

# INTERSTATIS: The STATIS method for interval valued data.

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The STATIS method, proposed by L'Hermier des Plantes and Escoufier, is used to analyze multiple data tables, each with information from the same set of individuals. The differences and similitudes between said tables are analyzed by means of a structure called the *compromise*. In this paper we present a new algorithm for applying the STATIS method when the input consists of interval data. This proposal is based on Moore's interval arithmetic and the Centers Method for Principal Component Analysis with interval data, proposed by Cazes. In addition to presenting the INTERSTATIS method in an algorithmic way, important implementation considerations are also discussed. Finally, an execution example is shown, alongside the interpretation of its results.

**Keywords:** INTERSTATIS, STATIS, Interval Arithmetic, Interval PCA, Interval Data, Data Mining.

## 1 Introduction

Given the flexibility and various applications of the Principal Component Analysis (PCA), L'Hermier des Plantes [15] and Escoufier [8, 12] worked, sequentially, in a generalized version of the method, to study multiple data tables. The method, named **STATIS**, is capable of analyzing several groups of tables, referring to the same variables or the same individuals (**STATIS DUAL**). The **STATIS** uses the PCA as part of the necessary transformations to reach a structure called the *compromise*, used in evaluating the differences and similitudes amongst the input tables.

Taking into account the potential of the **STATIS**, as an 3-index information analysis tool, the initiative of extending the method to the case of interval symbolic objects [3, 7] was born. These objects are meant to represent second order

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individuals, whose given *concepts* are much more complex than simple points in  $\mathbb{R}^n$ . For example, interval vectors, histograms, graphs, trees, rules, sets, functions, etc. The semantic and representation power possessed by these objects is evident, in comparison to the classic ones which handle only real numbers.

Although there already exist works in the field of symbolic methods for data analysis, like the generalizations of the Principal Components Analysis (PCA) [5, 11, 17],  $k$ -means [22], Multidimensional Scaling (MDS) [6] and Pyramidal Classification [18], the **STATIS** method has not been reformulated to handle symbolic objects. The first step consists in finding a way to generalize the **STATIS**, while guaranteeing that the classic method is an specific case of the symbolic proposal. This restriction is important since it ensures that the proposal has a sound statistical meaning.

Initially, Moore's Interval Arithmetic (IA) [4, 16] was proposed to perform operations between intervals. This arithmetic was created to handle, in a bounded way, the uncertainty in operations amongst non-exact quantities, and thus, provides a natural transition for the elemental operations –addition, subtraction, division and multiplication– from the classic case to the symbolic one. Besides, it is simple in its definition, implementation and complies with the fact that the operations between real numbers are specific cases of the IA, making it a good starting point for the generalization of the **STATIS**.

Additionally, knowing that the PCA is an integral part of the **STATIS**, it was necessary to have a PCA variant capable of handling interval valued data. To solve this need the Centers PCA (CPCA) by Cazes et al. [5] was used. This PCA consists in obtaining the principal components for the centers matrix and then projecting the *minima* and *maxima* in supplementary, giving as a result a representative hypercube for each individual, where its variation (in width, depth and height) describes the correspondent individual's variation.

Following is a small remark about the notation used thorough this paper:

