1 Topic

Linear Discriminant Analysis – Data Mining Tools Comparison (Tanagra, R, SAS and SPSS).

Linear discriminant analysis is a popular method in domains of statistics, machine learning and pattern recognition. Indeed, it has interesting properties: it is rather fast on large bases; it can handle naturally multi-class problems (target attribute with more than 2 values); it generates a linear classifier linear, easy to interpret; it is robust and fairly stable, even applied on small databases; it has an embedded variable selection mechanism. Personally, I appreciate linear discriminant analysis because we can have multiple interpretations (probabilistic, geometric), and thus highlights various aspects of supervised learning.

Discriminant analysis is both a descriptive and a predictive method¹. In the first case, we say Canonical Discriminant Analysis. We can consider the approach as a dimension reduction technique (a factor analysis). We want to highlight latent variables which explain the difference between the classes defined by the target attribute. In the second case, we can consider the approach as a supervised learning algorithm which intends to predict efficiently the class membership of individuals. Because we have a linear combination of the variables, we have a linear classifier. The purposes are therefore not intrinsically identical even if, when we analyze deeply the underlying formulas, we realize that the two approaches are closely related. Some bibliographic references maintain anyway the confusion by presenting them in a single framework.

Tanagra differentiates clearly the two approaches by providing two separate components: LINEAR DISCRIMINANT ANALYSIS (SPV LEARNING tab) for the prediction approach; CANONICAL DISCRIMINANT ANALYSIS (FACTORIAL ANALYSIS tab) for the descriptive (factorial) approach. It is the same for SAS software with respectively DISCRIM and CANDISC procedures². Others combine them. This is the case for SPSS and R, mixing results which refer to different goals. For specialists who know how to distinguish important elements depending on the context, this amalgam is not a problem. For beginners, it is a bit more problematic. One can be disturbed by results which do not seem directly related to the purposes of the study.

In this tutorial, we detail in a first time with the TANAGRA outputs about Predictive Linear Discriminant Analysis. In a second time, we compare them to the results of R, SAS and SPSS. The objective is to identify important information for predictive analysis i.e. get a simple classification system, get indications on the influence (for the interpretation) and the relevance of variables (statistical significance), and dispose of a variable selection mechanism.

2 Dataset

We use the « <u>alcohol.xls</u> » data file. We want to predict the alcohol type (Kirsch, Mirabelle and Pear) from their composition (butanol, etc.; 6 descriptors). The sample contains 77 instances.

¹ <u>http://en.wikipedia.org/wiki/Linear_discriminant_analysis</u>, <u>http://en.wikipedia.org/wiki/Discriminant_function_analysis</u> The distinction between the two approaches is clearly defined on the French version of Wikipedia (http://fr.wikipedia.org/wiki/Analyse_discriminante - http://fr.wikipedia.org/wiki/Analyse_discriminante_linéaire).

² http://support.sas.com/documentation/

3 Linear discriminant analysis under Tanagra

3.1 Importing dataset

After we launch Tanagra, we create a new diagram by clicking on the FILE / NEW menu. We select the "**alcohol.xls**" data file.

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Tanagra shows the number of instances (77) and the number of variables (7, including the class attribute TYPE) which are loaded.

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3.2 Linear discriminant analysis

The DEFINE STATUS enables to specify the status of the variables in the analysis: TYPE is the target attribute (TARGET); the others are the descriptors (INPUT).



We add the LINEAR DISCRIMINANT ANALYSIS (SPV LEARNING tab) into the diagram. We click on the contextual menu VIEW to obtain the results.

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3.2.1 Confusion matrix and resubstitution error rate

By applying the classifier to the learning sample, we obtain the confusion matrix: (9 + 6) = 15 instances are misclassified. The resubstitution error rate is 19.48% = 15 / 77.

Class	Classifier performances										
Error rate 0.1948											
Val	Values prediction Confusion matrix										
Value	Recall	1-Precision		KIRSCH	MIRAB	POIRE	Sum				
KIRSCH	1.0000	0.0000	KIRSCH	18	0	0	18				
MIRAB	0.7931	0.2813	MIRAB	0	23	6	29				
POIRE	0.7000	0.2222	POIRE	0	9	21	30				
	Sum 18 32 27 77										

Because we use the same dataset for the learning and the evaluation of the classifier, it is well known that the resubstitution error rate is *often* optimistic.

3.2.2 Statistical evaluation of the classifier

The Wilks' lambda statistic is used for the overall evaluation of the model. It evaluates the gap between the group centroids (the groups defined by the target attribute). When its value is close to 0, we expect that we get an efficient classifier. This point of view is closely related to the MANOVA³.

MANOVA

Stat	Value	p-value
Wilks' Lambda	0.1567	-
Bartlett C(12)	132.5414	0
Rao F(12, 138)	17.5556	0

In our case, $\Lambda = 0.1567$, this is a rather a good value (the worst value is 1). To evaluate the significance of the gap between the centroids, we use the Bartlett's C or the Rao's F transformations (C = 132.5414, d.f. = 12; χ^2 distribution; F = 17.5556, d.f. 1 = 12 and d.f. 2 = 138; Fisher distribution). At the 5% level, we reject the null hypothesis: the group centroids are significantly different.

By coupling this statistical test with the analysis of the confusion matrix, we understand that the good behavior of the model relies primarily on the situation of KIRSCH which we can detect perfectly. The descriptive analysis will confirm this result.

3.2.3 Classification functions

The following table gives the classification functions (Figure 1). They are used when we want classifying instances (KIRSCH, MIRAB or POIRE).

³ <u>http://en.wikipedia.org/wiki/Multivariate_analysis_of_variance</u>

	Clas	Classification functions							
Attribute	KIRSCH	MIRAB	POIRE						
MEOH	0.000659	0.015208	0.016407						
ACET	0.000445	0.004944	-0.00377						
BU1	-0.039342	0.556654	0.553048						
MEPR	0.186892	0.035901	0.102271						
ACAL	0.039174	-0.160881	-0.127328						
LNPRO1	6.378935	4.86937	5.34143						
constant	-24.686164	-25.141755	-29.631644						

Figure 1 – Classification functions - Model without variable selection

Let us consider a new unlabeled instance $\boldsymbol{\omega}$ to classify.

