Normalized k-means clustering of hyper-rectangles

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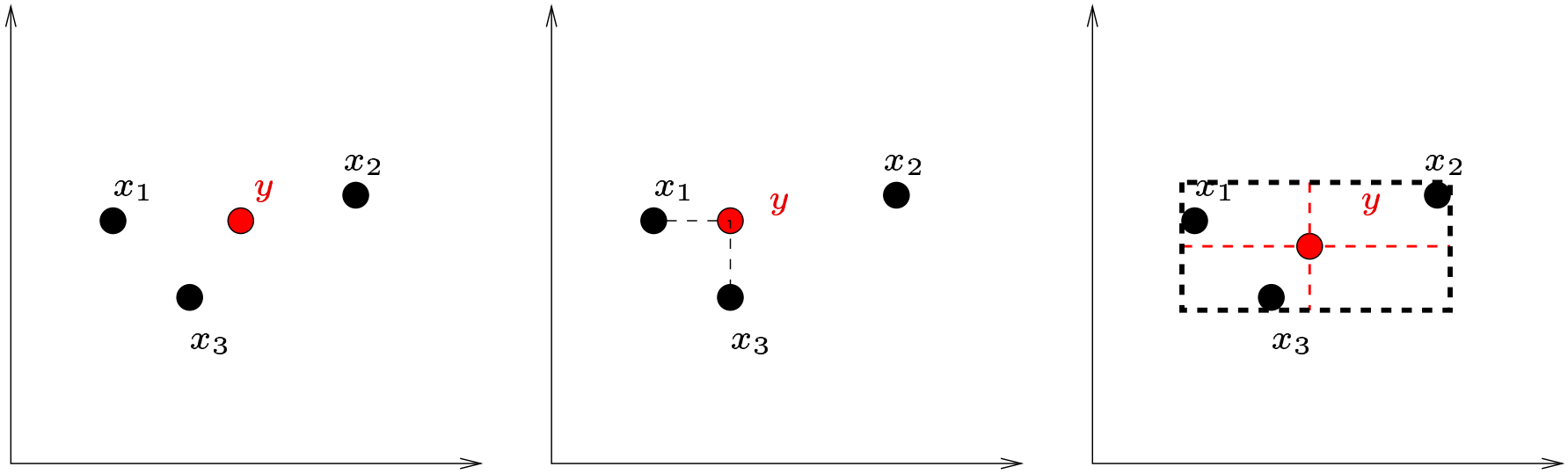
Introduction

Three different prototypes for points of $\mathbb{R}^p$ with L_1, L_2 or L_∞ distances :

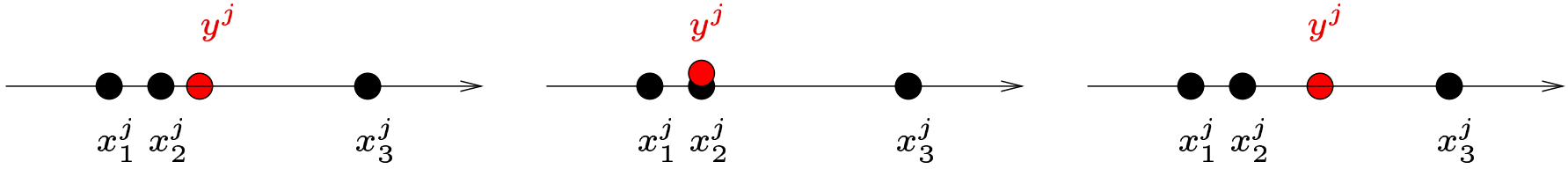


$\sum_{i=1}^{n} {d_2}^2(x_i, y)$ $\sum_{i=1}^{n} d_1(x_i, y)$ $\max_{i=1\ldots n} d_\infty(x_i, y)$

k-means Dynamical Clustering

Introduction

Three different measures of centrality y^j :



The mean | The median | The middle

Introduction

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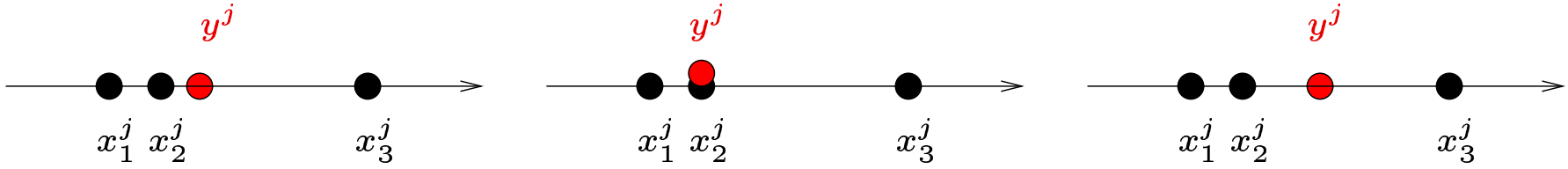
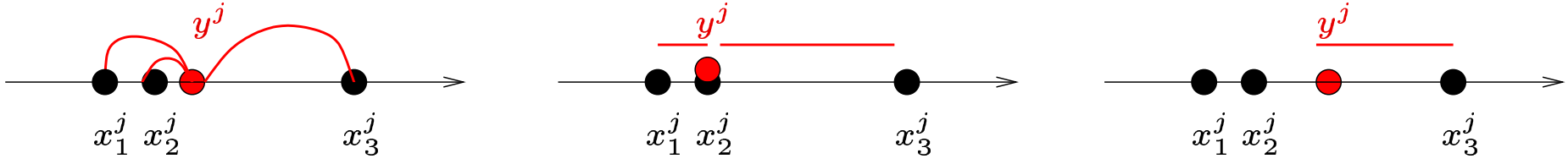


The mean | The median | The middle

Three different measures of dispersion σ^j :



The square deviation | The absolute deviation | The max deviation

Introduction

Normalized L_α distance between two $\mathbb{R}^p$-points:

$$d_\alpha(x_1, x_2) = \left(\sum_{j=1}^{p} \frac{1}{\sigma^j} |x_1^j - x_2^j|^\alpha\right)^{\frac{1}{\alpha}}$$

Three normalized k-means algorithms:

Prototype	Distance	Measure of dispersion
The "mean" $\mathbb{R}^p$-point	L_2-Euclidean	The square deviation from the mean
The "median" $\mathbb{R}^p$-point	L_1-City-Block	The absolute deviation from the median
The "middle" $\mathbb{R}^p$-point	L_∞-Max	The max deviation from the middle

Plan

Part 1 Interval data

Part 2 Comparing hyper-rectangles

Part 3 Define a class prototype

Part 3 Normalization

PART 1

Interval data

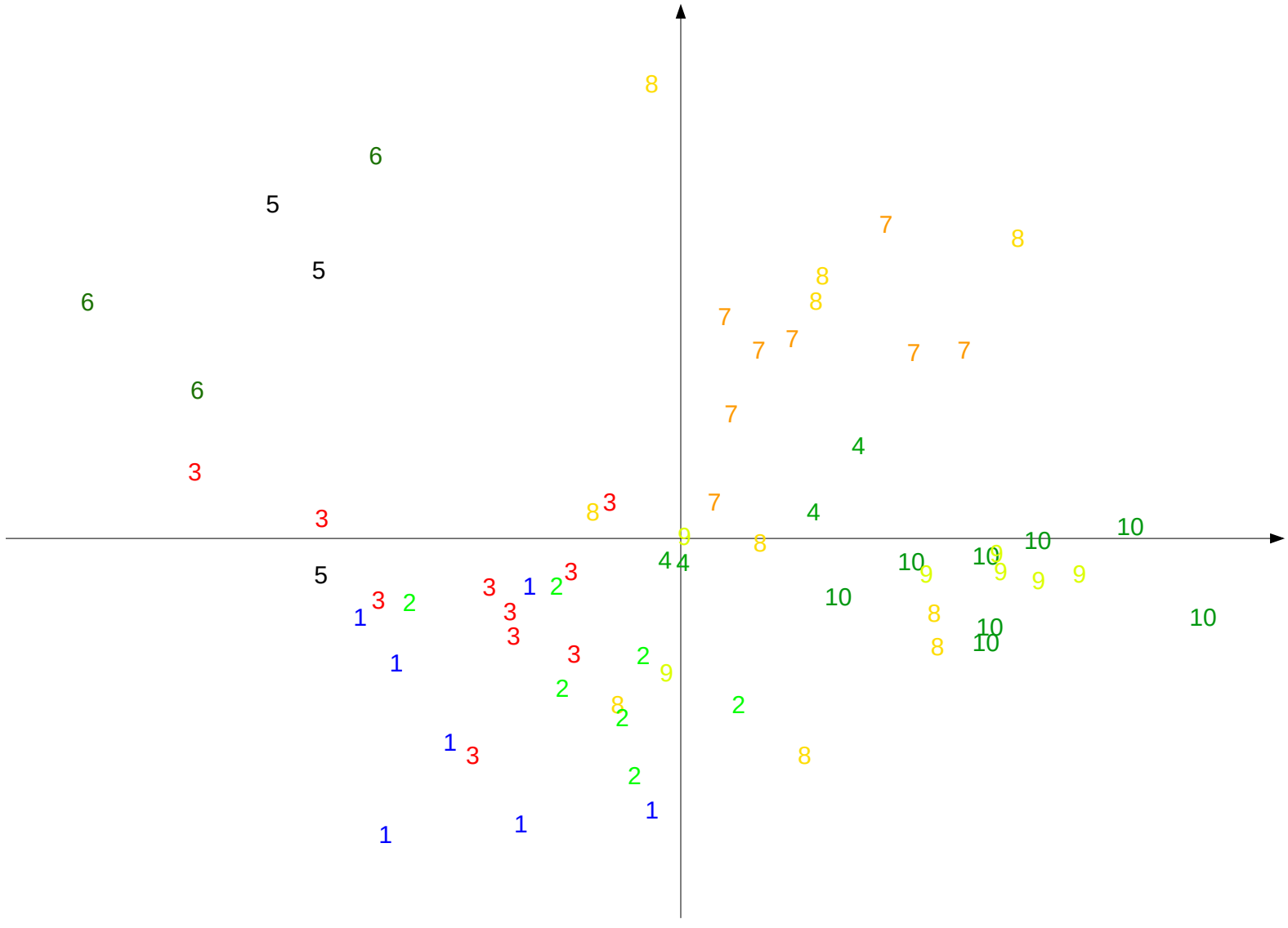
French Guyana Fish Example

- Mercury contamination in some Amerindian populations in French Guyana
- Data table : 67 fish of 10 different species described by 5 quantitative variables based on the mercury concentration (μg/g) in five organs (gills, liver, intestine, stomach, kidney)

Fish	liver	kidney	gills	intestine	stomach	species
1	-0.116	0.352	-1.214	-1.147	NA	ageneiosus brevifi li
2	-0.083	-0.457	-1.881	-1.171	-1.485	ageneiosus brevifi li
...	...	...	...	...	...	...
8	1.416	0.684	-1.439	-1.554	-0.874	cynodon gibbus
9	0.115	-0.509	-1.910	NA	-1.610	cynodon gibbus
...	...	...	...	...	...	...
67	1.813	1.953	-2.251	0.390	-0.651	doras micopoeus

