What if our data were intervals?

Lina Oliveira & M. Rosário Oliveira

CAMGSD, CEMAT, and Department of Mathematics, Instituto Superior Técnico

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"Theoretical derivation of interval principal component analysis",

Information Sciences, 2023

Conventional data/**Symbolic Data**:

- Each **object** is characterised by several **variables**
- Data is organized as an $n \times p$ matrix: rows correspond to **objects**, columns to **variables**

$$\begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix} \qquad \begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix}$$

For example,

x_{11} = real number $\qquad$ x_{11} = interval $[a, b]$ of real numbers

Conventional data/Symbolic Data:

Data matrix

$$\begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix}$$

random vector $\boldsymbol{X} = \begin{bmatrix} X_1 \\ \vdots \\ X_p \end{bmatrix} \rightarrow \mathbb{R}^p$

Data matrix

$$\begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix}$$

random vector $\boldsymbol{X} = \begin{bmatrix} X_1 \\ \vdots \\ X_p \end{bmatrix} \rightarrow \mathbb{IR}^p$

Random vector

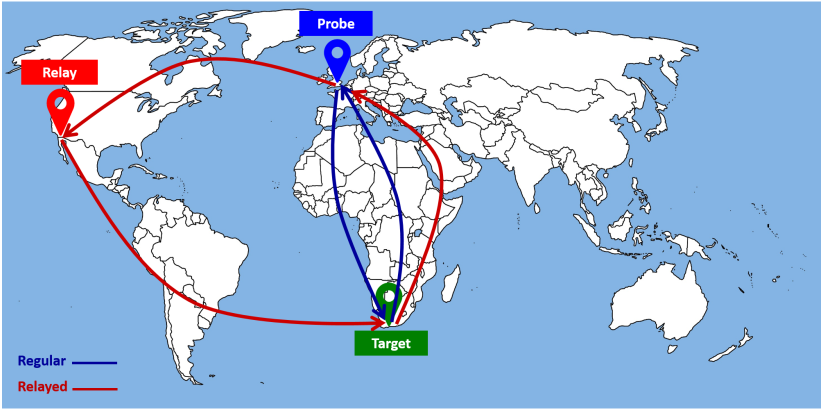
$[x_{11} \cdots x_{1p}]^T \in \mathbb{R}^p$ is a realisation of $\boldsymbol{X}$

Interval-valued random vector

$[x_{11} \cdots x_{1p}]^T \in \mathbb{IR}^p$ is a realisation of $\boldsymbol{X}$

WHY INTERVALS?

Detecting Internet traffic redirection attacks



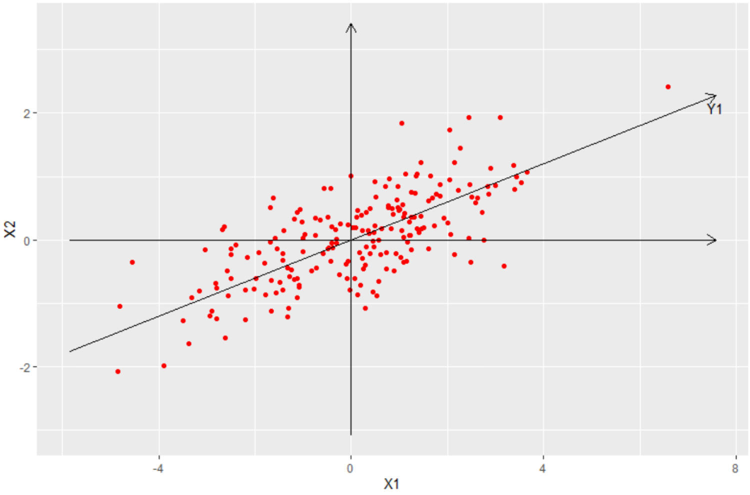
in A. Subtil, M.R. Oliveira, R. Valadas, A. Pacheco, and P. Salvador "Internet-Scale Traffic Redirection Attacks Using Latent Class Models", Intelligent Systems and Computing, 2020

Conventional data:

- Each **object** is characterised by several **variables**
- Data is organized as an $n \times p$ matrix: rows correspond to **objects**, columns to **variables**

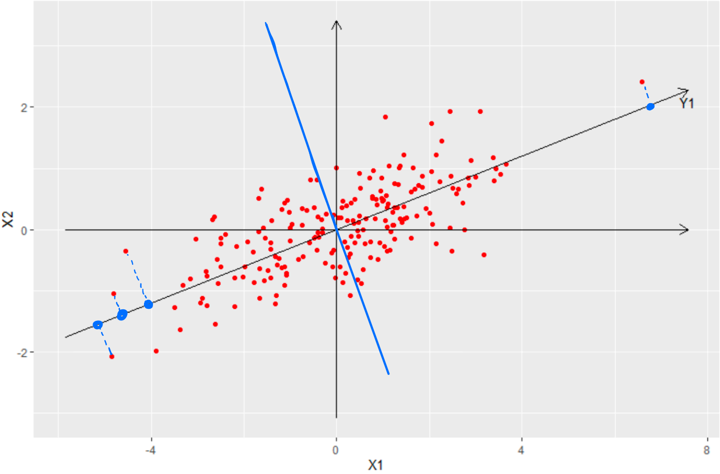
$$\text{Data matrix} \begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix} \qquad \text{random vector } \boldsymbol{X} = \begin{bmatrix} X_1 \\ \vdots \\ X_p \end{bmatrix} \to \mathbb{R}^p$$

Example: $\begin{bmatrix} x_{11} & \cdots & x_{1p} \end{bmatrix}^T \in \mathbb{R}^p$ is a realisation of $\boldsymbol{X}$.