MEOH	ACET	BU1	MEPR	ACAL	LNPRO1
707.0	131.0	15.0	28.0	9.0	4.89

We apply the classification function for each class value. For instance, for KIRSCH we have:

S(ω, **KIRSCH)** = 0.000659 x 707 + 0.000445 x 131 - 0.039342 x 15 + 0.186892 x 28 + 0.039174 x 9 + 6.378935 x 4.89 - 24.68616 = **12.0264**

We apply the function for each class, we obtain:

	KIRSCH	MIRAB	POIRE
S(.)	12.0264	17.9763	17.6072

MIRAB has the highest score [S(MIRAB) = 17.9763]. We assign the value MIRAB to this instance.

This classification operation is one of the main goals of the predictive analytics process.

3.2.4 Assessing the influence of the variables in the model

The influence of the predictive variables is not the same. The discriminant analysis can measure their contribution in the model. Tanagra shows these effects in the Statistical Evaluation part of the coefficients table (green).

	Classification functions St			Statistical	Evaluation		
Attribute	KIRSCH	MIRAB	POIRE	Wilks L.	Partial L.	F(2,69)	p-value
MEOH	0.000659	0.015208	0.016407	0.205214	0.763359	10.69497	0.00009
ACET	0.000445	0.004944	-0.00377	0.176705	0.88652	4.41622	0.015677
BU1	-0.039342	0.556654	0.553048	0.213115	0.73506	12.43496	0.000024
MEPR	0.186892	0.035901	0.102271	0.192667	0.813074	7.93155	0.000793
ACAL	0.039174	-0.160881	-0.127328	0.161541	0.969735	1.07671	0.346369
LNPRO1	6.378935	4.86937	5.34143	0.171693	0.912399	3.31241	0.042303
constant	-24.686164	-25.141755	-29.631644		-		

Remember that the overall lambda of the model is Λ = 0.1567 (Section 3.2.2).

The first column ("Wilks L.") indicates the lambda of the model if we remove the variable. For instance, if we remove MEOH from the classifier, the new value of the lambda for the model containing all the predictive variables except MEOH is $\Lambda_{\{-MEOH\}} = 0.205214$. The higher is the difference with the initial value of lambda, the most significant is the variable. "Partial lambda" is the ratio between these values. For instance, Partial L. $\{-MEOH\}$ = 0.1567 / 0.205214 = 0.763.

The last two columns are dedicated to the checking of the contribution of each variable. They are based on the comparison of the lambda with and without the variable that we intend to evaluate. For our dataset, only ACAL is not significant at the 5% level (p-value_{-ACAL} = 0.346369 > 5%).

3.3 Variable selection

We can select the relevant variables by using a stepwise approach.

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For this, we use the STEPDISC (FEATURE SELECTION tab) component. Tanagra can implement forward and backward strategies. We choose the forward strategy for our dataset. We start with the null model. We add sequentially the most significant variable as long as it is significant at the 1% level.

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Because we add STEPDISC after DEFINE STATUS 1 into the diagram, it searches the relevant variables among those defined as INPUT into the preceding component. We click on the VIEW menu to obtain the results, 3 variables are selected: BU1, MEPR, MEOH

Tanagra provides the details of the search processing. We will describe them later (cf. SAS outputs).

All we need to do is to add again the LINEAR DISCRIMINANT ANALYSIS component **after** STEPDISC into the diagram. Tanagra performs the learning process on the selected variables only.



The resubstitution error rate is 25.97%. It seems worse than the model with all the predictive attributes (19.48%). But we know that the resubstitution error rate is not a good indicator of the performance of the models. It often favors the complex model incorporating a large number of predictive variables. We must use resampling approach (e.g. cross validation, bootstrap) to obtain a reliable evaluation of the error rate enabling to compare the models.

Here are the coefficients of the new classification functions.

	Class	ification funct	ions	Statistical Evaluation			
Attribute	KIRSCH	MIRAB	POIRE	Wilks L.	Partial L.	F(2,72)	p-value
BU1	-0.19402	0.432081	0.43508	0.303303	0.66354	18.25443	0
MEPR	0.158883	0.016375	0.080243	0.251168	0.801272	8.92855	0.000344
меон	0.007296	0.018626	0.019405	0.248931	0.808472	8.52844	0.000474
constant	-5.235679	-13.841347	-16.982045				

Figure 2 – Classification functions – Model after variable selection

We apply the new model on the instance to classify (section 3.2.3, the unused variables are grayed):

MEOH	ACET	BU1	MEPR	ACAL	LNPRO1
707.0	131.0	15.0	28.0	9.0	4.89

We obtain the following scores. Here also, we assign the instance to the MIRAB class.

	KIRSCH	MIRAB	POIRE	
S(.)	1.4610	6.2670	5.5103	

3.4 Canonical discriminant analysis (factorial discriminant analysis)

Descriptive discriminant analysis is not the main topic of this tutorial. But we present nevertheless the outputs of Tanagra to better understand the results provided of the other tools.

We add the CANONICAL DISCRIMINANT ANALYSIS (FACTORIAL ANALYSIS tab) component into the diagram. Then we click on the VIEW menu to obtain the results.



3.4.1 Eigenvalues table

This table provides the eigenvalues for each factor. We have also the proportion of explained variance. The significance test of each factor is provided.

Roots and Wilks' Lambda

Root	Eigenvalue	Proportion	Canonical R	Wilks Lambda	CHI-2	d.f.	p-value
1	3.75959	0.9168	0.888762	0.156652	132.5414	12	0
2	0.3412	1	0.504381	0.7456	20.99	5	0.000814

3.4.2 Canonical coefficients

The raw canonical coefficients enable to calculate the coordinate of the individuals on the factors. The unstandardized coefficients can be applied on the untransformed values of the variables.