- How to cluster the 10 species

Classical or interval data representation



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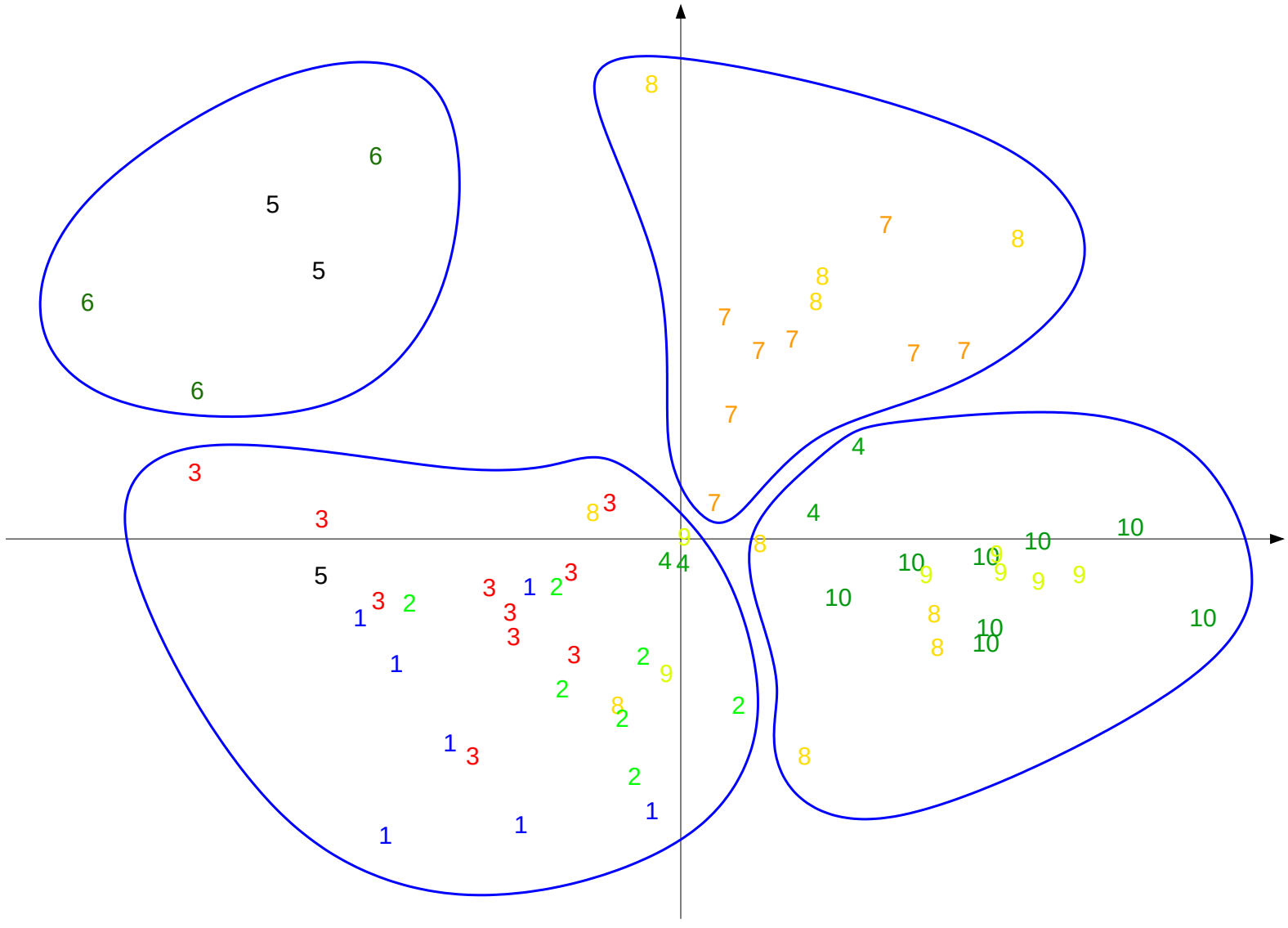

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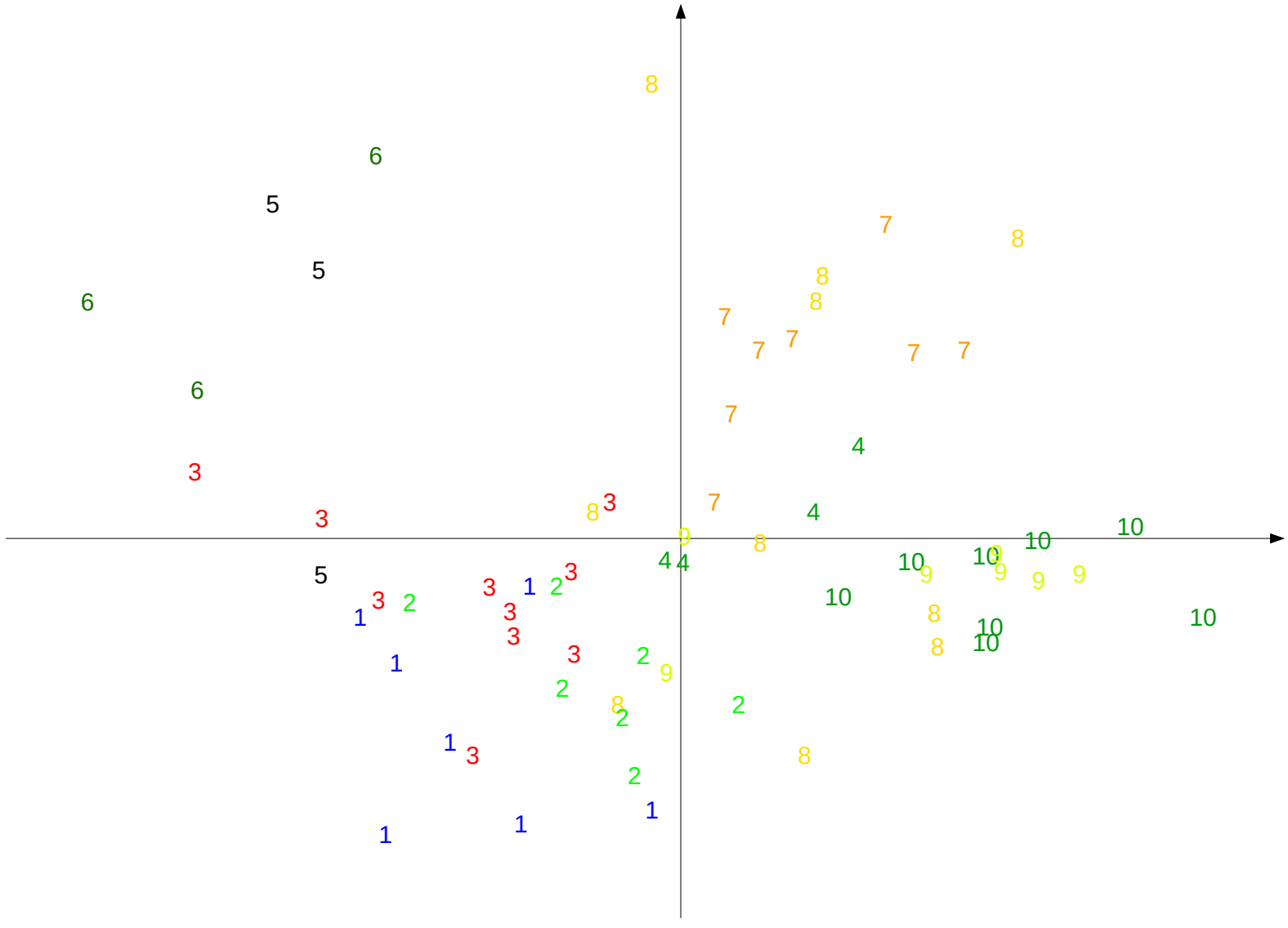

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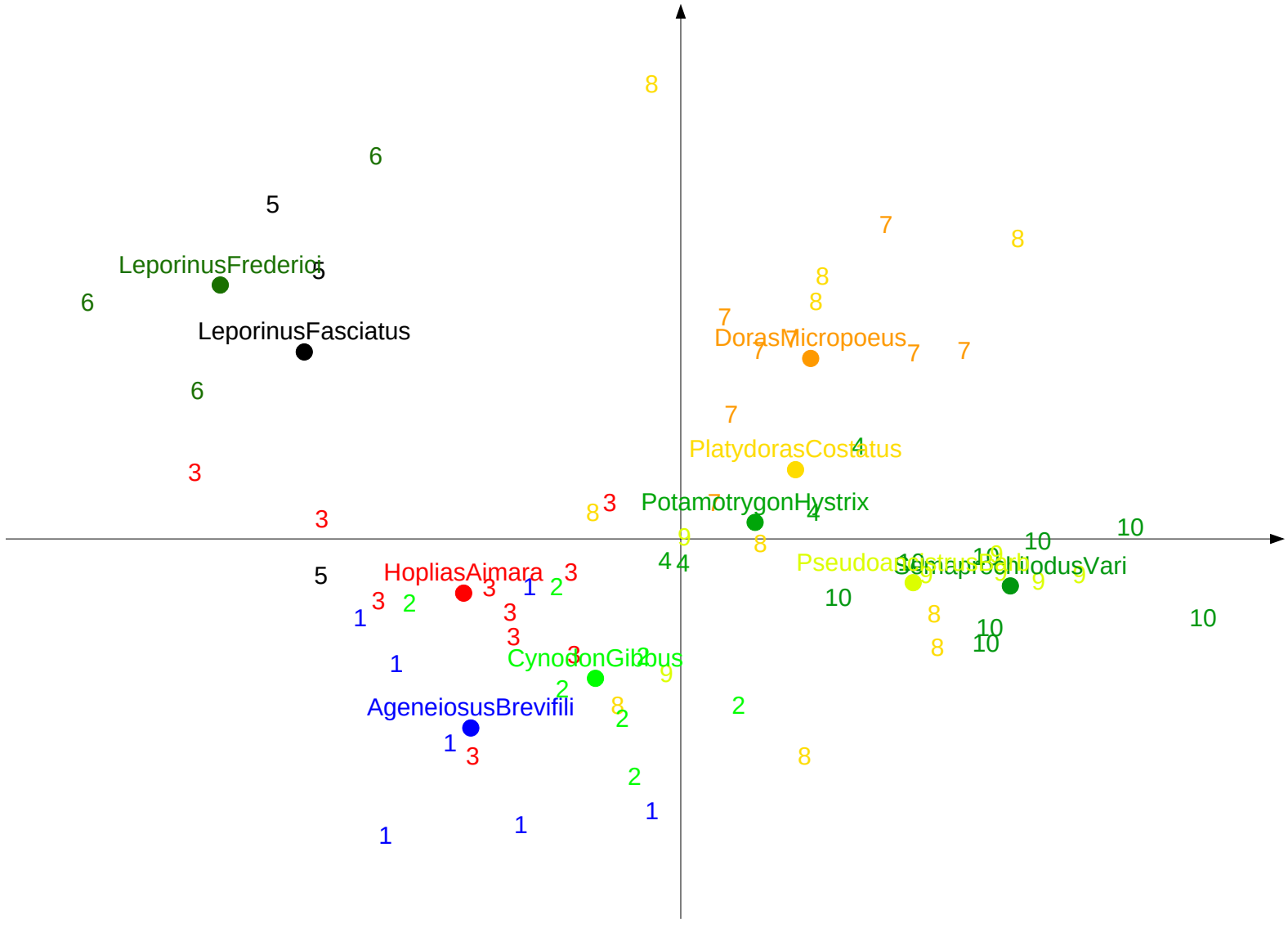

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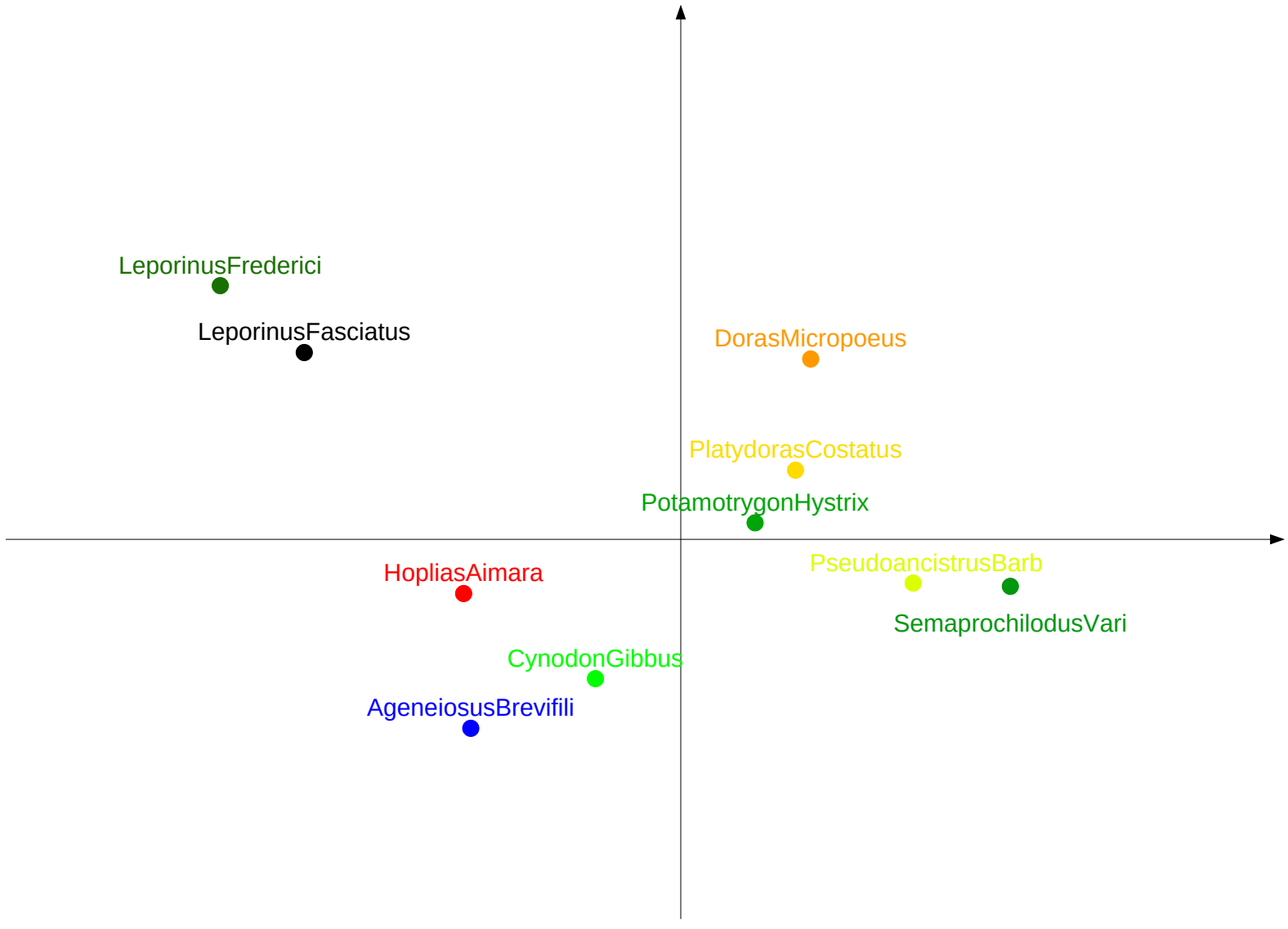