- $\mathbf{x} = [\underline{\mathbf{x}}, \overline{\mathbf{x}}] \in \mathcal{I}(\mathbb{R})$ : an interval in  $\mathbb{R}$  with *minima*  $\underline{\mathbf{x}}$  and *maxima*  $\overline{\mathbf{x}}$ .
- $\mathbf{V} = \{[\underline{\mathbf{v}}_1, \overline{\mathbf{v}}_1], [\underline{\mathbf{v}}_2, \overline{\mathbf{v}}_2], \dots, [\underline{\mathbf{v}}_n, \overline{\mathbf{v}}_n]\} \in \mathcal{I}(\mathbb{R}^n)$ : an interval vector in  $\mathbb{R}^n$ .
- $\mathbf{X} \in \mathcal{I}(\mathbb{M}^{n \times p})$ : a interval matrix  $\mathbf{X}$  with  $n$  individuals and  $p$  variables.
- Let  $\mathbf{a}, \mathbf{b} \in \mathcal{I}(\mathbb{R})$  :  $\mathbf{a} \hat{+} \mathbf{b}, \mathbf{a} \hat{-} \mathbf{b}, \mathbf{a} \hat{\times} \mathbf{b}, \mathbf{a} \hat{/} \mathbf{b}, \sqrt{\hat{\mathbf{a}}}$ : the IA operations for the addition, subtraction, multiplication, division and square root.
- In the case of the dot product between symbolic matrices, its definition is analog to the dot product between real matrices, but using the IA multiplication.

Note as well the use of boldface to denote interval valued variables. For example,  $\mathbf{X}$  denotes an interval matrix, while  $X$  stands for a classic matrix. This provision facilitates distinguishing between both cases throughout the paper.

## 2 INTERSTATIS with IA and Centers PCA

This first version of the INTERSTATIS for interval data, works by replacing the conventional –or classic– operations, with their IA counterparts. Also, the CPCA, with its interval inputs and outputs, replaces the classic PCA method.

During the preprocessing phase of the input matrices, it is a requisite to center them. For this step the Rodríguez [19] intervals mean was used. It follows:

**Definition 2.1** (Intervals Mean). Let  $\mathbf{Y}$  be an interval valued variable, defined over  $E = \{1, 2, \dots, n\}$  for  $\mathbf{Y} = \{[y_1, \bar{y}_1], [y_2, \bar{y}_2], \dots, [y_n, \bar{y}_n]\}$ , the mean is defined as:

$$\bar{\mathbf{Y}} = \left[ \frac{1}{n} \sum_{i=1}^n y_i, \frac{1}{n} \sum_{i=1}^n \bar{y}_i \right].$$

Following, the INTERSTATIS algorithm using IA and CPCA, as a generalization of the version presented by González and Rodríguez in [10].

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### INTERSTATIS with AI and CPCA

**Input:**  $r$  data tables (matrices)  $\mathbf{X}_k \in \mathcal{I}(\mathbb{M}^{n \times p_k})$  individuals  $\times$  variables of size  $n \times p_k$ , centered with respect to  $D$  (using Definition 2.1 for the means), where

- $n$  is the number of individuals, the same in the  $r$  measurements.
- $p_k$  is the number of variables in the  $k$ th measuring.
- $D = \text{diag}(1/n, 1/n, \dots, 1/n)$  is the weights matrix, invariant for the  $r$  measurements.
- $l = \sum_{k=1}^r p_k$  is the amount of variables in all tables.

**Output:** the following tables are generated:

- $\mathbf{T} \in \mathcal{I}(\mathbb{M}^{r \times r})$  with the correlations between tables (step 4).
- $\mathbf{E}_v \in \mathcal{I}(\mathbb{M}^{l \times l})$  with the evolution of the variables (step 7).
- $\mathbf{M}_i \in \mathcal{I}(\mathbb{M}^{n \times l})$  with the average individuals (step 7).
- $\mathbf{E}_i \in \mathcal{I}(\mathbb{M}^{rn \times l})$  with the evolution of the individuals (step 11).

**Interstructure:** (steps 1-4). Given that the individuals in the  $r$  measurements are the same, it is possible to compare their spatial distribution by means of the  $\mathbf{W}_i = \mathbf{X}_i \hat{\times} \mathbf{X}_i^T$  matrices. For this, the metric defined by the internal product is used

$$\langle \mathbf{W}_i, \mathbf{W}_j \rangle_{\phi} = \text{trace}(\mathbf{W}_i \hat{\times} \mathbf{W}_j) = \langle \vec{\mathbf{W}}_i \hat{\times} \vec{\mathbf{W}}_j \rangle_I$$

where  $\vec{\mathbf{W}}_i \in \mathcal{I}(\mathbb{R}^{n^2})$  is the vector formed by all the rows of the  $\mathbf{W}_i$  matrix, for  $i = 1, 2, \dots, r$ .