Coefficients	Unstand	Unstandardized		rdized					
Attribute	Root n1	Root n2	Root n1	Root n2					
MEOH	-0.0033821	-0.000571	-0.6811478	-0.1150081					
ACET	0.0000465	0.0066574	0.0051822	0.7420478					
BU1	-0.1322048	0.0162599	-0.6469978	0.0795743					
MEPR	0.0256226	-0.053361	0.3454686	-0.7194653					
ACAL	0.0404876	-0.0297884	0.2160076	-0.1589256					
LNPRO1	0.2791911	-0.3894401	0.2753705	-0.3841107					
constant	1.89673943	3.17877051	-						

Figure 3 – Raw canonical coefficients

For the instance ω with the following description:

aniaal Discriminant Function

MEOH	ACET	BU1	MEPR	ACAL	LNPRO1
707.0	131.0	15.0	28.0	9.0	4.89

The coordinate on the first factor is,

```
Axe 1 = -0.0033821 x 707 + 0.0000465 x 131 - 0.1322048 x 15 + 0.0256226 x 28 + 0.0404876 x 9 + 0.2791911 x 4.89 + 1.89673943 = -0.0243
```

On the second factor, **Axe 2** = -0.000571 x 707 + ... - 0.3894401 x 4.89 + 3.17877051 = **0.2245**



By applying these functions on the individuals of the learning sample, we obtain a representation of the instances into the two first axes. By coloring the points according to its group membership, we can evaluate the class separability. We note that KIRSCH does not overlap of the others. This confirms the results of the confusion matrix obtained earlier (section 3.2.1).

3.4.3 Canonical structure

The canonical structure corresponds to the correlation between the variables and the factors. There are different ways to compute this correlation: ignoring the class membership (TOTAL); controlling the class membership (WITHIN); highlighting the class membership (BETWEEN).

Root		Root n1		Root n2			
Descriptors	Total	Within	Between	Total	Within	Between	
MEOH	-0.890038	-0.676771	-0.991413	-0.206864	-0.296316	-0.130768	
ACET	0.044423	0.021247	0.138243	0.560792	0.505278	0.990398	
BU1	-0.939650	-0.787683	-0.997447	-0.118534	-0.187184	-0.071407	
MEPR	-0.171747	-0.086008	-0.378992	-0.738951	-0.697111	-0.925400	
ACAL	-0.159216	-0.073841	-0.929377	-0.111430	-0.097353	-0.369131	
LNPRO1	0.521401	0.272151	0.968743	-0.235265	-0.231331	-0.248066	

Factor Structure Matrix - Correlations

At a first glance, we observe that: (1) the distinction between KIRSCH and the others relies mainly on MEOH and BU1 on the first axis; (2) the distinction between MIRAB and POIRE on the second axis is due to ACET and MEPR.

These results are consistent with the predictive approach where BU1, MEPR and MEOH were the selected variables after the STEPDISC FORWARD process at 1% level.

3.4.4 Class means on canonical variables

Tanagra provides the means on the axis of the three groups.

ТҮРЕ	Root n1	Root n2
KIRSCH	3.439733	-0.031885
MIRAB	-0.981483	0.674773
POIRE	-1.115073	-0.63315
Sq Canonical corr.	0.789898	0.2544

Group centroids on the canonical variables

It is especially interesting to visualize the class centroids within the graphical representation of the individuals. We observe that the closest group centroid to the instance to classify with the coordinates (-0.0243, 0.2245) is MIRAB (-0.981483, 0.674773).



3.4.5 Classification rule – Method 1

How to assign the individual with the coordinates (-0.0243, 0.2245) to one of the classes? Visually, we observe that the MIRAB centroid (-0.981483, 0.674773) is the closest to the instance to classify (with the coordinates: -0.0243, 0.2245). But we must confirm this visual impression with calculations.

To obtain a classification consistent with the one of the predictive discriminant analysis, we need – in addition to the group centroids - to know the proportion of the groups into the learning sample.

ТҮРЕ	Proportion
KIRSCH	0.233766
MIRAB	0.376623
POIRE	0.389610

For the instance ω that we want to classify, we calculate the squared generalized distance to the centroids:

$$D^{2}(\omega, c) = \sum_{k=1}^{K} [f_{k}(\omega) - \mu_{kc}]^{2} - 2 \times \ln \pi_{c}$$

Where *c* is one the classes, K is the number of factors, $f_k(\omega)$ is the coordinate of the instance on the factor k, μ_{kc} is the conditional mean of the class *c* on the factor k, π_c is the proportion of the class *c* in the learning sample.

Thus, for the various classes, we obtain:

 $D^{2}(\omega, \text{KIRSCH}) = (-0.0243 - 3.439733)^{2} + (0.2245 + 0.031885)^{2} - 2 \ln(0.233766) = 14.9723$ $D^{2}(\omega, \text{MIRAB}) = (-0.0243 + 0.981483)^{2} + (0.2245 - 0.376623)^{2} - 2 \ln(0.376623) = 3.0719$ $D^{2}(\omega, \text{POIRE}) = (-0.0243 + 1.115073)^{2} + (0.2245 + 0.63315)^{2} - 2 \ln(0.389610) = 3.8106$

We assign the individual to the class for which the centroid is the closest. In this case, this is MIRAB since $D^2(\omega, MIRAB)$ takes the smallest value.

Furthermore, we can calculate the posterior probability of the class membership:

$$P(Y = y/X) = \frac{\exp[-0.5 \times D^2(y)]}{\sum_u \exp[-0.5 \times D^2(u)]}$$

For the instance above:

 $P(Y(\omega) = KIRSCH / X) = 0.00056 / 0.36459 = 0.00154$ $P(Y(\omega) = MIRAB / X) = 0.21525 / 0.36459 = 0.59039$ $P(Y(\omega) = POIRE / X) = 0.14878 / 0.36459 = 0.40807$

We assign the instance $\boldsymbol{\omega}$ to the most likely group.

3.4.6 Classification rule - Method 2

By developing the formulas above and by multiplying them by -0.5, we obtain a linear classification functions based on the factorial coordinates. They are equivalent to the classification function provided by the predictive discriminant analysis, to within a constant which does not depend to the class membership. So, the classification characteristic is exactly the same.

We have:

$$S'(\omega, c) = \sum_{k=1}^{K} f_k(\omega) \times \mu_{kc} - \frac{1}{2} \sum_{k=1}^{K} \mu_{kc}^2 + \ln \pi_c$$

For the instance ω to classify:

S'(\omega, KIRSCH) = -0.0243 x 3.439733 + 0.2245 x (-0.031885) - (3.439733² + (-0.031885)²)/2 + ln(0.233766) = -7.4606 **S'(\omega, MIRAB**) = -0.0243 x (-0.981483) + 0.2245 x 0.674773 - ((-0.981483)² + 0.674773²)/2 + ln(0.376623) = -1.5105 **S'(\omega, POIRE**) = -0.0243 x (-1.115073) + 0.2245 x (-0.63315) - ((-1.115073)² + (-0.63315) ²)/2 + ln(0.389610) = -1.8798

We assign the instance to the MIRAB class. The result is necessarily consistent with that of the predictive discriminant analysis (sections 3.2.3 and 3.4.5).