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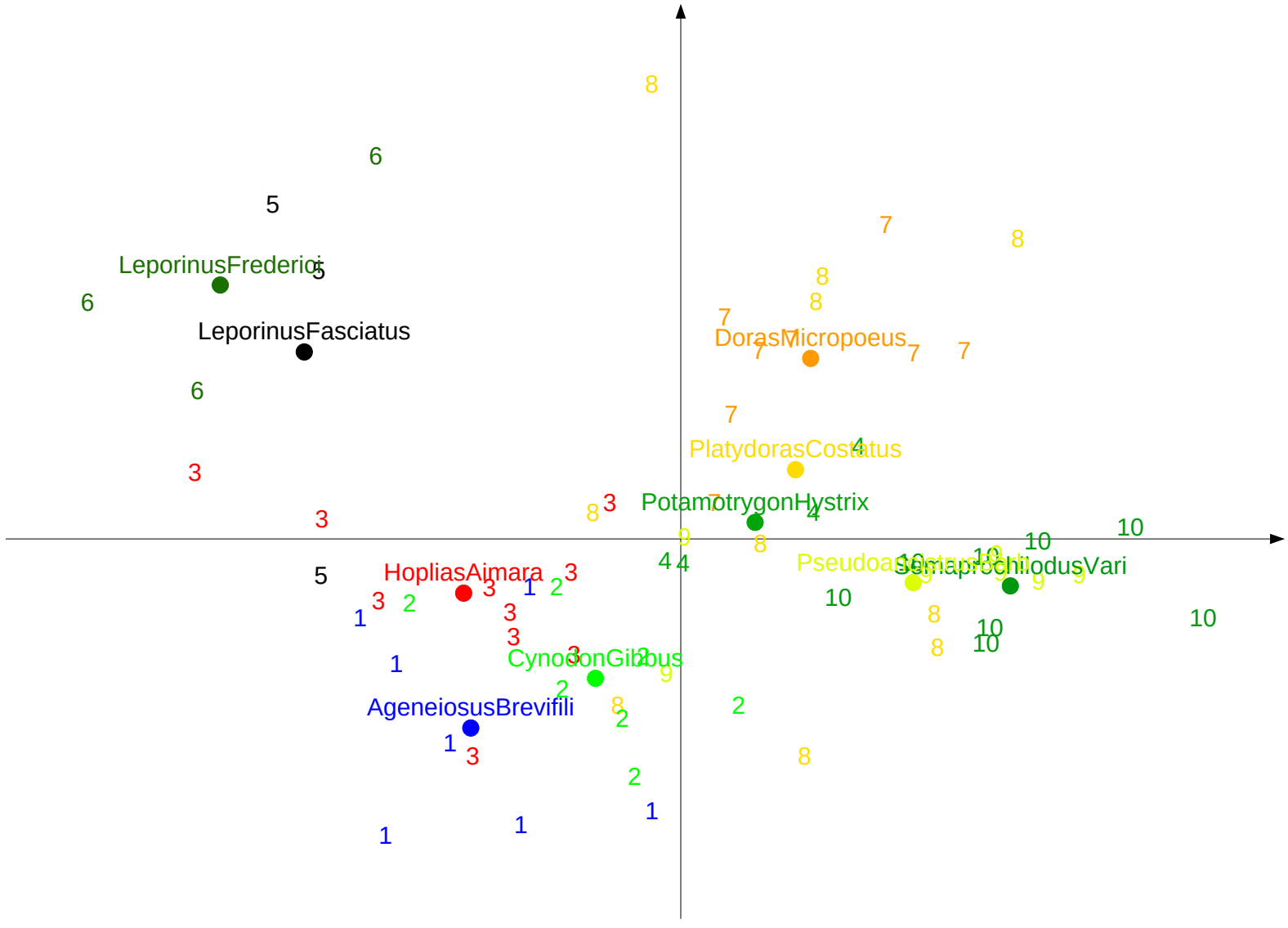

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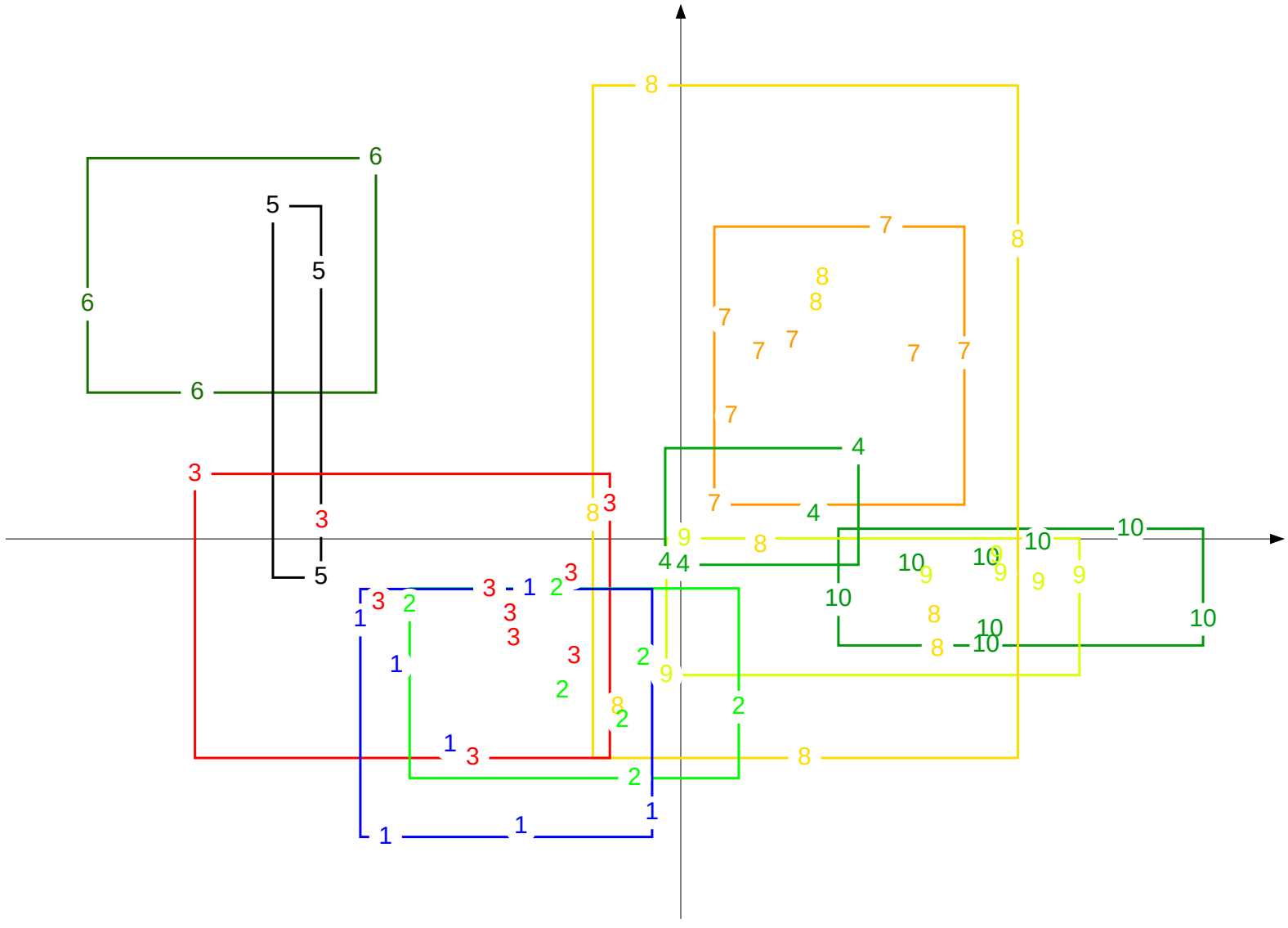

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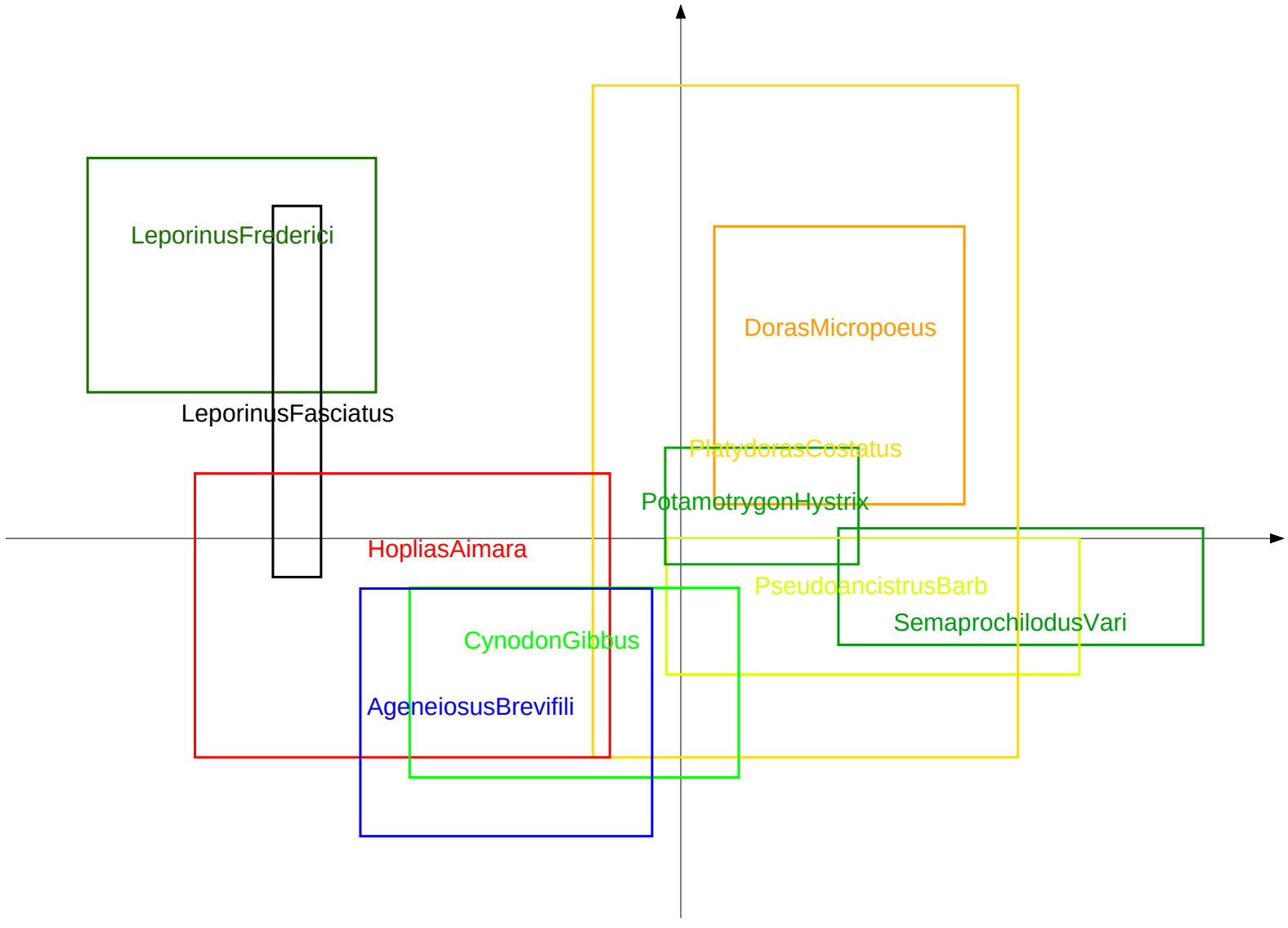