**Step 1:** Compute the  $\mathbf{W}_i \in \mathcal{I}(\mathbb{M}^{n \times n})$  matrices, given by  $\mathbf{W}_i = \mathbf{X}_i \widehat{\times} \mathbf{X}_i^T$  for  $i = 1, 2, \dots, r$ .

**Step 2:** Generate the following matrix

$$\mathbf{X} = \left[ \vec{\mathbf{W}}_1 \mid \vec{\mathbf{W}}_2 \mid \dots \mid \vec{\mathbf{W}}_r \right]_{\mathcal{I}(n^2 \times r)}$$

**Step 3:** Perform a CPCA for the triplet  $(\mathbf{X}, D_{\frac{1}{\sigma^2}}, \frac{1}{n^2} I_n^2)$ .

Store the resulting principal components as

$$\mathbf{T} = [\mathbf{PC}_1, \mathbf{PC}_2, \dots, \mathbf{PC}_r]_{\mathcal{I}(r \times r)}.$$

Also store the first eigenvector, noted by  $u = (u_1, u_2, \dots, u_r)$ , and the first eigenvalue  $\lambda_1$ , both real, to use them later on in the creation of the *compromise*. It is not necessary to convert these to interval data since the IA defines operations between interval and real values.

**Step 4:** Plot the correlations circle from the  $\mathbf{T}$  matrix. Each point represents a data table, where close points mean similar individual configurations, and parallel vectors represent homothetic configurations.

**Intrastructure:** (steps 5-12). The evolutive study of the individuals and the variables is performed through the *compromise*  $\sum_{k=1}^r \beta_k \mathbf{W}_k$  product of the CPCA with parameters  $(\tilde{\mathbf{X}}, I_l, D)$ , where  $\beta_k$  is defined in step 5 and  $\tilde{\mathbf{X}}$  is defined as:

$$\tilde{\mathbf{X}} = \left[ \beta_1 \widehat{\times} \mathbf{X}_1 \mid \beta_2 \widehat{\times} \mathbf{X}_2 \mid \dots \mid \beta_r \widehat{\times} \mathbf{X}_l \right]_{\mathcal{I}(n \times l)}$$

**Evolution of the variables:** (steps 5-9)

**Step 5:** Compute  $\beta = (\beta_1, \beta_2, \dots, \beta_r) = \frac{1}{\sqrt{\lambda_1}} u$ .

**Step 6:** Compute the blocks matrix  $\tilde{\mathbf{X}}$  as follows:

$$\tilde{\mathbf{X}} = \left[ \beta_1 \widehat{\times} \mathbf{X}_1 \mid \beta_2 \widehat{\times} \mathbf{X}_2 \mid \dots \mid \beta_r \widehat{\times} \mathbf{X}_l \right]_{\mathcal{I}(n \times l)}$$

**Step 7:** Perform a CPCA for  $(\tilde{\mathbf{X}}, I_l, D)$ . Store the principal components  $\mathbf{M}_i$  and the principal correlations  $\mathbf{E}_v$ , in the following way

$$\mathbf{M}_i = [\mathbf{C}_1, \mathbf{C}_2, \dots, \mathbf{C}_l]_{\mathcal{I}(n \times l)} \quad y \quad \mathbf{E}_v = [\mathbf{PC}_1, \mathbf{PC}_2, \dots, \mathbf{PC}_n]_{\mathcal{I}(l \times l)}.$$

**Step 8:** Plot the correlations circle from  $\mathbf{E}_v$ , in which it is possible to study the evolution of the variables.

**Step 9:** Plot the principal plane based on  $\mathbf{M}_i$ , in which the  $n$  average individuals (see definition in [13]) are represented.