3.4.7 Classification rule - Return on the original variables - Method 3

In the previous section, the classification functions are a linear combination of the factors. These last ones are a linear combination of the original variables. So, we can produce a classification function defined on the original predictive variables.

The classification functions on factors are the following:

Score function 1	KIRSCH	MIRAB	POIRE
f1	3.439733	-0.981483	-1.115073
f2	-0.031885	0.674773	-0.633150
Const	-7.369825	-1.685824	-1.764742

For instance, we have for KIRSH: **S'(KIRSH)** = 3.439733 x f1 -0.031885 x f2 - 7.369825

The factors **F1** are **F2** are linear combinations of original predictive attributes (Figure 3). We can thus produce a new version of the classification functions defined on the predictive attributes S'(.):

Score function 2	KIRSCH	MIRAB	POIRE
MEOH	-0.011615	0.002934	0.004133
ACET	-0.000052	0.004447	-0.004267
BU1	-0.455268	0.140729	0.137123
MEPR	0.089836	-0.061155	0.005214
ACAL	0.140216	-0.059838	-0.026286
LNPRO1	0.972760	-0.536805	-0.064744
constant	-0.946902	-1.402493	-5.892384

We can compare them to the classification functions obtained from the predictive linear discriminant analysis S(.) (Figure 1). We observe that the coefficients of S() and S'() are different, but the gap between the classes is the same for each variable.

	S() - Analyse prédictive				S'() - Déduite de l'analyse descriptive			Eca	rts entre coeffi	cients
Attribute	KIRSCH	MIRAB	POIRE		KIRSCH	MIRAB	POIRE	KIRSCH	MIRAB	POIRE
MEOH	0.000659	0.015208	0.016407		-0.011615	0.002934	0.004133	0.0123	0.0123	0.0123
ACET	0.000445	0.004944	-0.003770		-0.000052	0.004447	-0.004267	0.0005	0.0005	0.000
BU1	-0.039342	0.556654	0.553048		-0.455268	0.140729	0.137123	0.4159	0.4159	0.4159
MEPR	0.186892	0.035901	0.102271		0.089836	-0.061155	0.005214	0.0971	0.0971	0.0973
ACAL	0.039174	-0.160881	-0.127328		0.140216	-0.059838	-0.026286	-0.1010	-0.1010	-0.1010
LNPRO1	6.378935	4.869370	5.341430		0.972760	-0.536805	-0.064744	5.4062	5.4062	5.4062
constant	-24.686164	-25,141755	-29.631644	1	-0.946902	-1.402493	-5,892384	-23,7393	-23,7393	-23,739

This is the reason for which we have not the same score value for the individual ω

 $S(\omega, KIRSCH) \neq S'(\omega, KIRSCH)$; $S(\omega, MIRAB) \neq S'(\omega, MIRAB)$; $S(\omega, POIRE) \neq S'(\omega, POIRE)$

But the difference depends on the individual and not to the class membership.

 $[S(\omega, KIRSCH) - S'(\omega, KIRSCH)] = [S(\omega, MIRAB) - S'(\omega, MIRAB)] = [S(\omega, POIRE) - S'(\omega, POIRE)]$

In the end, the instances are classified in identical way. This is the most important.

4 Discriminant analysis under SAS

4.1 Proc DISCRIM

We perform the same analysis under SAS 9.3 using PROC DISCRIM. We use the following commands.

```
proc discrim data = alcohol;
    class type;
    var MEOH ACET BU1 MEPR ACAL LNPRO1;
    priors proportional;
run;
```

The **PRIORS** option enables to use the proportion measured on the learning set as classes' prior distribution in the learning process.

METHOD = NORMAL (multivariate normal distribution) and POOL = YES (used the pooled covariance matrix) are two important options for which the default values were used.

Overall description. SAS provides a description of the problem that we handle. We observe, among others, the proportion of classes into the learning sample.



Distances between the group centroids. We have the squared generalized distance between the group centroids.

Generalized Squared Distance to TYPE									
From TYPE	KIRSCH	MIRAB	POIRE						
KIRSCH	2.90687	21.99954	22.99300						
MIRAB	22.95339	1.95302	3.61372						
POIRE	24.01465	3.68153	1.88522						

The distance between the centroids of the same group is not null. In addition it is not symmetric!

This is really surprising. This is because the proportion of the groups is used in the formula⁴. For instance, the distance of the KIRSCH with itself is obtained with (see section 3.4.4 for the values of the centroids):

 $D^{2}(KIRSCH, KIRSCH) = (3.439733 - 3.439733)^{2} + (-0.031885 + 0.031885)^{2} - 2 \times \ln(0.233766) = 2.90687$

The generalized distance is not symmetric. For instance, between KIRSCH and MIRAB:

 $D^{2}(KIRSCH, MIRAB) = (3.439733 + 0.981483)^{2} + (-0.031885 - 0.674773)^{2} - 2 \times \ln(0.233766) = 22.95339$ $D^{2}(MIRAB, KIRSCH) = (-0.981483 - 3.439733)^{2} + (0.674773 + 0.031885)^{2} - 2 \times \ln(0.376623) = 21.99954$

Classification functions. SAS provides the same classification functions as Tanagra.

Lin	Linear Discriminant Function for TYPE					
Variable	Label	KIRSCH	MIRAB	POIRE		
Constant		-24.68616	-25.14175	-29.63164		
MEOH	MEOH	0.0006591	0.01521	0.01641		
ACET	ACET	0.0004450	0.00494	-0.00377		
BU1	BU1	-0.03934	0.55665	0.55305		
MEPR	MEPR	0.18689	0.03590	0.10227		
ACAL	ACAL	0.03917	-0.16088	-0.12733		
LNPRO1	LNPRO1	6.37894	4.86937	5.34143		

But SAS does not provide any information about the relevance of the variables.

Confusion matrix and resubstitution error rate. Last, SAS provides the confusion matrix.