SODAS Software

- The data table obtained with DB2SO method of SODAS software

species	liver	kidney	gills	intestine	stomach
ageneiosus brevifi li	[-0.80:0.34]	[-1.50:0.35]	[-1.88:-1.21]	[-1.45:-0.48]	[-1.49:-1.05]
Cynodon Gibbus	[0.12:1.59]	[-0.51:1.18]	[-1.91:-1.44]	[-1.75:-0.68]	[-1.61:0.22]
Hoplias Aimara	[-0.44:0.90]	[-0.17:1.60]	[-1.98:-1.53]	[-2.17:-0.71]	[-2.36:-0.93]
Potamitrigon Hystrix	[0.66:2.01]	[0.77:2.15]	NA	[-0.50:0.23]	[-0.80:-0.69]
Leporinus Fasciatus	[-0.98:-0.58]	[-0.32:0.35]	[-3.00:-2.63]	NA	[-2.11:-2.76]
Leporinus Frederici	[-0.82:-0.04]	[-0.95:-0.19]	[-3.27:-2.55]	[-1.74:-1.42]	[-2.03:-0.55]
Doras Micropoeus	[1.34:2.12]	[1.47:2.69]	[-2.38:-2.21]	[-1.99:0.39]	[-1.45:-0.24]
Platidoras Costatus	[0.41:2.42]	[-0.02:2.75]	[-2.90:-1.27]	[-1.22:0.38]	[-1.41:-0.49]
Pseudoancistrus Barbatus	[1.26:2.84]	[-0.99:0.99]	NA	[-0.31:0.68]	[-0.71:0.12]
Semaprochilodus Vari	[2.70:3.96]	[1.11:1.91]	[-1.79:-1.40]	[-0.91:0.52]	[-0.74:0.22]

- Each of the $n = 10$ species i is an hyper-rectangle of $\mathbb{R}^p$ (here $p = 5$) noted:

$$x_i = \prod_{j=1}^{p} \underbrace{[a_i^j, b_i^j]}_{x_i^j}$$

PART 2

Comparing hyper-rectangles

Several approaches

- Simple Euclidean distance or more generally Minkowsky distance $\Rightarrow$ lower and upper bound are used independantly

species	Axis1	Axis2
AgeneiosusBrevifi li	[-1,957:-0,175]	[0,306:1,819]
CynodonGibbus	[-1,656:0,354]	[0,302:0,302]
DorasMicropoeus	[-2,967:-0,433]	[-0,397:1,337]
HopliasAimara	[-0,095:1,085]	[-0,554:0,158]
LeporinusFasciatus	[-2,491:-2,197]	[-2,031:0,236]
...	...	...

Axis1		Axis2	
-1,957	-0,175	0,306	1,819
-1,656	0,354	0,302	0,302
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- Elaborated distances taking into account both position and span of the intervals $\Rightarrow$ Explicit formulas for the optimum class prototype ?

The Hausdorff distance

The Hausdorff distance between two sets $A, B \subset \mathbb{R}^p$ is :

$$d_{H,\alpha}(A, B) = \max(h(A, B), h(B, A))$$

with

$$h(A, B) = \sup_{u \in A} \inf_{v \in B} d_\alpha(u, v)$$

$\Rightarrow$ Depends on the distance d_α (L_1,L_2...L_∞) chosen to compare two points of $\mathbb{R}^p$

Mathematical properties

Here A and B are two hyper-rectangles of $\mathbb{R}^p$ noted:

$$A = \prod_{j=1}^{p} A_j,\ B = \prod_{j=1}^{p} B_j$$

where $A_j = [a_j, b_j]$ and $B_j = [\alpha_j, \beta_j]$ are intervals of $\mathbb{R}$.

- *Property 1.* In the one dimensional space we can drop the subscript α and:

$$d_H(A_j, B_j) = \max(|a_j - \alpha_j|, |b_j - \beta_j|)$$

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- *Property 1.* In the one dimensional space we can drop the subscript α and:

$$d_H(A_j, B_j) = \max(|a_j - \alpha_j|, |b_j - \beta_j|)$$

- *Property 2.* With the L_∞ distance, we have the following relation between the Hausdorff distance $d_{H,\infty}$ in p dimensions and d_H in one dimension:

$$d_{H,\infty}(A, B) = \max_{j=1,\ldots,p} d_H(A_j, B_j)$$

Two distances between hyper-rectangles

We are able to give an explicit formula of the optimum class prototype with:

- The L_∞ Hausdorff distance:
  $$d_{H,\infty}(A,B) = \max_{j=1,\ldots,p} \underbrace{\max(|a_j - \alpha_j|, |b_j - \beta_j|)}_{d_H(A_j, B_j)}$$
  $\Rightarrow$ In the particular case of intervals reduced to single points, the L_∞ Hausdorff distance is the well-known L_∞ distance between $\mathbb{R}^p$ points

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- The Hausdorff-based distance:
$$d(A,B) = \sum_{j=1}^{p} \underbrace{\max(|a_j - \alpha_j|, |b_j - \beta_j|)}_{d_H(A_j,B_j)}$$
$\Rightarrow$ In the particular case of intervals reduced to single points, this distance is the well-known L_1 City-Block distance between $\mathbb{R}^p$ points

Example

num	species	Axis1	Axis2
1	AgeneiosusBrevifi li	[-1,957:-0,175]	[0,306:1,819]
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- Comparing species 1 and 2 in one dimension:

  $d_H(x_1^1, x_2^1) = \max(|-1,957+1,656|, |-0,175-0,354|) = 0,529$

  $d_H(x_1^2, x_2^2) = 1,517$

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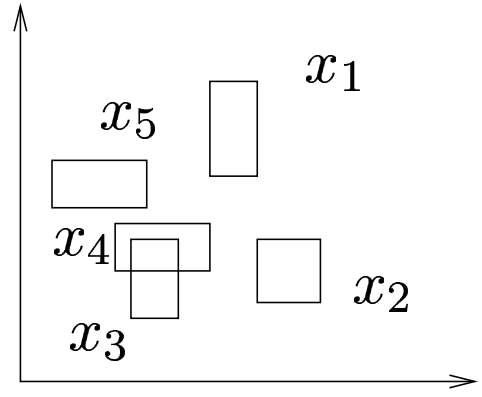
  $d_H(x_1^2, x_2^2) = 1,517$
- Comparing species 1 and 2 in two dimensions:
  - with the L_∞ Hausdorff distance:
    $d_{H,\infty}(x_1, x_2) = \max(0,529, 1,517)$
  - with the Hausdorff-based distance:
    $d(x_1, x_2) = 0,529+1,517$

PART 3

Define a class prototype

Define a class prototype



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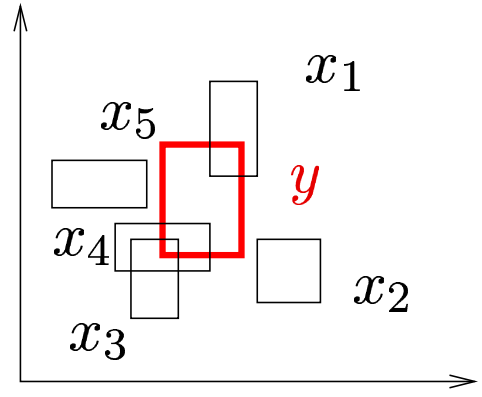

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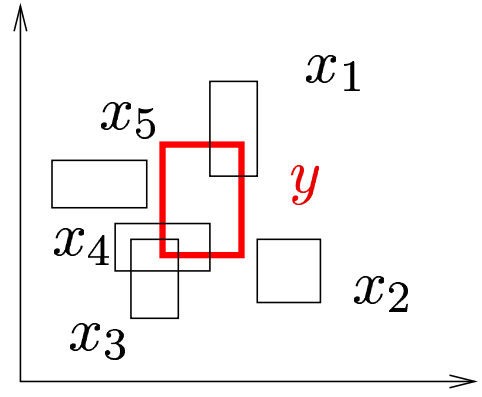

- Adequacy criterion f between y and $C = \{x_1, ..., x_5\}$
- A distance between hyper-rectangles y and x_i

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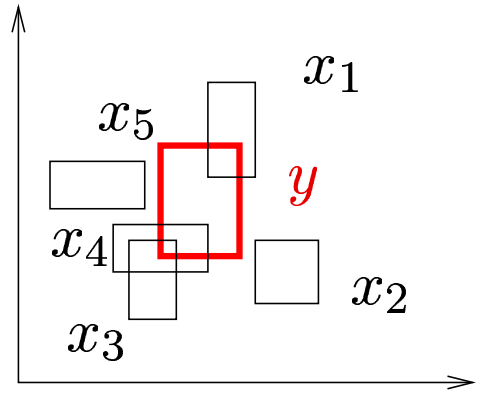

- Adequacy criterion f between y and $C = \{x_1, ..., x_5\}$
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$\Rightarrow$ Find an explicit formula for the prototype y which optimizes f

IFCS Krakow 2002

- Distance between hyper-rectangles: $d(x_i, y) = \sum_{j=1}^{p} d_H(x_i^j, y^j)$

  $\Rightarrow$ Not an Hausdorff distance between $\mathbb{R}^p$-sets

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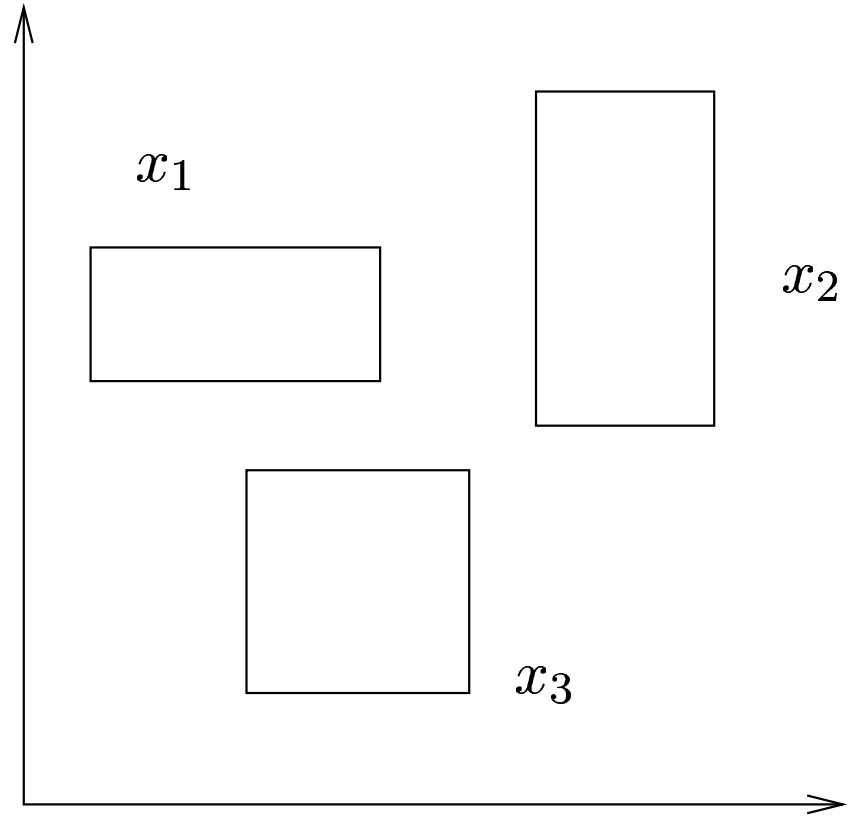
- Explicit formula of the minimizer $\hat{y} = \prod_{j=1}^{p} [\hat{\mu}^j - \hat{\lambda}^j, \hat{\mu}^j + \hat{\lambda}^j]$:

$$\begin{aligned} \hat{\mu}^j &= median\{m_i^j \mid i \in C\} \\ \hat{\lambda}^j &= median\{l_i^j \mid i \in C\} \end{aligned}$$

with m_i^j and l_i^j the midpoints and the half-lengths of the intervals x_i^j

An example



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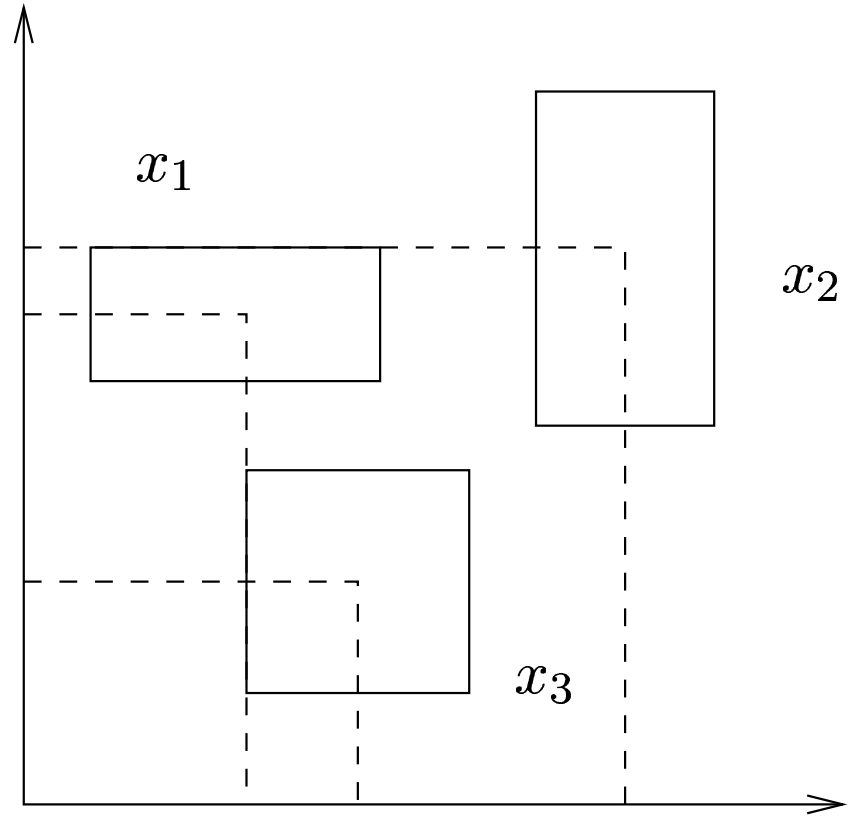

