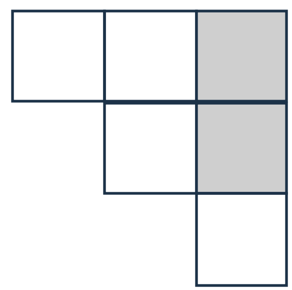
$H_{0_{1,3}}$ $H_{1_{1,3}}$



$H_{0_{2,3}}$ $H_{1_{2,3}}$



$H_{0_{1,(2,3)}}$ $H_{1_{1,(2,3)}}$



$H_{0_{(1,2),3}}$ $H_{1_{(1,2),3}}$

THEORETICAL PROPERTIES OF THE PROCEDURE

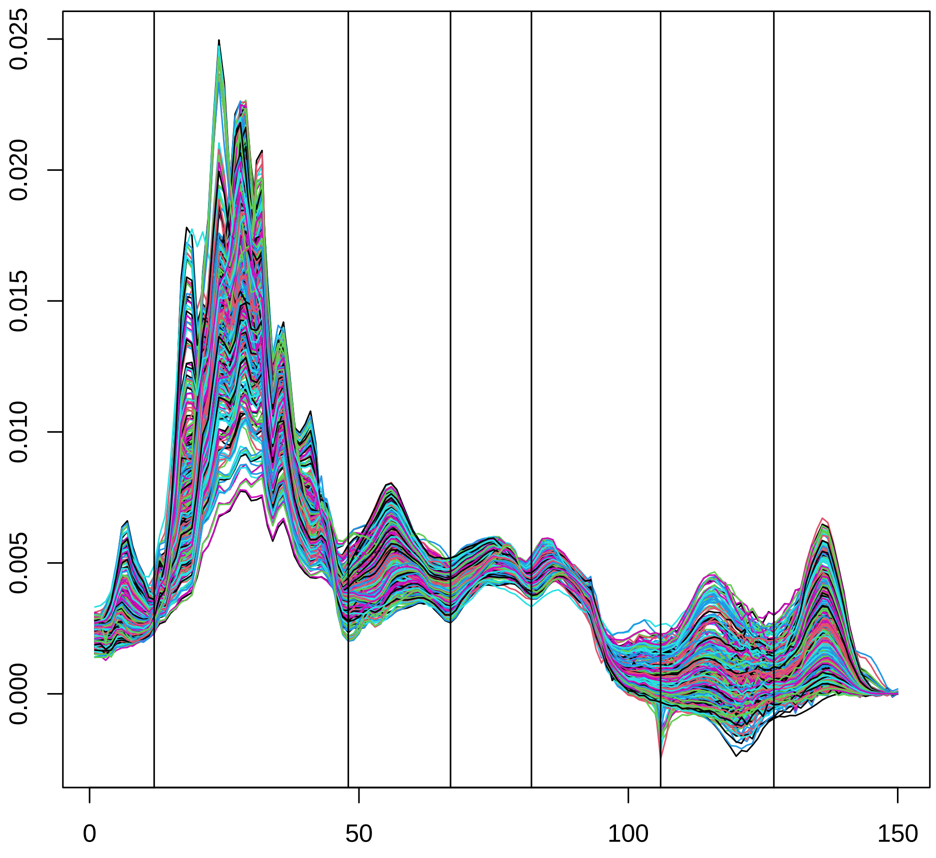
Theorem 1 *The adjusted p-value $\tilde{p}_{m,m'}$ is provided with the following error control: for all non-overlapping intervals of blocks $\mathcal{J}_{\mathcal{I}} = \cup_{i=m}^{m+h}\{\mathcal{J}_i\}$ and $\mathcal{J}_{\mathcal{I}'} = \cup_{i=m'}^{m'+h'}\{\mathcal{J}_i\}$, with $1 \leq m \leq m+h < m' \leq m'+h' \leq M$, $\forall \alpha \in (0,1)$*