Y1
X2
2
0
-2
-4
0
4
8
X1

Work with these blue data instead!



Principal Component Analysis (PCA)

covariance matrix $\quad \boldsymbol{\Sigma} = \left[\mathrm{cov}(X_i, X_j)\right] \qquad i, j = 1, \ldots, p$

$\boldsymbol{\Sigma} = \boldsymbol{\Sigma}^T \qquad \boldsymbol{\Sigma}$ is symmetric

$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \qquad \leftarrow$ eigenvalues of $\boldsymbol{\Sigma}$

$\boldsymbol{\Gamma} = [\gamma_1 | \gamma_2 | \ldots | \gamma_p] \qquad \leftarrow$ eigenvectors $\quad \boldsymbol{\Gamma}\boldsymbol{\Gamma}^T = \boldsymbol{I} = \boldsymbol{\Gamma}^T\boldsymbol{\Gamma}$

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \qquad \leftarrow \text{eigenvalues of } \boldsymbol{\Sigma}$$

$$\boldsymbol{\Gamma} = [\gamma_1|\gamma_2|\dots|\gamma_p] \qquad \leftarrow \text{eigenvectors in } \mathbb{R}^p$$

$$\boldsymbol{\Gamma}^T \boldsymbol{\Sigma} \boldsymbol{\Gamma} = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_p) \quad \Rightarrow \quad \gamma_i^T \boldsymbol{\Sigma} \gamma_i = \lambda_i, \quad i = 1, \dots, p.$$

$$\gamma_1 = \arg\max_{\|\gamma\|=1} \gamma^T \boldsymbol{\Sigma} \gamma$$

$$\begin{cases} \gamma_j = \arg\max_{\|\gamma\|=1} \gamma^T \boldsymbol{\Sigma} \gamma \\ \gamma^T \gamma_i = 0, \quad i = 1, \dots, j-1, \end{cases} \qquad j > 1$$

principal components of $\boldsymbol{X} \in \mathbb{R}^p$

$$Y_1 = \gamma_1^T \boldsymbol{X}, \quad Y_2 = \gamma_2^T \boldsymbol{X}, \quad \dots, \quad Y_p = \gamma_p^T \boldsymbol{X}$$

Symbolic data:

How to reduce dimensionality/How to find an SPCA?

- Data is organized as an $n \times p$ matrix, where rows correspond to **objects**, columns to **interval-valued variables**:

$$\text{Data matrix} \begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix}, \qquad \text{e.g., } x_{11} = [a_{11}, b_{11}]$$

$$\text{random vector } \boldsymbol{X} = \begin{bmatrix} X_1 \\ \vdots \\ X_p \end{bmatrix} \to \mathbb{IR}^p$$

Example: $\begin{bmatrix} x_{11} & \cdots & x_{1p} \end{bmatrix}^T \in \mathbb{IR}^p$ is a realisation of X.

What do we need?

$\mathbb{IR}^p$ **Principal components of $\boldsymbol{X}$**

$$Y_1 = \gamma_1^T \boldsymbol{X}, \quad Y_2 = \gamma_2^T \boldsymbol{X}, \quad \ldots, \quad Y_p = \gamma_p^T \boldsymbol{X}$$

$$Y_1 = \gamma_1^T \boldsymbol{X} = \gamma_1^T \begin{bmatrix} X_1 \\ \vdots \\ X_p \end{bmatrix} = \gamma_1^T \begin{bmatrix} [a_1, b_1] \\ \vdots \\ [a_p, b_p] \end{bmatrix}$$

1. Define $\mathbb{IR}^p$
2. interval arithmetic, linear combinations of intervals
3. "orthogonality"

- Definition of $\mathbb{IR}^p$

Let

$$\mathbb{IR} = \{[a, b] : a, b \in \mathbb{R}, a \leq b\}$$

be the set of all real closed and bounded intervals,

$[a, b]$ seen as a point (C, R) in $\mathbb{R}^2$

$$C = \frac{a+b}{2} \qquad \text{centre of } [a, b]$$

$$R = b - a \qquad \text{range of } [a, b]$$

- Definition of $\mathbb{IR}^p$

Let

$$\mathbb{IR}^p = \mathbb{IR} \times \mathbb{IR} \times \cdots \times \mathbb{IR}$$

be the cartesian product of p copies of $\mathbb{IR}$.