**Evolution of the individuals:** (steps 10-12)

**Step 10:** Compute the IND matrix, defined by blocks as:

$$\text{IND} = \begin{bmatrix} \mathbf{W}_1 \\ \mathbf{W}_2 \\ \vdots \\ \mathbf{W}_r \end{bmatrix}_{\mathcal{I}(rn \times n)}$$

**Step 11:** Compute the coordinates for the individuals throughout the different tables, noted as  $\mathbf{E}_i$ , through the following matrix product:

$$\mathbf{E}_i = \text{IND} \widehat{\times} \mathbf{M}_i$$

**Step 12:** Plot the principal plane using  $\mathbf{E}_i$ . In this chart, one can study the evolution of the individuals.

The following results prove that the classical STATIS is a particular case of the INTERSTATIS with IA and CPCA.

**Definition 2.2** (Classical and interval matrix equivalence). Let  $X \in \mathbb{M}^{n \times p}$  and  $\mathbf{Y} \in \mathcal{I}(\mathbb{M}^{n \times p})$ . Then,  $X$  is matrix-equivalent to  $\mathbf{Y}$ , noted by  $X \equiv \mathbf{Y}$  if

$$X \equiv \mathbf{Y} \iff \forall x_{ij} \in X, \forall \mathbf{y}_{ij} \in \mathbf{Y} : x_{ij} = \underline{\mathbf{y}_{ij}} = \overline{\mathbf{y}_{ij}}$$

with  $i = \{1, 2, \dots, n\}$  and  $j = \{1, 2, \dots, p\}$ .

**Lemma 2.1.** *The classic PCA is a particular case of the CPCA [19].*

**Lemma 2.2.** *The classic operations  $\{+, -, \times, /, \sqrt{\cdot}\}$  are particular cases of the IA [16].*

**Theorem 2.3.** *The classic STATIS is a particular case of the INTERSTATIS with IA and CPCA.*

*Proof.* Let  $X \in \mathbb{M}^{n \times p}$  y  $\mathbf{Y} \in \mathcal{I}(\mathbb{M}^{n \times p})$  with  $X \equiv \mathbf{Y}$ .

By lemma 2.1 the steps 3, 4, 7, 8, 9 and 12 are equivalent for the classic and the symbolic case. By lemma 2.2, the steps 1 y 11 are equivalent in the same way. Step 5 involves only real values, and the remaining steps, 2, 6 and 10, don't perform any arithmetic calculations since they are only block reordering of matrices.

Therefore, when the involved interval matrices are logically equivalent to matrices in  $\mathbb{M}^{n \times p}$  –according to definition 2.2– the classic and the symbolic case are equivalent.  $\square$

**Corollary 2.4.** *Let  $X \in \mathbb{M}^{n \times p}$  and  $\mathbf{Y} \in \mathcal{I}(\mathbb{M}^{n \times p})$  with  $X \equiv \mathbf{Y}$ , then the output of the STATIS taking  $X$  as input, is the same as the INTERSTATIS output, taking  $\mathbf{Y}$  as input.*

### 3 Experiments

This section is concerned with the data used in the tests and the interpretation of the correspondent results.

For the experiments a data table based on the wine data by Abdi [1] was generated. This table describes the criteria from three different wine experts, on six different types of wines, depending on the type of oak barrels used in their aging process. For each wine sample, the intensity of a given flavor is defined in a scale from 1 to 10. Also, for the generated table, the center of each one of its entries is the same as the correspondent entry in the original data table. Mathematically, let  $X$  be the classic wines table and  $\mathbf{Y}$  the test data matrix, then

$$\forall x_{ij} \in X, \forall \mathbf{y}_{ij} \in \mathbf{Y} : x_{ij} = m(\mathbf{y}_{ij}),$$

with  $i = \{1, 2, \dots, n\}$ ,  $j = \{1, 2, \dots, p\}$  and where  $m(\mathbf{y})$  is the middle point or center of the interval  $\mathbf{y}$ .