Classi	ficat	ion Sum	The DIS(mary for	CRIM Pro Calibrat	oce ior	edure 1 Data 1 Disci	: W	ORK	ALC	OH
noou	Nu	Number of Observations and Percent Classified								
	Fro	om TYPE	KIRSCH	I MIRA	в	POI	RE	То	tal	
	KIF	RSCH	18	3 0 0	0	0	0	100	18 00	
	MIRAB		0.00) 2	23		6	100	29	
	POIRE		0.00) 79.3	9	20.	69 21	100	30	
	_		0.00	30.0	00	70.	00	100	.00	
	10	tal	23.38	3 3 3 41.5	52 56	35.	06	100	.00	
	Priors		0.23377	0.3766	52	0.389	61			
		En	or Count	Ectimate		for TV	DF			
		LI	KIRSCH	MIRAB	P	OIRE	Т	otal		
		Rate	0.0000	0.2069	0	.3000	0.1	1948		
		Priors	0.2338	0.3766	0	.3896				

⁴ http://www.math.wpi.edu/saspdf/stat/chap25.pdf

4.2 Variable selection with STEPDISC

SAS proposes STEPDISC, a tool for the variable selection which is consistent with the linear discriminant analysis principle. We perform a forward selection at 1% level (METHOD = FORWARD, SLENTRY = 1%):

We compare the detailed results with those of Tanagra (Figure 4).

De	Detailed results						
N°	d.f	Best	Sol.1	Sol.2	Sol.3	Sol.4	Sol.5
1	(2, 74)	BU1 L:0.299 F:86.75 p:0.0000	BU1 L:0.299 F:86.75 p:0.0000	MEOH L:0.363 F:64.82 p:0.0000	LNPRO1 L:0.771 F:10.98 p:0.0001	MEPR L:0.838 F:7.16 p:0.0014	ACET L:0.918 F:3.29 p:0.0429
2	(2, 73)	MEPR L:0.249 F:7.34 p:0.0012	MEPR L:0.249 F:7.34 p:0.0012	MEOH L:0.251 F:6.95 p:0.0017	ACET L:0.275 F:3.17 p:0.0478	LNPRO1 L:0.276 F:3.05 p:0.0535	ACAL L:0.298 F:0.18 p:0.8353
3	(2, 72)	MEOH L:0.201 F:8.53 p:0.0005	MEOH L:0.201 F:8.53 p:0.0005	ACET L:0.228 F:3.26 p:0.0443	LNPRO1 L:0.232 F:2.68 p:0.0751	ACAL L:0.249 F:0.05 p:0.9543	
4	(2, 71)		ACET L:0.181 F:4.02 p:0.0222	LNPRO1 L:0.182 F:3.71 p:0.0294	ACAL L:0.191 F:1.95 p:0.1504	-	

Figure 4 – Detailed results - Stepdisc at 1% level - Tanagra

Step 1: SAS picks BU1 after having listed the contributions of the candidate variables.

	The STEPDISC Procedure Forward Selection: Step 1										
			Stat	istics	for En	try,	DF = 2	2, 7	4		
Varia	ble	Labe	el	R-So	quare	F١	/alue	Pr	> F	Tole	erance
MEOH	1 1	MEC	н	0	.6366		64.82	<.(0001		1.0000
ACET	1	ACE	Г	0	.0816		3.29	0.0)429		1.0000
BU1	F	BU1		0	.7010		86.75	<.(0001		1.0000
MEPF	۱ s	MEP	R	0	.1622		7.16	0.0	0014		1.0000
ACAL	. /	ACA	L	0	.0232		0.88	0.4	199		1.0000
LNPR	01 I	LNPF	RO1	0	.2288		10.98	<.(0001		1.0000
	Variable BU1 will be entered.										
	BU1	000	BU1	200	MEOH	42	LNPRO	1	MEPR	020	ACET
(2, 74)	F:86	.75	F:8	.299 6.75 .0000	F: 64.	63 82 000	F: 10.9	71 98 001	F:7.	.038 .16 .0014	F: 3.2

SAS provides R-Square = $1 - \Lambda$. For instance, R-Square(MEOH) = 1 - 0.363 = 0.6366. The F statistic is the same as Tanagra, it enables to check the significance of the variable e.g. F(MEOH) = 64.82, with the p-value(MEOH) = 0.0001. The tolerance statistic characterizes the redundancy with the variables already included in the model. At the first step, the initial set of selected variables is empty. There is no possible redundancy. It is therefore equal to 1 for all variables.

BU1 has the highest "F Value", and it is significant at the 1% level. It is thus included in the model. In the forward process, this decision is unchangeable. We cannot remove this variable later.

SAS pursues with the assessment of the current model

Multivariate Statistics					
Statistic	Value	F Value	Num DF	Den DF	Pr > F
Wilks' Lambda	0.298992	86.75	2	74	<.0001
Pillai's Trace	0.701008	86.75	2	74	<.0001
Average Squared Canonical Correlation	0.350504				

The <u>stepdisc documentation</u> explains the reading of the various statistics (Pillai, Average Squared Canonical Correlation) provided by SAS. There is one variable at this step. Thus, the "F Value" is the same as the one of the BU1 variable in the table "Stepdisc Procedure – Step 1" above.

Step 2: SAS evaluates the contribution of the remaining variables. The "Partial R-Square" compares the lambda of the models containing or not an additional variable e.g. for MEOH, Partial R-Square(MEOH) = $1 - 0.251 / 0.299 \approx 0.160$.

MEPR is the best variable according the "Partial R-Square" (or according to the F Value). It is significant at the 1% level. It is approved.



We note also, even if this is not taken into account for the selection, that MEPR is weakly correlated with the already introduced variable because its tolerance is 0.9046. It means that the squared correlation between BU1 and MEPR is $r^2 = 1 - 0.9046 = 0.0954$.

For the overall evaluation of the model with 2 (BU1, MEPR) predictive variables, we have:

Va That E	Variable(s) That Have Been Entered				
BU1	MEPR				
Multivar	iate Statist	tics			
Statistic	Value	F Value	Num DF	Den DF	Pr > F
Wilks' Lambda	0.248931	36.66	4	146	<.0001
Pillai's Trace	0.851978	27.46	4	148	<.0001
Average Squared Canonical Correlation	0.425989				

SAS continues until it is no more possible to add variables. It then produces a table summarizing the process (Figure 5). The values (Wilks lambda, F Value) are consistent with those of Tanagra.