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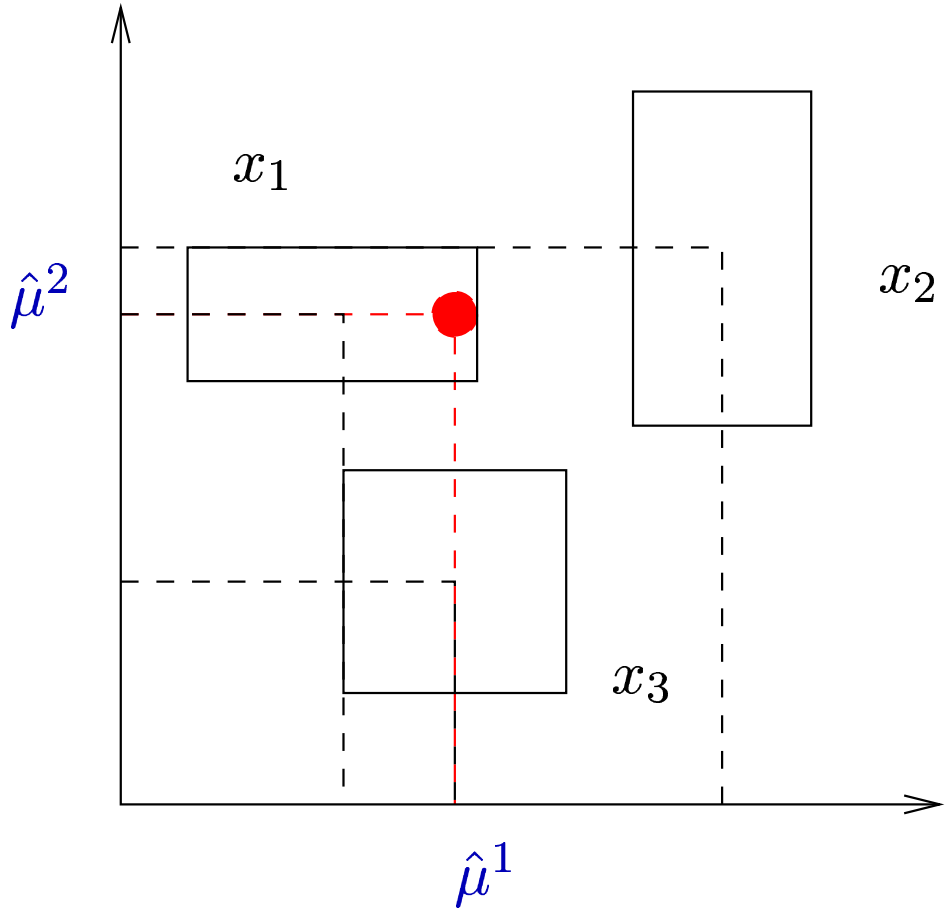

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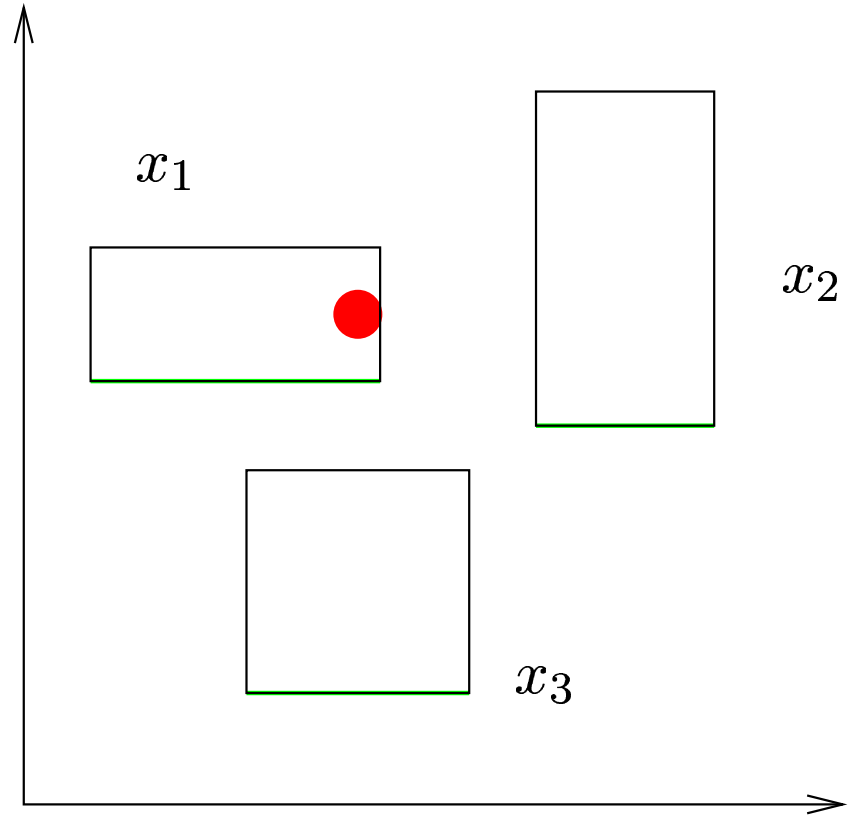

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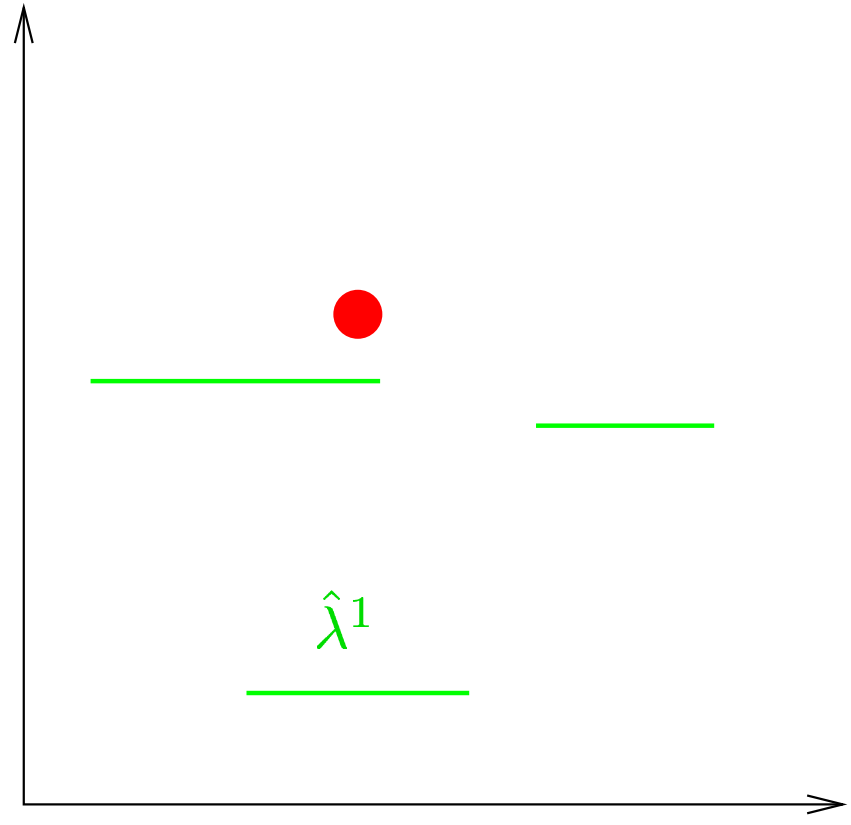

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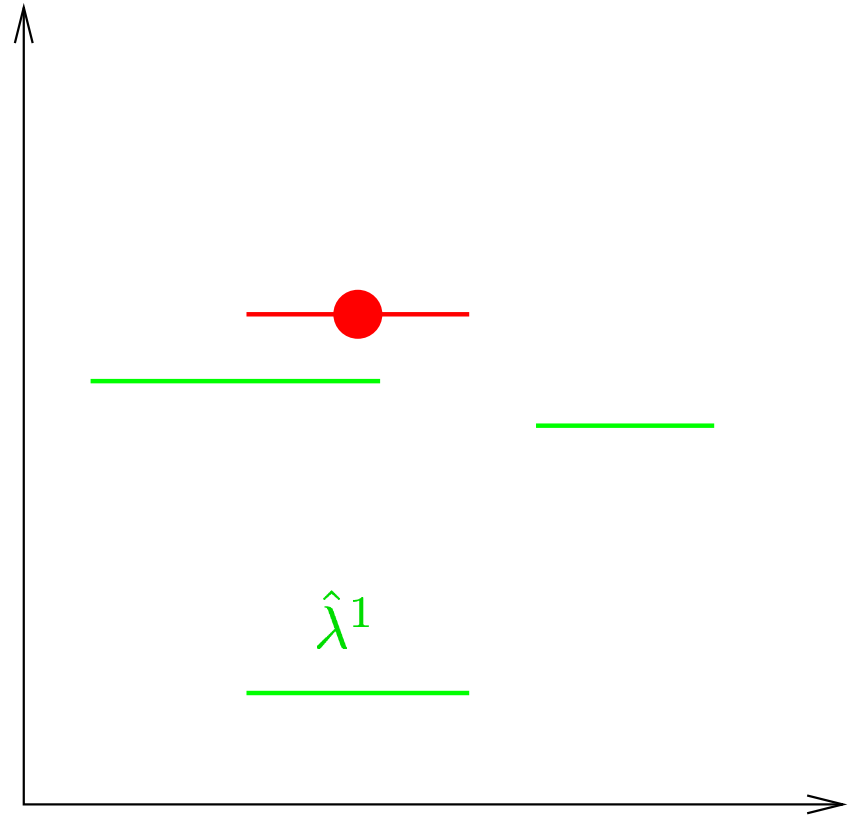

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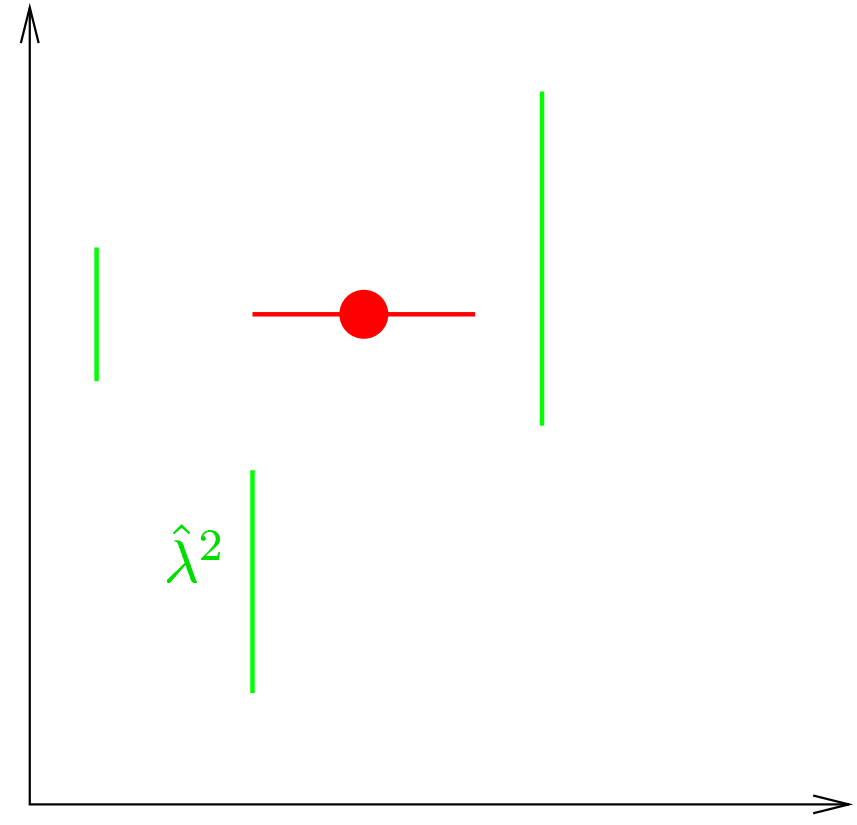