This property for the test table is based on the way the CPCA works. As mentioned earlier, said method projects, for each interval, the center and then the *minima* and *maxima* in supplementary. Therefore, if the center –for each entry– of the test table is equal to the value in the original table, the individuals will have a similar spatial placement in the experiment.

Table 2 shows the test table, for which, the width of any of its elements is not greater than 1. This helps to keep the results compact.

The INTERSTATIS was initially coded in Mathematica 6.0, and then in C++, using the Libaa [9] library to handle the interval valued data, LAPACK [2] to compute the eigensystems and PLplot [14] for charting. The charts in this paper were generated in Mathematica.

#### 3.1 Interpretation of the results

Each of the figures presents the output of the STATIS using the original data table, alongside the output of the INTERSTATIS using the test table, with the first two axes used for plotting.

Analyzing figure 1b, the test data produces a very similar output to that of the STATIS, given that experts 1 and 2 are correlated given their similitude, leaving expert 3 on its own. Nonetheless, the distance between the groups of tables is variable, as a consequence of the use of interval data. For example, the closeness of the borders for experts 2 and 3 indicates a similar behavior in said borders, nonexistent in the classic case. It is precisely this capability of handling a level of uncertainty, the advantage of this symbolic proposal, since it analyzes not only the variation amongst individuals, but their internal variation as well.

Figure 2b presents a very similar correlations structure in comparison to the one generated by the STATIS, showing three groupings of variables, but in the symbolic case overlapping occurs amongst said groups. It should be noted that the representations for the variables, in both figure 2a and 2b, are near the

borders of the circle, clear sign of marked correlations. It follows that results drawn upon them are thus valid.

In the average individuals plane (figures 3a and 3b) the additional information provided by the INTERSTATIS can be appreciated, through the size of the rectangles, given that their size is proportionate to the average size of the represented individual.

In the last step (figures 4a and 4b) the evolution of the individuals is studied, that is, their changes throughout all the tables or measurements. Given the amount of rectangles present ( $r \times n$ ), this plane should ideally be plotted using a subset of the individuals, to aid in its interpretation. For example, visualize the evolution of a pair of individuals to better appreciate their variation and interaction. Although this technique is valid in both cases, it has an even larger impact in the symbolic approach, since it tends to saturate the plot rapidly.

It is important to remark that the symbolic proposal adds analysis information without sacrificing that already provided by the classic method, that is, produces more information by the use of intervals. Nevertheless, the interpretation complexity is increased as well.

An important aspect that heavily affects the output of the method is the width of the input intervals. Even though the size of the rectangles is useful because it represents the variation of an individual or a variable, it becomes a problem if it becomes too large and thus, the input tables should be normalized so that the width of its elements is reduced.

Another relevant aspect of symbolic analysis, which adds value to the proposal, lies in its ability to reveal possible interactions between individuals or variables, hidden in the results obtained through the classic methods. For example, when overlapping between individuals occurs, a more elaborate relationship amongst them is revealed, instead of just that expressed by closeness of points in the plane. There is also the case when in the classic output, the points are clearly separated, but in the symbolic results they overlap, thus changing the results of the interpretation. These situations are not strange, considering that traditional methods use averaging or sampling to represent groups of individuals—in big sets of data—, therefore incurring in information loss.

## 4 Conclusions and future work

A new proposal for applying the STATIS method when the input data consists of interval valued data was proposed. This proposal exploits the additional semantic provided by symbolic objects, permitting the method to handle internal variation in the input data, therefore allowing the use of representations which better reflect the true nature of that which is measured. It was also proved that the STATIS is a particular case of the proposed INTERSTATIS with IA and CPCA, thus validating its statistical usefulness.

Another important benefit resides in the use of symbolic objects *per se*, given that they can be used to compact copious amounts of data, while minimizing data loss during the process. Once these symbolic objects are created, the

INTERSTATIS –as well as any other symbolic method– allows the exploration and analysis of the totality (or a majority) of the individuals present in the original data table, thereby eliminating the bias introduced by sampling, which affects traditional methods.