	SAS								-	ΓΑΝΑ	GRA		
											N	d.f	Best
	Forward Selection Summary								1	(2, 74)	BU1 L:0.299 F:86.75		
									Average Squared				p:0.0000
Step	Number In	Entered	Label	Partial R-Square	F Value	Pr > F	Wilks' Lambda	Pr < Lambda	Canonical Correlation	Pr > ASCC	2	(2, 73)	MEPR L:0.249
1	1	BU1	BU1	0.7010	86.75	<.0001	0.29899190	<.0001	0.35050405	<.0001			p: 0.0012
2	2	MEPR	MEPR	0.1674	7.34	0.0012	0.24893122	<.0001	0.42598921	<.0001			MEOH
3	3	MEOH	MEOH	0.1915	8.53	0.0005	0.20125392	<.0001	0.45385985	<.0001	3	(2, 72)	L:0.201 F:8.53 p:0.0005

Figure 5 – Summary of the selection process - Stepdisc forward at 1% level

The selected variables are: BU1, MEPR and MEOH.

5 Discriminant Analysis under R – Ida() [MASS package]

We use the **Ida()** procedure of the « MASS » package to perform the linear discriminant analysis. This package is automatically installed with R.

5.1 Importing the dataset

The **read.xlsx()** command of the package "xlsx"⁵ enables to read a data file in the Excel format (XLS or XLSX). The summary() command describes shortly the variables of the dataset.

```
library(xlsx)
#sheetIndex: number of the sheet to read
#header: the first row corresponds to the name of the variables
alcohol.data <- read.xlsx(file="alcohol.xls",sheetIndex=1,header=T)
print(summary(alcohol.data))</pre>
```

We obtain the main features of the variables.

⁵ http://cran.r-project.org/web/packages/xlsx/index.html

R Console				
> print(summa:	ry(alcohol.data))		•
TYPE	MEOH	ACET	BU1	MEPR
KIRSCH:18 1	Min. : 3.0	Min. : 13.0	Min. : 0.20	Min. : 9.00
MIRAB :29	1st Qu.: 620.0	1st Qu.:127.0	1st Qu.: 9.30	1st Qu.:26.00
POIRE :30 1	Median : 910.0	Median :181.0	Median :17.00	Median :33.00
1	Mean : 845.6	Mean :211.7	Mean :14.74	Mean :35.76
;	3rd Qu.:1087.0	3rd Qu.:287.0	3rd Qu.:20.00	3rd Qu.:46.00
1	Max. :1548.0	Max. :495.0	Max. :30.00	Max. :72.00
ACAL	LNPR01			
Min. : 2.0	0 Min. :3.30	0		
1st Qu.: 8.6	0 1st Qu.:4.28	0		
Median :11.0	0 Median :5.26	0		
Mean :12.5	1 Mean :5.30	1		=
3rd Qu.:15.0	0 3rd Qu.:6.22	0		
Max. :28.0	0 Max. :8.01	0		
>				
1				*
•				•

TYPE is the categorical attribute (3 values) that we want to explain.

5.2 Using the Ida() procedure

We load the MASS⁶ package. We start the lda() procedure on the learning sample.

```
#linear discriminant analysis
library(MASS)
alcohol.lda <- lda(TYPE ~ ., data = alcohol.data)
print(alcohol.lda)</pre>
```

Ida() provides: the proportions of the classes; the conditional mean of the variables according to the classes; the unstandardized coefficients of the canonical functions (Section 3.4.2), without the constant term; the proportion of variance explained by each factor.

🥂 R Console	×
Call:	*
lda(TYPE ~ ., data = alcohol.data)	
Prior probabilities of groups: KIRSCH MIRAB POIRE	
0.2337662 0.3766234 0.3896104	
Group means:	
MEON ACEI DUI MEPR ACAL LNPROI NTDSCH 378 6044 218 0167 1 511111 32 06667 11 16667 6 231111	
MTRAR 939 1379 247 3448 17 906897 30 55172 12 54138 4 883103	
POIRE 1035.4000 173.3667 19.620000 43.00000 13.27333 5.145667	
Coefficients of linear discriminants:	
LD1 LD2	
MEOH 3.382089e-03 0.0005710473	
ACET -4.649248e-05 -0.0066573606	
BU1 1.322048e-01 -0.0162598664	
MEPR -2.562255e-02 0.0533609640	
ACAL -4.048757e-02 0.0297883525	
LNPRO1 -2./91911e-01 0.389440048/	
Proportion of trace:	=
LD1 LD2	
0.3100 0.0032	-
	. ►

⁶ http://cran.r-project.org/web/packages/MASS/index.html

In principle, **Ida()** seems only intended to the descriptive analysis. But as we have seen above, the connection between the descriptive analysis and the predictive analysis is strong (section 3.4.5). Thus, the **predict()** command enables to assign individual to the classes. The classification properties are identical to those of Tanagra or SAS i.e. each individual is assigned to the same group whatever the tool used.

5.3 Prediction

The **predict()** enables to apply the classifier on the individuals.

```
#prediction on the training set
pred.lda <- predict(alcohol.lda,newdata=alcohol.data)
print(attributes(pred.lda))</pre>
```

The object has 3 main properties: 'class', 'posterior' and 'x'.



'class' is a vector, its length is n = 77. It provides the predicted value for each individual of the sample. For instance, we show here the predicted values for the first 6 individuals.

R Console		3
<pre>> head(pred.lda\$class) [1] KIRSCH KIRSCH KIRSCH KIRSCH KIRSCH KIRSCH Levels: KIRSCH MIRAB POIRE ></pre>		*
<	Þ	

'posterior' is a matrix with n = 77 rows and 3 columns (because the class attribute has 3 values). Each column corresponds to the posterior probability of the class membership. For the first 6 instances, we have the following values:

R Console	
<pre>> head(pred.lda\$posterior)</pre>	
	▶

'x' provides the canonical coordinates of the instances. This is a matrix with 77 rows and 2 columns (because we have two factors). Here are the values for the first 6 instances:

<u>R</u> R Console	
> head(pred.	lda\$x)
LD1	LD2
1 -4.091901	-0.2497072
2 -3.887575	-0.1277995
3 -3.503543	-1.1199342
4 -3.475565	0.7129591
5 -3.107675	-0.7864612
6 -3.602823	-0.9710812
>	-
	►

5.4 Confusion matrix

To obtain the confusion matrix, we create a contingency table from the observed values of the class attribute and the predictions of the model.

```
#confusion matrix
mc.lda <- table(alcohol.data$TYPE,pred.lda$class)
print(mc.lda)</pre>
```

We have the same matrix as Tanagra (section 3.2.1) and SAS (section 4.1).