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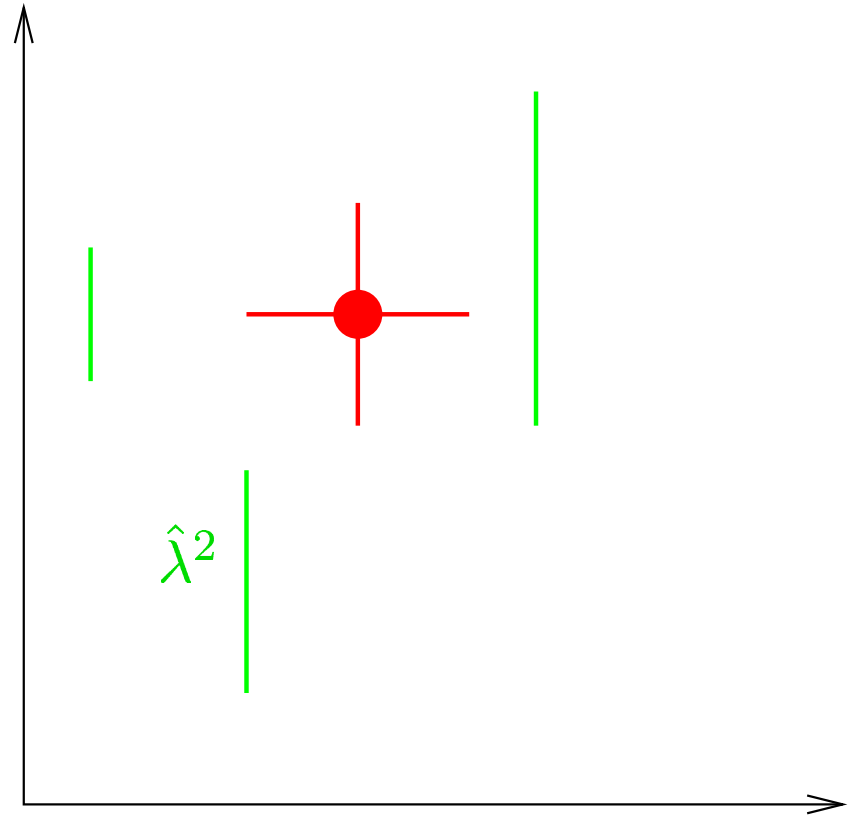

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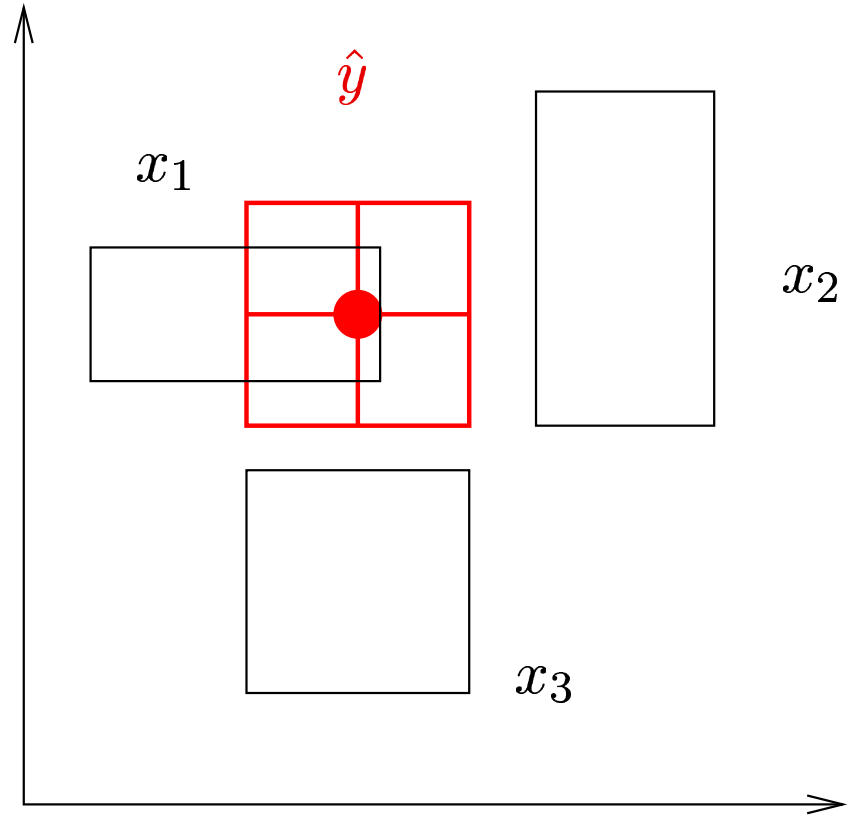

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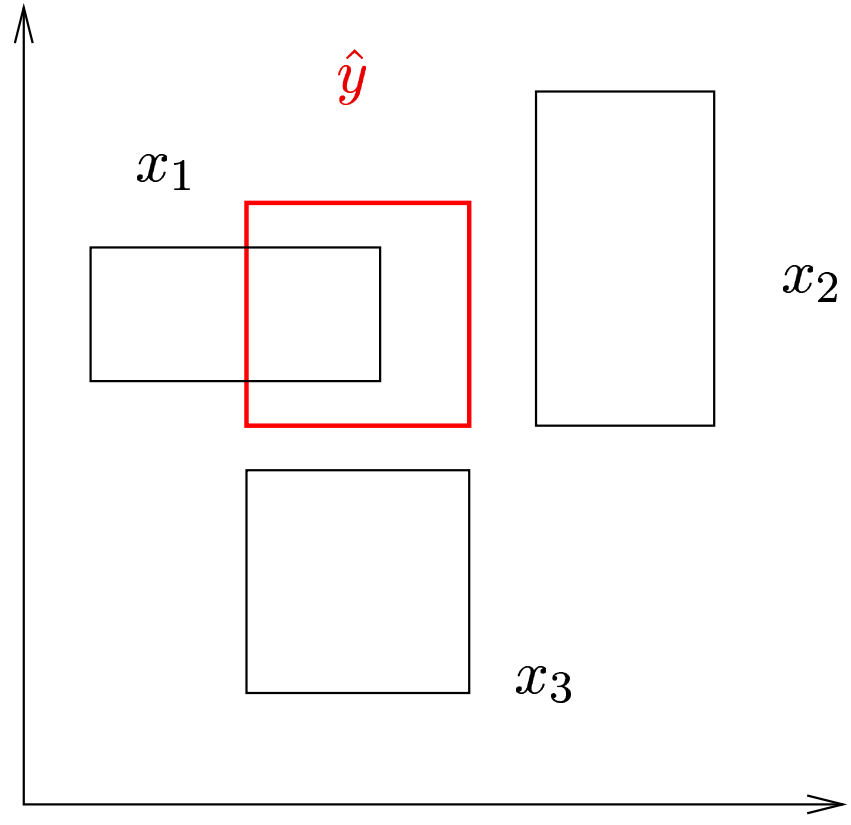

IFCS Chicago 2004

- L_∞ Hausdorff distance: $d_{H,\infty}(x_i, y) = \max_{j=1...p} d_H(x_i^j, y^j)$

  $\Rightarrow$ "Real" Hausdorff distance between $\mathbb{R}^p$-sets

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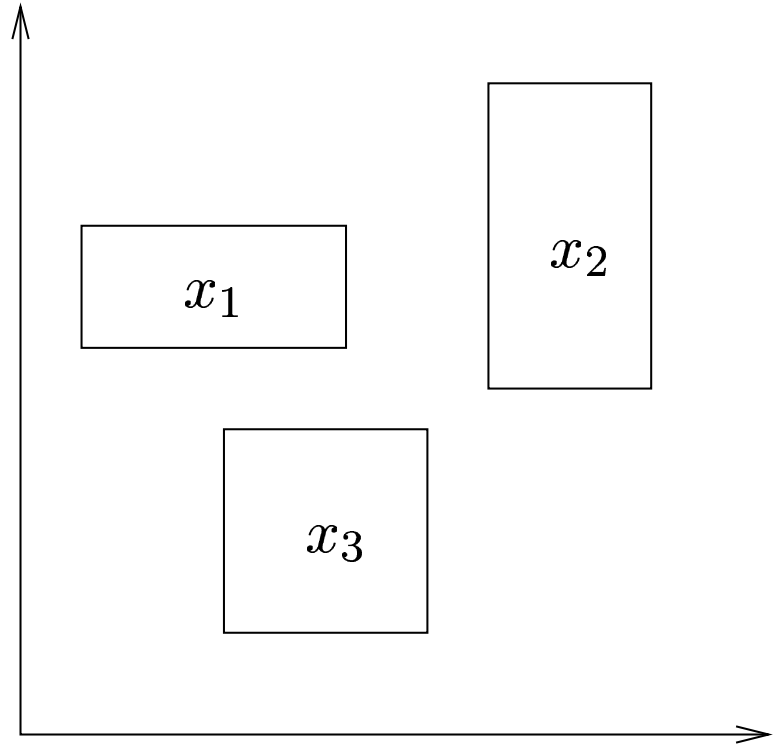
- Explicit formula of *a* minimizer $\hat{y} = \prod_{j=1}^{p} [\hat{\alpha}^j, \hat{\beta}^j]$:

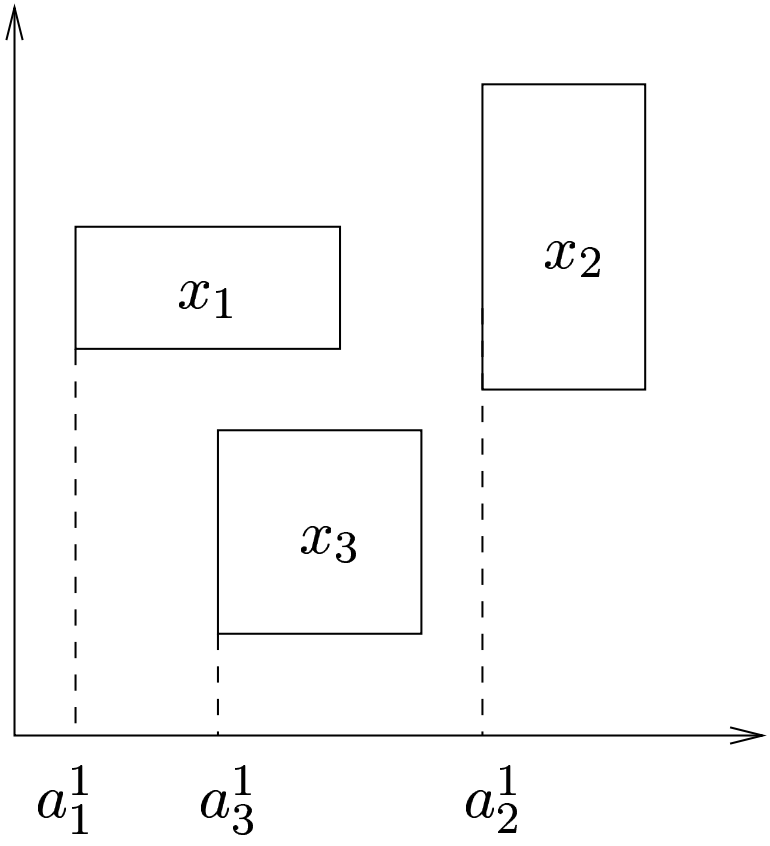
$$\begin{aligned} \hat{\alpha}^j &= \frac{\max_{i \in C} a_i^j + \min_{i \in C} a_i^j}{2} \\ \hat{\beta}^j &= \frac{\max_{i \in C} b_i^j + \min_{i \in C} b_i^j}{2} \end{aligned}$$