With regards to future work, although the obtained results have been positive, there exist other interval arithmetics (and modifications of these) that could help make the output of the INTERSTATIS more compact. There is also room for research concerning the preprocessing of the input data to make the interval widths smaller. For this work, a maximum width of 1 was chosen, to help alleviate the increasing size of the rectangles in the results. Also, a careful study of those operations which increment the width of the results would be useful as well. Finally, a generalization of the STATIS method to treat histogram valued data is an open problem.

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Wine	Expert 1			Expert 2			Expert 3				
	Barrel	Fruit	Wood	Coffee	Red Fruit	Roast	Vanilla	Wood	Fruit	Butter	Wood
1	1	1	6	7	2	5	7	6	3	6	7
2	2	5	3	2	4	4	4	2	4	4	3
3	2	6	1	1	5	2	1	1	7	1	1
4	2	7	1	2	7	2	1	2	2	2	2
5	1	2	5	4	3	5	6	5	2	6	6
6	1	3	4	4	3	5	4	5	1	7	5

Table 1: Abdi's Wines [1].

Wine	Barrel	Expert 1			Expert 2			Expert 3			
		Fruit	Wood	Coffee	Red Fruit	Roast	Vanilla	Wood	Fruit	Butter	Wood
1	1	[0.9, 1.1]	[5.8, 6.2]	[6.5, 7.5]	[2, 2]	[4.9, 5.1]	[6.5, 7.5]	[5.8, 6.2]	[2.9, 3.1]	[5.9, 6.1]	[6.8, 7.2]
2	2	[4.8, 5.2]	[2.9, 3.1]	[2, 2]	[4, 4]	[3.9, 4.1]	[3.6, 4.4]	[2, 2]	[3.9, 4.1]	[3.8, 4.2]	[3, 3]
3	2	[5.4, 6.6]	[0.8, 1.2]	[0.95, 1.05]	[4.8, 5.2]	[1.85, 2.15]	[0.9, 1.1]	[0.8, 1.2]	[6.8, 7.2]	[1, 1]	[0.9, 1.1]
4	2	[6.9, 7.1]	[0.75, 1.25]	[1.85, 2.15]	[6.9, 7.1]	[2, 2]	[0.6, 1.4]	[1.7, 2.3]	[2, 2]	[1.8, 2.2]	[1.8, 2.2]
5	1	[1.9, 2.1]	[5, 5]	[3.6, 4.4]	[2.7, 3.3]	[5, 5]	[6, 6]	[4.4, 5.6]	[1.9, 2.1]	[6, 6]	[5.8, 6.2]
6	1	[2.8, 3.2]	[3.8, 4.2]	[3.6, 4.4]	[2.9, 3.1]	[4.75, 5.25]	[3.9, 4.1]	[4.6, 5.4]	[0.9, 1.1]	[6.9, 7.1]	[5, 5]

Table 2: Test data (widths  $\leq 1$ ).