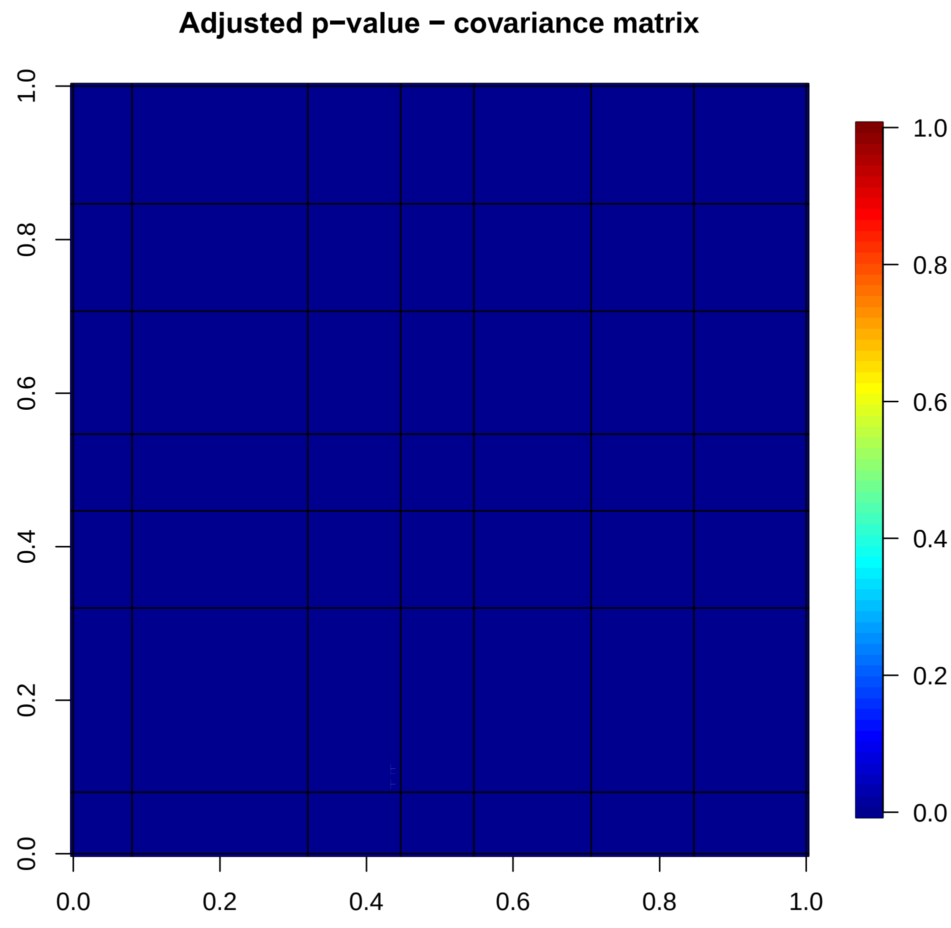
$$\text{if } H_{0,m,m'} \text{ is true } \forall (m,m') \in \mathcal{I} \times \mathcal{I}',$$
$$\limsup_{n \to \infty} \mathbb{P}\left[\exists (m,m') \in \mathcal{I} \times \mathcal{I}' : \tilde{p}_{m,m'} \leq \alpha\right] \leq \alpha.$$

Theorem 2 *The adjusted p-value $\tilde{p}_{m,m'}$ is consistent, that is: for all non-overlapping intervals of blocks $\mathcal{J}_{\mathcal{I}} = \cup_{i=m}^{m+h}\{\mathcal{J}_i\}$ and $\mathcal{J}_{\mathcal{I}'} = \cup_{i=m'}^{m'+h'}\{\mathcal{J}_i\}$, with $1 \leq m \leq m+h < m' \leq m'+h' \leq M$, $\forall \alpha \in (0,1)$*

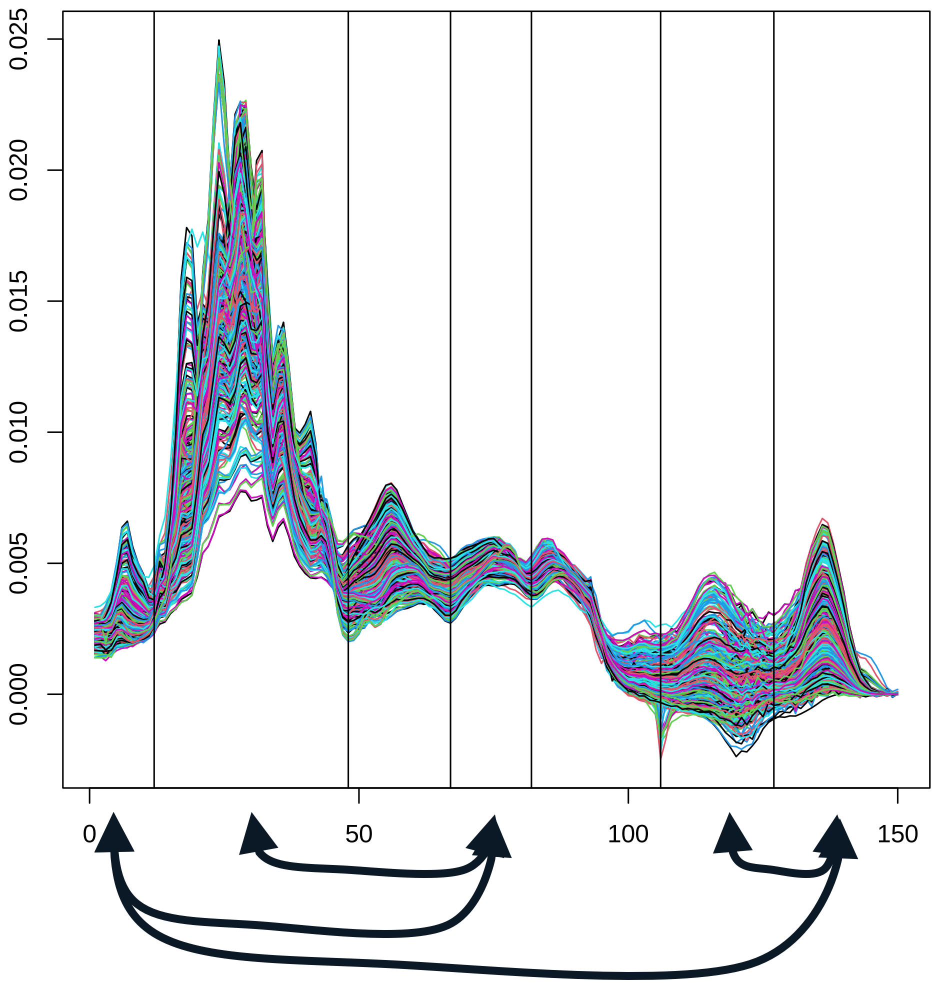
$$\text{if } H_{0,m,m'} \text{ is false } \forall (m,m') \in \mathcal{I} \times \mathcal{I}',$$
$$\lim_{n \to \infty} \mathbb{P}\left[\forall (m,m') \in \mathcal{I} \times \mathcal{I}' : \tilde{p}_{m,m'} \leq \alpha\right] = 1.$$