Ŗ R Consol	e					3
> #confu > mc.lda > print(sion ma <- tab mc.lda)	trix le(alco	ohol.da	ata\$TYPE,pred.lda\$cla	155)	*
KIRSCH MIRAB POIRE	KIRSCH 18 0 0	MIRAB 0 23 9	POIRE 0 6 21			•
•					•	

We can compute the error rate,

```
#error rate
print(1-sum(diag(mc.lda))/sum(mc.lda))
```

We have 19.48%

R Console	x
<pre>> #error rate > print(1-sum(diag(mc.lda))/sum(mc.lda))</pre>	*
[1] 0.1948052 >	-
< >	

5.5 Variable selection

We use the proceduree **greedy.wilks()** of the package « klaR »⁷ for the variable selection.

```
#variable selection
library(klaR)
alcohol.forward <- greedy.wilks(TYPE ~ .,data=alcohol.data, niveau = 0.01)</pre>
```

⁷ http://cran.r-project.org/web/packages/klaR/index.html

print(alcohol.forward)

At each step, R provides the F statistic for the additional variable (**F.statistics.diff**), and the F statistic for the model with the current set of selected variables (**F.statistics.overall**).

```
R Console
                                                                            > library(klaR)
> alcohol.forward <- greedy.wilks(TYPE ~ ., data = alcohol.data, niveau = 0.01)
> print(alcohol.forward)
Formula containing included variables:
TYPE ~ BU1 + MEPR + MEOH
<environment: 0x00000000773d558>
Values calculated in each step of the selection procedure:
  vars Wilks.lambda F.statistics.overall p.value.overall F.statistics.diff p.value.diff
1 BU1
         0.2989919
                              86.74917
                                        3.975561e-20
                                                             86.749173 3.975561e-20
                                                                                      Ξ
2 MEPR
         0.2489312
                               36.65654
                                          3.402765e-21
                                                               7.340239 1.235768e-03
                                        7.226240e-23
3 MEOH
         0.2012539
                              29.49819
                                                               8.528444 4.692630e-04
```

The process is consistent with those of Tanagra and SAS (Figure 5).

We perform a new analysis on the variables selected by the **greedy.wilks()** procedure. This last one provides directly the formula with only the relevant variables. This feature is really useful if the initial number of candidate variables is very large.

```
#2nd model after variable selection
alcohol.lda.fwd <- lda(alcohol.forward$formula, data = alcohol.data)
print(alcohol.lda.fwd)</pre>
```

We obtain a new version of the model.

🥂 🥂 R Console 📃 🗖 🗖	x
Call: Ida(alcohol.forward\$formula, data = alcohol.data)	*
Prior probabilities of groups: KIRSCH MIRAB POIRE 0.2337662 0.3766234 0.3896104	
Group means:	
KTRSCH 1 511111 32 06667 378 6944	
MTRAB 17,906897 30,55172 939,1379	
POIRE 19.620000 43.00000 1035.4000	
Coefficients of linear discriminants: LD1 LD2	
BU1 0.149874251 -0.0313069489	
MEPR -0.025447467 0.0759388778	
MEOH 0.002809521 0.0002065334	
Proportion of trace: LD1 LD2 0.9516 0.0484	•
I < 1	•i

We apply this model on the sample to obtain the corresponding confusion matrix and error rate.

```
#2nd confusion matrix
mc.lda.fwd <- table(alcohol.data$TYPE,predict(alcohol.lda.fwd,newdata=alcohol.data)$class)
print(mc.lda.fwd)
#2nd error rate
print(1-sum(diag(mc.lda.fwd))/sum(mc.lda.fwd))</pre>
```

We obtain:

R Cons	ole				3
> mc.ld > print	a.fwd <- (mc.lda.:	table fwd)	(alcoho	ol.data\$TYPE,predict(\$	^
	KIRSCH	MIRAB	POIRE		
KIRSC	H 18	0	0		
MIRAB	0	22	7		
POIRE	1	12	17		
>					
> #2nd	error rat	te			
> print	(1-sum (d:	iag(mc	.lda.fv	vd))/sum(mc.lda.fwd))	
[1] 0.2	597403				
>					-
•				•	

6 Discriminant analysis under SPSS

We use the French version of SPSS 12.0.1. We import the "alcohol.xls" data file. We transform TYPE in a numerical attribute before (KIRSCH = 1, MIRAB = 2, POIRE = 3)⁸.

🔲 alcoh	🗃 alcohol.sav - Editeur de données SPSS 📃 🗖 🔀										
Fichier Ed	Fichier Edition Affichage Données Transformer Analyse Graphes Outils Fenêtre Aide										
1 : TYPE 1											
	TYPE	MEOH	ACET	BU1	MEPR	ACAL	LNPR01	V8			
1	1	3.0	15.0	.2	9.0	9.0	5.86				
2	1	23.0	13.0	.8	9.0	2.0	6.67				
3	1	65.0	96.0	.4	9.0	4.0	5.31				
4	1	279.0	66.0	.9	36.0	4.8	5.45				
5	1	292.0	210.0	1.1	34.0	8.0	4.08				
6	1	371.0	414.0	1.2	39.0	9.0	6.22				
7	1	393.0	287.0	1.8	41.0	9.7	6.47				
8	1	394.0	217.0	1.0	31.0	8.6	6.31				
9	1	418.0	62.0	.8	24.0	7.0	5.83				
10	1	426.0	204.0	1.3	37.0	8.6	6.07				
11	1	465.0	267.0	1.5	39.0	17.0	8.01				
12	1	469.0	226.0	1.6	35.0	8.0	6.21				
13	1	475.0	172.0	1.9	33.0	14.0	6.30				
14	1	498.0	343.0	2.3	42.0	21.0	6.59				
15	1	507.0	397.0	3.3	30.0	21.0	5.98				
16	1	523.0	367.0	2.6	45.0	25.0	6.67				
17	2	546.0	119.0	12.0	28.0	7.4	3.30	-			
Af	fichage d	es données ,	Affichage d	es variab 🔳							
				5	5PSS processeu	ır est prêt					

6.1 Construction of the model including all the predictive variables

We click on the **ANALYSE / CLASSIFICATION / ANALYSE DISCRIMINANTE** menu. We set into the settings dialog:

⁸ See also "<u>Annotated SPSS Output – Discriminant Analysis</u>".