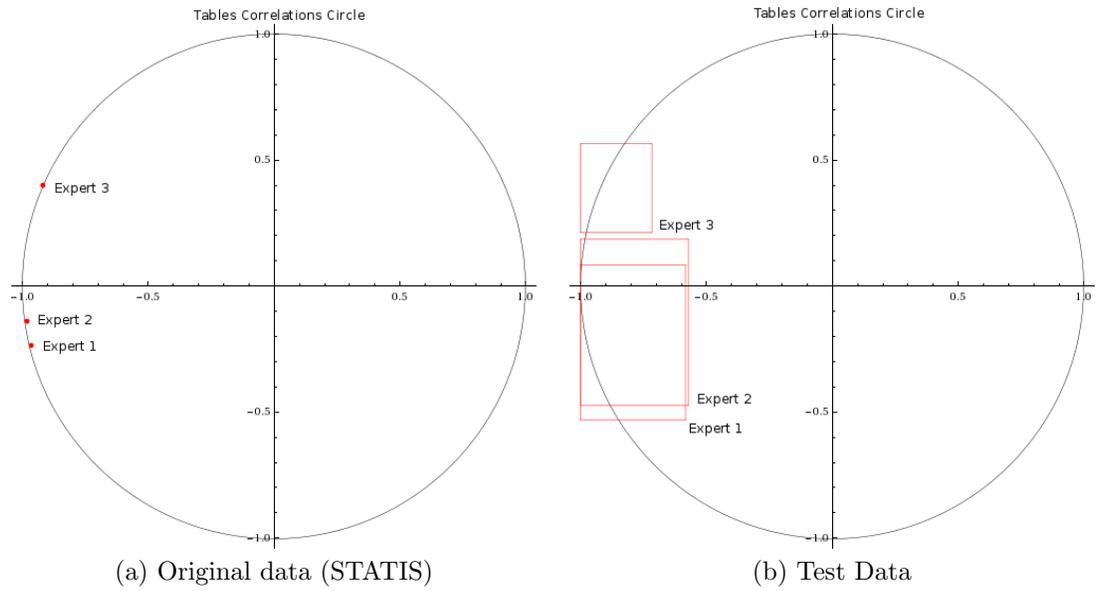


Figure 1: Comparison of the correlations amongst data tables.

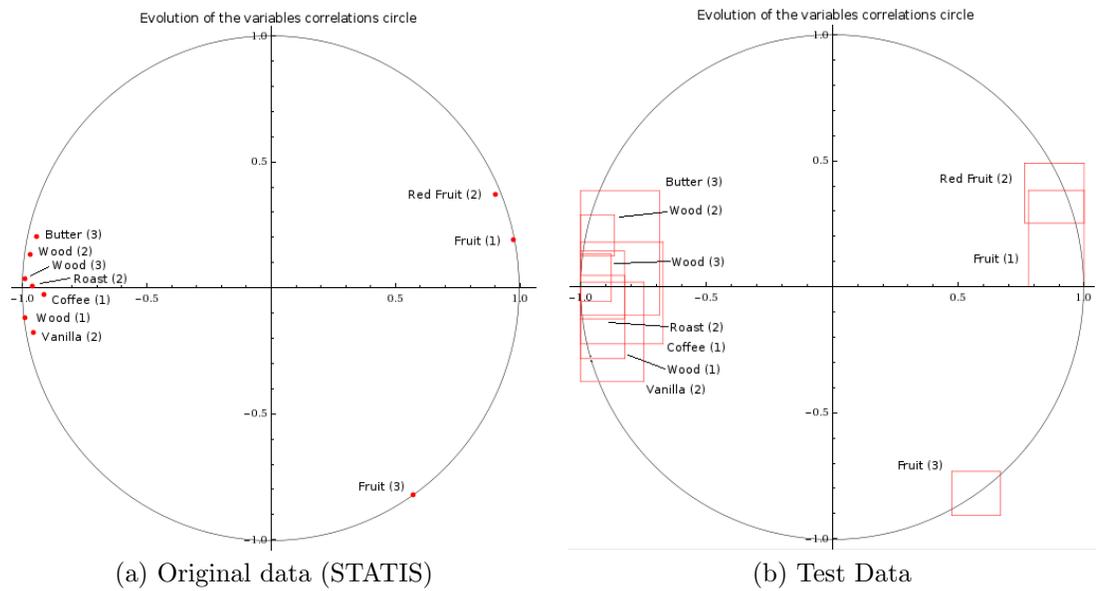


Figure 2: Evolution of the variables comparison.