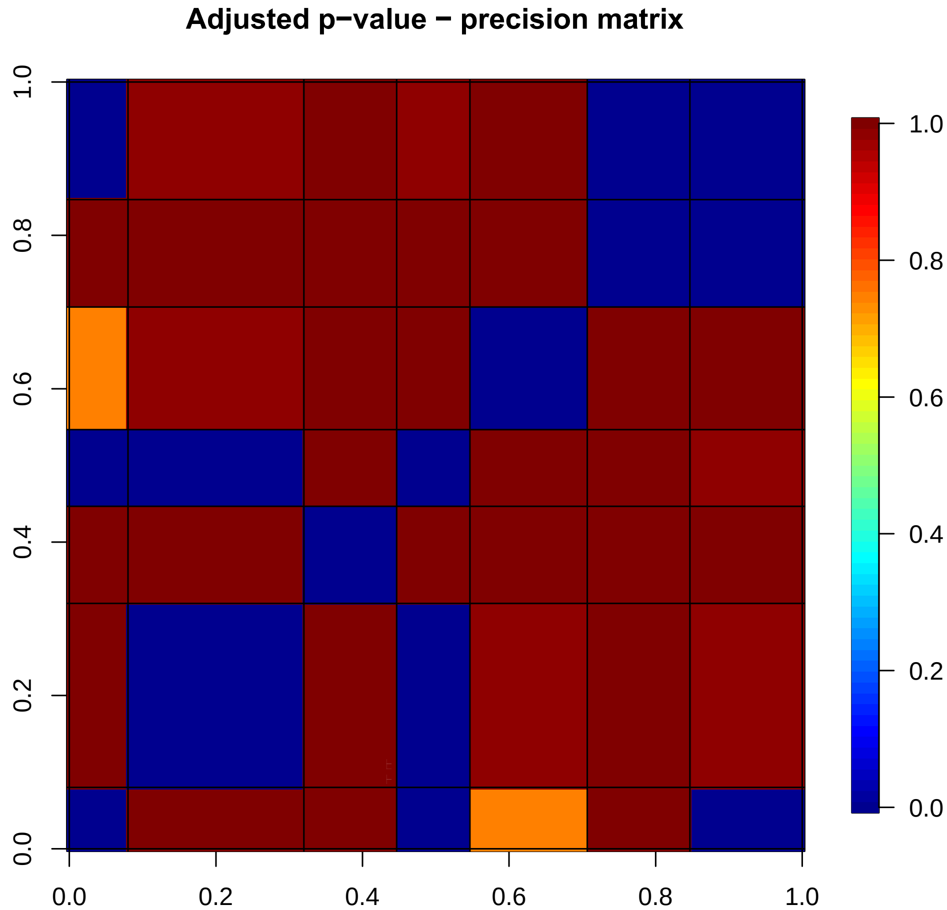
FRUITS PUREES DATASET INDEPENDENCE





FRUITS PUREES DATASET CONDITIONAL INDEPENDENCE





DISCUSSION

- Two methods for performing inference on the covariance structure of functional data:
  - A test of linear independence.
  - test of conditional linear independence.
- A novel way to adjust for multiplicity when testing blocks of the covariance/precision matrix.
- The adjustment method can be plugged-in with every available testing procedure.

Future works

- How to define blocks when they are not available?
- How to extend the procedure without relying on a basis expansion?

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