with a_i^j and b_i^j the lower and upper bounds of the intervals x_i^j

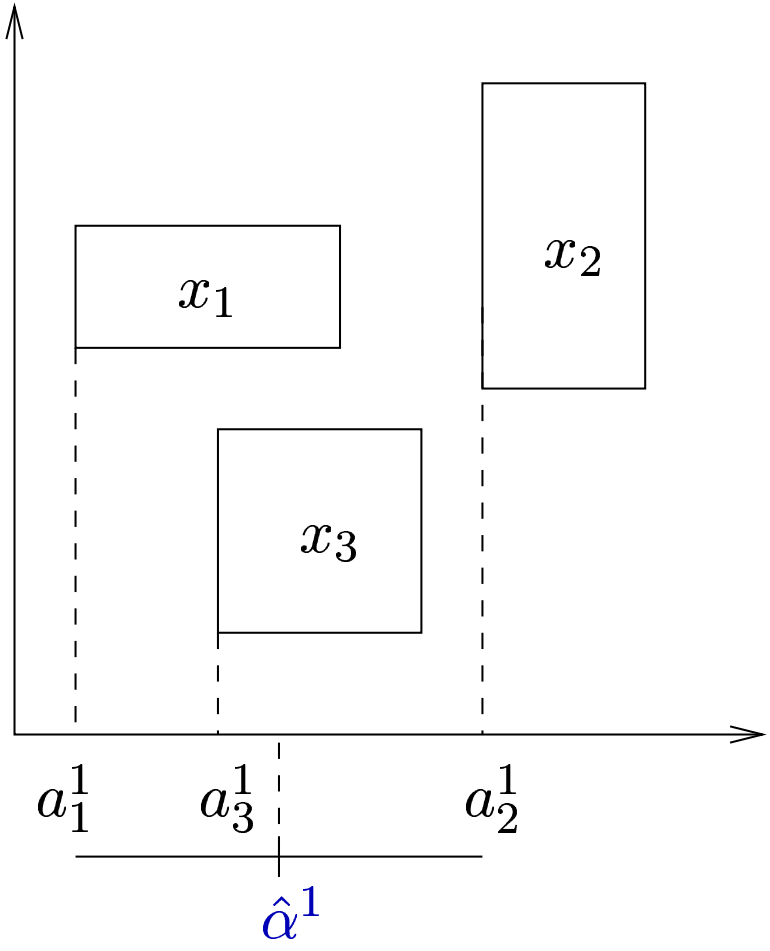
An example



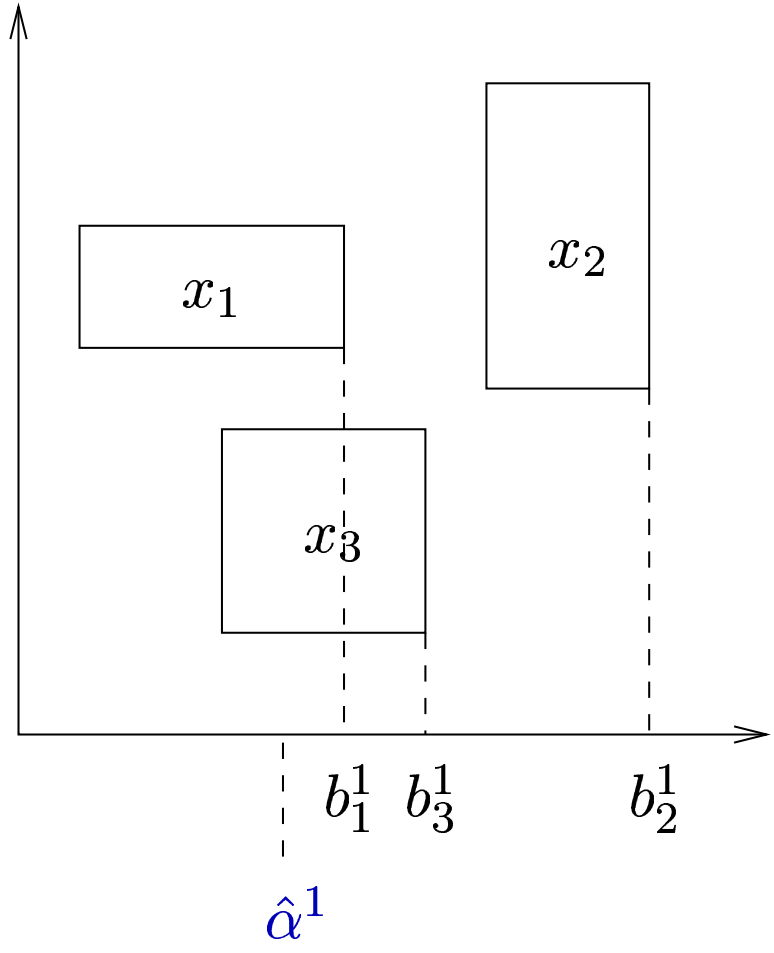
An example



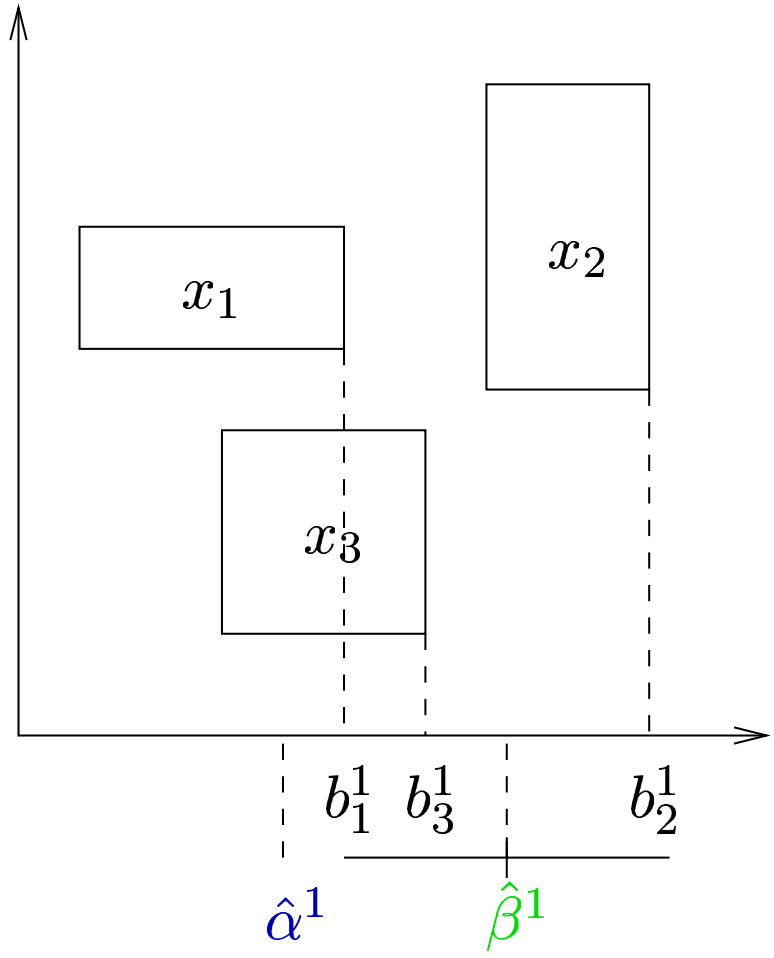
An example



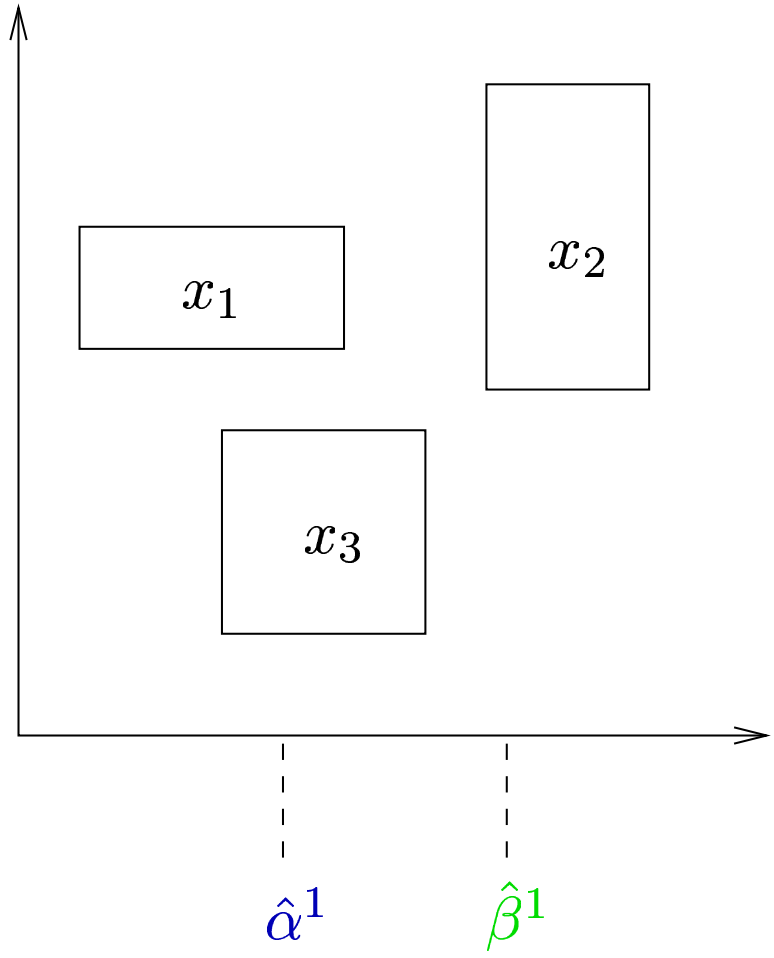
An example



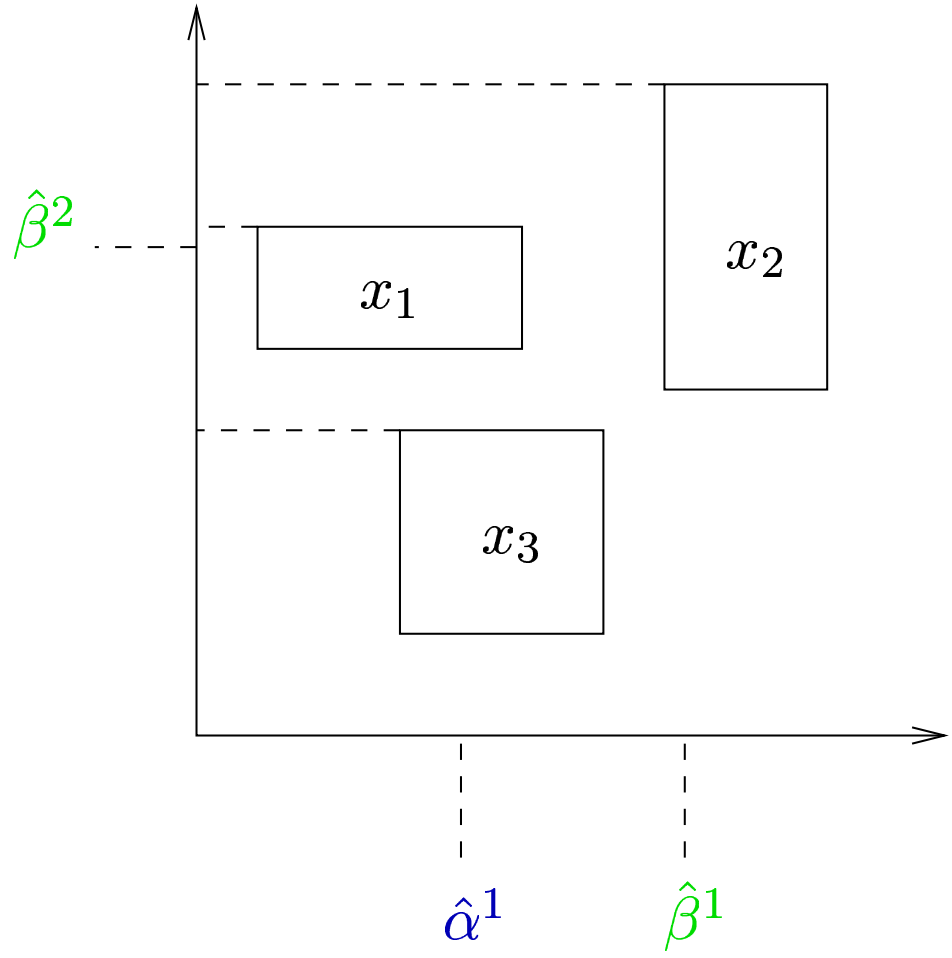
An example



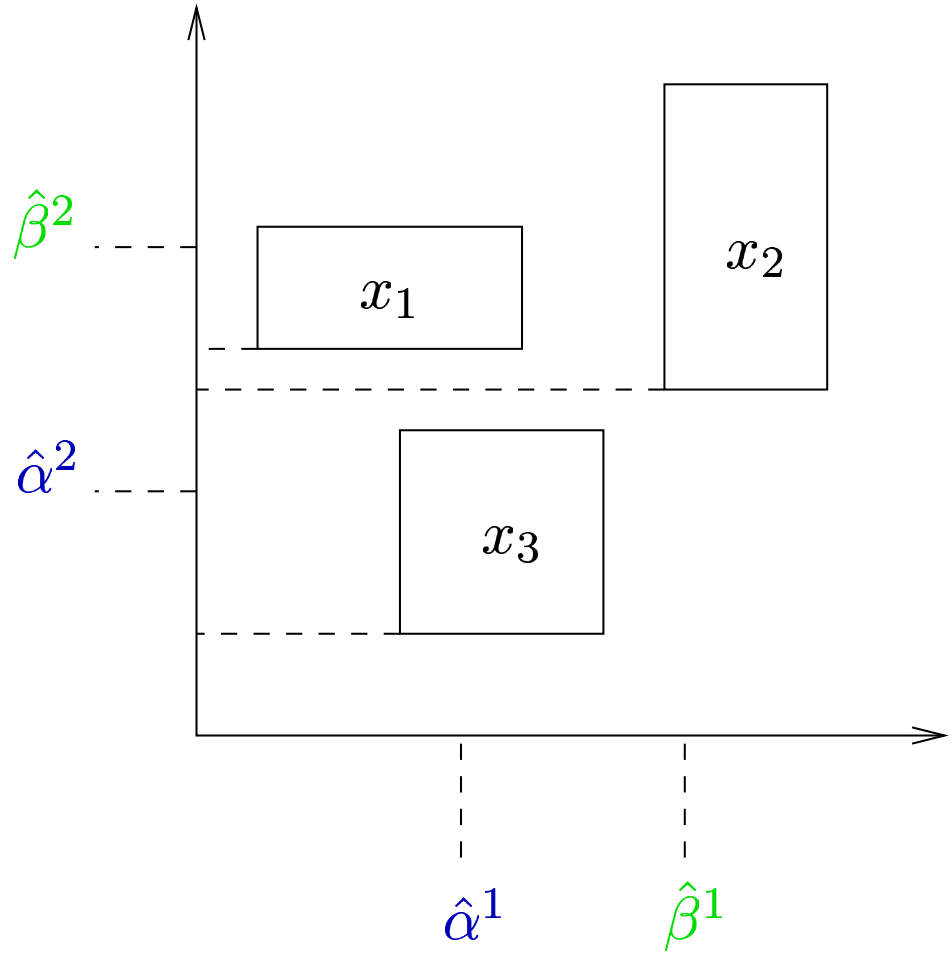
An example



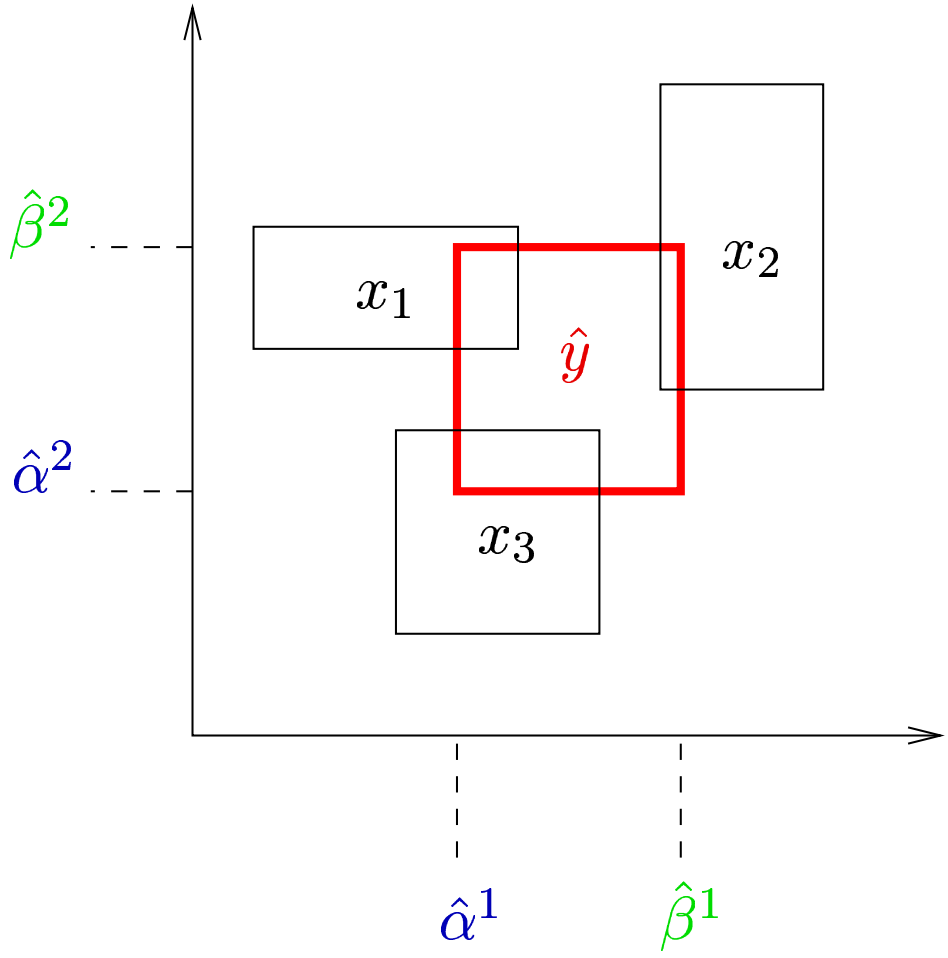
An example



An example



An example

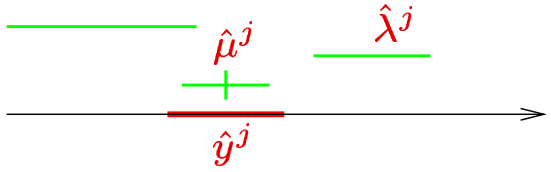


PART 4

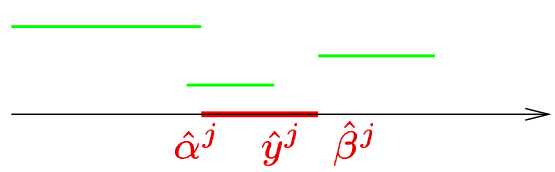
Normalization

Measure of centrality and dispersion

Two “central” intervals $\hat{y}^j$:



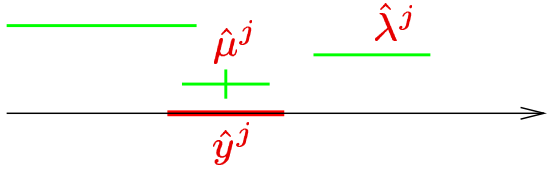
The “median” interval



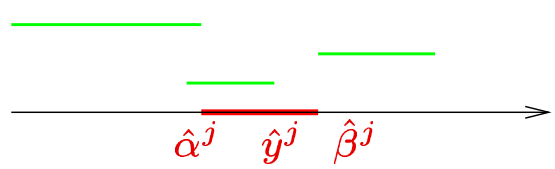
The “middle” interval

Measure of centrality and dispersion

Two "central" intervals $\hat{y}^j$:



The "median" interval



The "middle" interval

Two measures of dispersion σ^j from a "central" interval:

The "star":

$$\sum_{i=1}^{n} d_H(x_i^j, \hat{y}^j)$$

$$\Downarrow$$

$$\sigma^j = \sum_{i=1}^{n} \max(|a_i^j - \hat{\mu}^j + \hat{\lambda}^j|, |b_i^j - \hat{\mu}^j - \hat{\lambda}^j|)$$

The "radius":

$$\max_{i=1\ldots n} d_H(x_i^j, \hat{y}^j)$$

$$\Downarrow$$

$$\sigma^j = \max_{i=1\ldots n} \max(|a_i^j - \hat{\alpha}^j|, |b_i^j - \hat{\beta}$$

Normalized distance or data table

Initial data table $(x_i^j)_{n\times p}$

$$x_i^j = [a_i^j, b_i^j]$$

$$d_H(x_i^j, x_{i'}^j)$$

Normalized distance or data table

Initial data table $(x_i^j)_{n\times p}$

$$x_i^j = [a_i^j, b_i^j]$$

$$d_H(x_i^j, x_{i'}^j)$$

$$\Downarrow$$

Normalized distance

$$\sum_{j=1}^{p} \frac{1}{\sigma^j} d_H(x_1^j, x_2^j)$$

$$\max_{j=1\ldots p} \frac{1}{\sigma^j} d_H(x_1^j, x_2^j)$$

Normalized distance or data table

Initial data table $(x_i^j)_{n\times p}$

$$x_i^j = [a_i^j, b_i^j]$$

$$d_H(x_i^j, x_{i'}^j)$$

$$\Downarrow$$

Normalized distance

$$\sum_{j=1}^{p} \frac{1}{\sigma^j} d_H(x_1^j, x_2^j)$$

$$\max_{j=1\ldots p} \frac{1}{\sigma^j} d_H(x_1^j, x_2^j)$$

Normalized data table $(z_i^j)_{n\times p}$

$$z_i^j = [\frac{a_i^j}{\sigma^j}, \frac{b_i^j}{\sigma^j}]$$

$$d_H(z_i^j, z_{i'}^j)$$

Normalized distance or data table

Initial data table $(x_i^j)_{n\times p}$