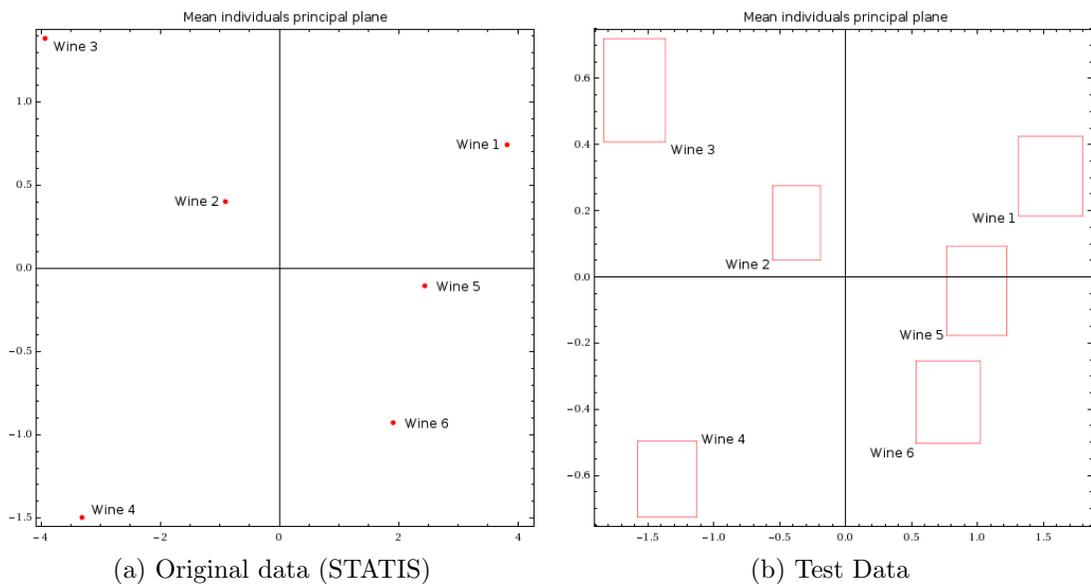


Figure 3: Comparison of the average individuals.

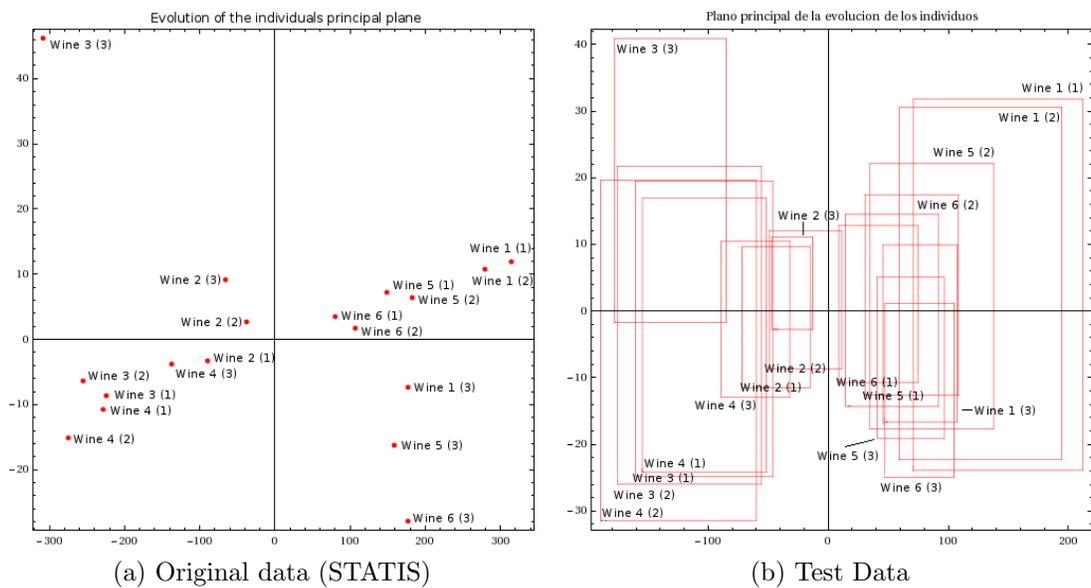


Figure 4: Evolution of the individuals comparison.