🗖 Analyse discriminante		×
	Critère de regroupement :	ОК
		Coller
	Dennin intervene	Restaurer
	Variables explicatives :	Annuler
•	ACET	Aide
	Entrer les variables simultanément This is a méthode pas à pas	
	Variable de filtrage : Filtre	
Statistiques	Méthode Classement Enregistrer	

We set TYPE in « **Critère de regroupement** », the range (Définir intervalle) of the value is MIN = 1 to MAX = 3. All the others variables are predictive variables « **Variables explicatives** ». At the moment, we do not perform a variable selection « **Entrer les variables simultanément** ».

Analyse discriminante: Statistiques 🛛 🗙						
Caractéristiques Moyennes ANOVA à 1 facteur Test de Box Coefficients de la fonction Fisher Non standardisés	Matrices Corrélations intra-classe Covariance intra-classe Covariance de chaque classe Covariance totale Poursuivre Annuler Aide					

Then, we click on the « **Statistiques** » button. We ask the "Fisher" classification function.

From the initial dialog box, we click on the « **Classements** » button. We want to estimate the prior probabilities of the groups from the proportion measured on the learning sample. We use the pooled covariance matrix.

Analyse discriminante : Classement		
Probabilités a priori C Egales pour toutes les classes C A calculer selon les effectifs	Utiliser la matrice d'inertie Intra-classe De chaque classe	Poursuivre Annuler
Afficher Résultats par observation Limiter les observations aux premières : Récapitulatif Classification par élimination Remplacer les valeurs manquantes par la moyenne	Diagrammes Toutes classes combinées Classe par classe Carte des régions d'affectation	

We validate these settings. A new window describing the results of the calculations appears.

SPSS mixes the outputs of the canonical analysis and predictive analysis. This is not a problem. Indeed, the two approaches can converge as we shown previously. We must know simply discern the appropriate information in the outputs. We have the eigenvalues related to the factors and the tests of significance.



Then, we have: (1) the canonical functions; (2) the canonical structure; (3) the conditional centroids.



Secondly, we have the results in the predictive point of view.

We have, among others, the classification functions: the "Fisher's Linear Discriminant Functions" according to SPSS.

	TYPE						
	1	2	3				
MEOH	.001	.016	.015				
ACET	.000	004	.005				
BU1	039	.553	.557				
MEPR	.187	.102	.036				
ACAL	.039	127	161				
LNPR01	6.379	5.341	4.869				
(Constante)	-24.686	-29.632	-25.142				

Coefficients des fonctions de classement

Fonctions discriminantes linéaires de Fisher

6.2 Variable selection

To perform a variable selection, we must restart the analysis by modifying the treatment of the independent variables. We select the stepwise approach. We click on the "Méthode" button.

🗖 Analyse discriminante	×
Critère de regroupement :	ОК
	Coller
Deinin intervalie	Restaurer
Variables explicatives :	Annuler
	Aide
C Entrer les variables simultanément	
Variable de filtrage :	
Statistiques <u>Méthode</u> Classement Enregistrer	

Only the bidirectional approach is available i.e. at each step, we check if the adding of a variable does not imply the removing of another already selected variable. Two significance levels enable to guide the process: 0.01 for the adding, 0.05 for the removing. We select the Wilks' lambda (Méthode) to obtain consistent results with the other tools.

Méthode	Critéres	Poursuiv
Eambda de Wilks	🔿 Choisir la valeur de F	A number
C Variance résiduelle	Introduction : 3.84 Elimination : 2.71	Annulei
🔿 Distance de Mahalanobis	,	Aide
Plus petit rapport F	Choisir la probabilité de F	
🔿 V de Rao	Entrée : .01 Elimination : .05	
V à introduire : 0		
Afficher]
Récapitulation des étapes	Test F des distances entre couples	

R.R.

A table summarizes the process. It is very similar to the table provided by the procedure **greedy.wilks**() (KlaR package) under R.

		Lambda de Wilks							
						F exact			
Pas	Introduite	Statistique	ddl1	ddl2	ddl3	Statistique	ddl1	ddl2	Signification
1	BU1	.299	1	2	74.000	86.749	2	74.000	.000
2	MEPR	.249	2	2	74.000	36.657	4	146.000	.000
3	MEOH	.201	3	2	74.000	29.498	6	144.000	.000

Then we have more details on the various versions of the models. As we seen above, the tolerance criterion enables to evaluate the redundancy between the selected variables. It varies between 0 and 1. The higher is the value, the weaker is the redundancy between the variables.

Pas		Tolérance	Signification du F pour éliminer	Lambda de Wilks
1	BU1	1.000	.000	
2	BU1	.899	.000	.838
	MEPR	.899	.001	.299
3	BU1	.811	.000	.303
	MEPR	.830	.000	.251
	MEOH	.781	.000	.249

Variables de l'analyse

In the last column, we have the Wilks' lambda of the model if we remove a variable.

Last, a table provides a full detailed description of the process. We observe for instance that BU1 is the best variable in the first step. It proposes the weaker value of the Wilks' lambda (0.299). In the second step, MEPR is the most interesting (0.249). Etc.

				Signification	
			Tolérance	du F pour	Lambda
Pas		Tolérance	minimale	introduire	de Wilks
0	MEOH	1.000	1.000	.000	.363
	ACET	1.000	1.000	.043	.918
	BU1	1.000	1.000	.000	.299
	MEPR	1.000	1.000	.001	.838
	ACAL	1.000	1.000	.420	.977
	LNPR01	1.000	1.000	.000	.771
1	MEOH	.846	.846	.002	.251
	ACET	1.000	1.000	.048	.275
	MEPR	.899	.899	.001	.249
	ACAL	.975	.975	.835	.298
	LNPR01	.996	.996	.053	.276
2	MEOH	.781	.781	.000	.201
	ACET	.995	.895	.044	.228
	ACAL	.966	.886	.954	.249
	LNPR01	.996	.896	.075	.232
3	ACET	.940	.738	.022	.181
	ACAL	.801	.647	.150	.191
	LNPR01	.966	.758	.029	.182

Variables absentes de l'analyse

7 Conclusion

Discriminant analysis is an attractive method. It is available in almost all statistical software. In this tutorial, we tried to highlight the similarities and the differences between the outputs of Tanagra, R, SAS, and SPSS software. The main conclusion is that, if the presentation is not always the same, ultimately we have exactly the same results. This is the most important.