$$\mathbb{IR} \longleftrightarrow \mathbb{R}^2$$

Let $\mathbf{X} = (X_1, ..., X_p)^T$ be an **interval-valued random vector**

$$X_1 \quad \leftrightarrow \quad (C_1, R_1), \qquad \ldots, \qquad X_p \quad \leftrightarrow \quad (C_p, R_p)$$

$$\boldsymbol{C} = \begin{bmatrix} C_1 \\ C_2 \\ \vdots \\ C_p \end{bmatrix} \qquad \boldsymbol{R} = \begin{bmatrix} R_1 \\ R_2 \\ \vdots \\ R_p \end{bmatrix}$$

1. Definition of $\mathbb{IR}^p = \mathbb{IR} \times \mathbb{IR} \times \cdots \times \mathbb{IR} \longleftrightarrow \mathbb{R}^{2p}$

Let $\mathbf{X} = (X_1, ..., X_p)^T = (\boldsymbol{C}^T, \boldsymbol{R}^T)^T = \begin{bmatrix} \boldsymbol{C} \\ \boldsymbol{R} \end{bmatrix}$ be an **interval-valued random vector** with realisations in $\mathbb{R}^{2p}$

$$X_1 \quad \leftrightarrow \quad (C_1, R_1), \qquad \ldots, \qquad X_p \quad \leftrightarrow \quad (C_p, R_p)$$

$$\boldsymbol{C} = \begin{bmatrix} C_1 \\ \vdots \\ C_p \end{bmatrix} = \frac{1}{2}\left(\begin{bmatrix} a_1 \\ \vdots \\ a_p \end{bmatrix} + \begin{bmatrix} b_1 \\ \vdots \\ b_p \end{bmatrix} \right) = \frac{1}{2}(\boldsymbol{A} + \boldsymbol{B}) \qquad \text{random vector of centres}$$

$$\boldsymbol{R} = \begin{bmatrix} R_1 \\ \vdots \\ R_p \end{bmatrix} = \boldsymbol{B} - \boldsymbol{A} \qquad \text{random vector of ranges}$$

- **Moore's interval arithmetic**

For $X = [a, b] = (C, R)$, $\quad Y = [c, d] = (C', R')$ in $\mathbb{IR}$, define

$$X + Y = (C + C', R + R') \qquad = \{x + y \colon x \in X, y \in Y\}$$

$$\alpha X = (\alpha C, |\alpha| R)$$

Linear combination

For $\boldsymbol{X} \in \mathbb{IR}^p$ and $\boldsymbol{\alpha} \in \mathbb{R}^p$, define

$$\boldsymbol{\alpha}^T \boldsymbol{X} = \sum_{i=1}^{p} \alpha_i X_i = (\boldsymbol{\alpha}^T \boldsymbol{C}, |\boldsymbol{\alpha}|^T \boldsymbol{R})^T = \Big(\sum_{i=1}^{p} \alpha_i C_i, \sum_{i=1}^{p} |\alpha_i| R_i\Big)$$

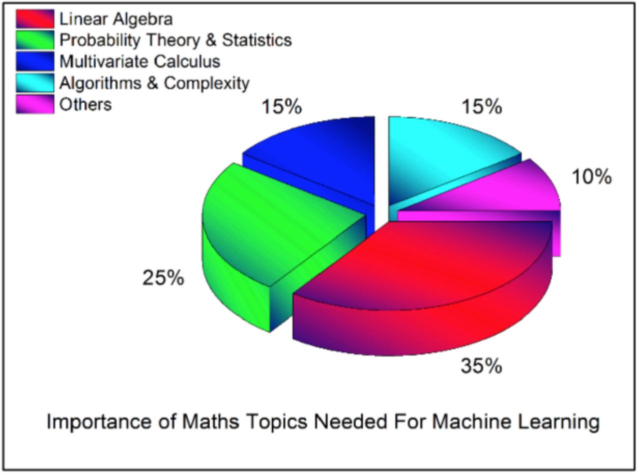
Theorem

The p orthogonal-pcs of $\boldsymbol{X}$ *are* $Y_1, \cdots, Y_p$ *with* $Y_i = \gamma_i^T \boldsymbol{X}$, *where* $\gamma_i \in \mathbb{R}^p$ *is*

$$\gamma_i = \arg\max_{l=1,\ldots,2^p} \left(\gamma_{il}^T \boldsymbol{\Sigma}_{CC} \gamma_{il} + \gamma_{il}^T \boldsymbol{M}_{RR} \gamma_{il} \right) ,$$

and γ_{il}, $l = 1, \ldots, 2^p$, *solves a subproblem:*

$$\gamma_{il} = \begin{cases} \arg\max_{\gamma:||\gamma||=1} \left(\gamma^T \boldsymbol{\Sigma}_{CC} \gamma + \gamma_{il}^T \boldsymbol{M}_{RR} \gamma_{il} \right) \\ \gamma^T \gamma_j = 0, \; j = 1, \ldots, i-1 \;\; \text{if} \;\; i > 1 \end{cases} ,$$



(by Wale Akinfaderin, `https://tinyurl.com/y6hc9sh8`)