$$x_i^j = [a_i^j, b_i^j]$$

$$d_H(x_i^j, x_{i'}^j)$$

$$\Downarrow$$

Normalized distance

$$\sum_{j=1}^{p} \frac{1}{\sigma^j} d_H(x_1^j, x_2^j)$$

$$\max_{j=1\ldots p} \frac{1}{\sigma^j} d_H(x_1^j, x_2^j)$$

Normalized data table $(z_i^j)_{n\times p}$

$$z_i^j = [\frac{a_i^j}{\sigma^j}, \frac{b_i^j}{\sigma^j}]$$

$$d_H(z_i^j, z_{i'}^j)$$

$$\Downarrow$$

Initial distance

$$\sum_{j=1}^{p} d_H(z_1^j, z_2^j)$$

$$\max_{j=1\ldots p} d_H(z_1^j, z_2^j)$$

Normalized distance or data table

Initial data table $(x_i^j)_{n\times p}$

$$x_i^j = [a_i^j, b_i^j]$$

$$\frac{1}{\sigma^j} \quad d_H(x_i^j, x_{i'}^j)$$

$$\Downarrow$$

Normalized distance

$$\sum_{j=1}^{p} \frac{1}{\sigma^j} d_H(x_1^j, x_2^j)$$

$$\max_{j=1\ldots p} \frac{1}{\sigma^j} d_H(x_1^j, x_2^j)$$

=

Normalized data table $(z_i^j)_{n\times p}$

$$z_i^j = [\frac{a_i^j}{\sigma^j}, \frac{b_i^j}{\sigma^j}]$$

$$d_H(z_i^j, z_{i'}^j)$$

$$\Downarrow$$

Initial distance

$$\sum_{j=1}^{p} d_H(z_1^j, z_2^j)$$

$$\max_{j=1\ldots p} d_H(z_1^j, z_2^j)$$

Normalized distance or data table

Initial data table $(x_i^j)_{n\times p}$

$$x_i^j = [a_i^j, b_i^j]$$

$$\frac{1}{\sigma^j} \quad d_H(x_i^j, x_{i'}^j) \quad = \quad d_H(z_i^j, z_{i'}^j)$$

$$\Downarrow \qquad\qquad\qquad \Downarrow$$

Normalized distance | Initial distance

$$\sum_{j=1}^{p} \frac{1}{\sigma^j} d_H(x_1^j, x_2^j) \quad = \quad \sum_{j=1}^{p} d_H(z_1^j, z_2^j)$$

$$\max_{j=1\ldots p} \frac{1}{\sigma^j} d_H(x_1^j, x_2^j) \quad = \quad \max_{j=1\ldots p} d_H(z_1^j, z_2^j)$$

Normalized data table $(z_i^j)_{n\times p}$

$$z_i^j = [\frac{a_i^j}{\sigma^j}, \frac{b_i^j}{\sigma^j}]$$

Conclusion

- General approach for the “normalization” of k-means (dynamical clustering) algorithms
- Two normalized k-means methods for hyper-rectangles clustering:

Prototype	Distance	Measure of dispersion
The “median” hyper-rectangle	Hausdorff-based	The “star” from the “median” hyper-rectang
The “middle” hyper-rectangle	L_∞-Hausdorff	The “radius” deviation from the “middle” hyper-re

- Explicit formula for prototypes with a real L_1 or L_2 Hausdorff distance between hyper-rectangles ?

Normalized k-means clustering of hyper-rectangles

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