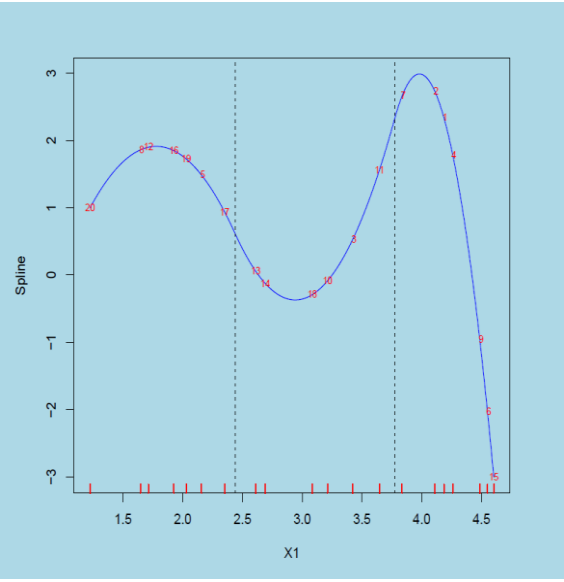
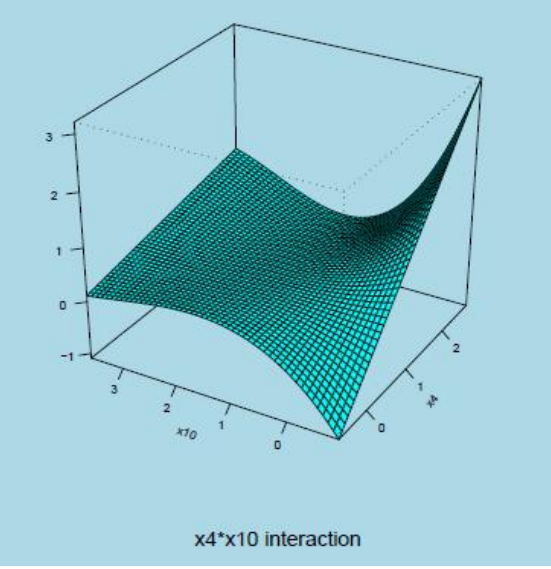
PLSS for Nonlinear Prediction and Data Analysis

Developed during the last decade at the Montpellier 2 university under the direction of J. F. Durand, the PLSS package (PLSS for Partial Least-Squares Splines) allows to construct statistical models of prediction whose domain of interest concerns many scientific and industrial areas such as chemistry, near infrared spectroscopy, sensometrics, econometrics, marketing, credit scoring.

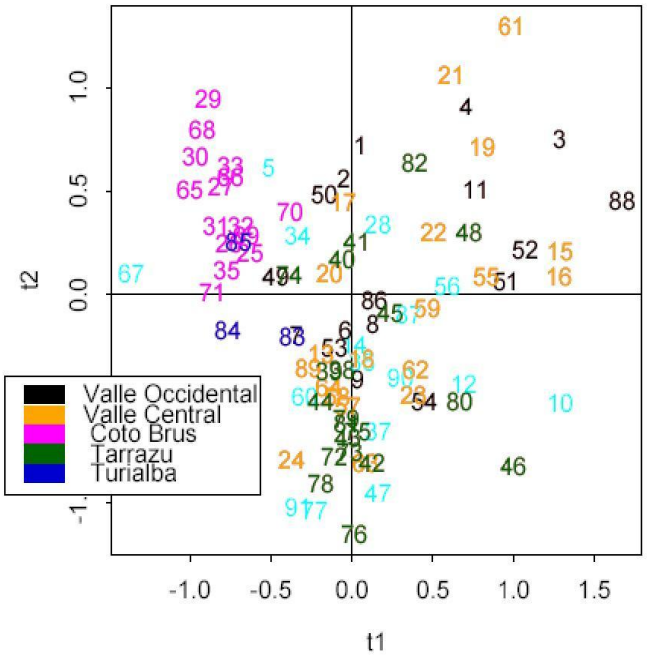
Inheriting good properties from the Partial Least-Squares Linear models (PLSL) elaborated by H. and S. Wold during the eighties, PLSS differentiates itself from other methods as an efficient prediction tool in the following difficult statistical context : a set of predictors characterized by their large number, sometimes several hundred, and also by their heterogeneous nature (a mixture of continuous, categorical and binary variables), all measured on few observations used to predict one or several responses that can be continuous, leading in that case to regression models, or categorical, leading to decision models.

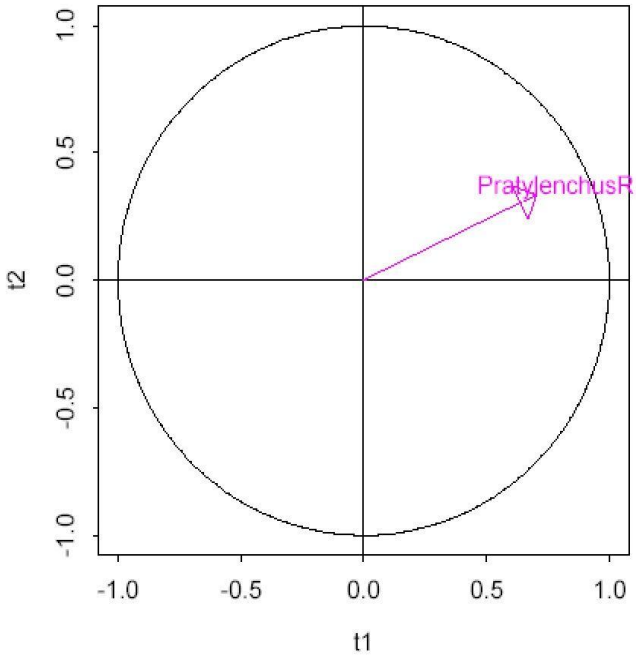
PLSS is new in the sense that transforming the predictors with spline functions (piecewise polynomials), allows the models to capture nonlinear relationships between the responses and the most influential predictors called the main effects variables and their possible interactions.





Besides its characteristics of a prediction tool, PLSS proposes to look at the data through 2-D maps called the "component scatterplots" and built from latent variables or principal components.





Principal components used to predict the responses, are few synthetic variables that are the sum of the non-linearly transformed predictors and their eventual relevant interactions.

The timing of the prediction process can be split up into 3 steps:

1. Set up the aims of the problem and the associated schedule conditions.
2. The building-model phase: a (a)-(b) round-trip until obtaining a training data set leading to validated models.
   a) Building an evolutionary data base following the retained schedule conditions.
   b) Data processing by the PLSS package and validation or not of the models built on the data at hand.

3. Elaborate some scenarios of prediction. A scenario allows the user to enter new real or fictive data and test the validated models.

Some industry/research contracts :

2008 - Institut Français du Pétrole: Forecasting oil production by using an adaptive design of experiments.

2008 - Institut Français de la vigne et du vin : Elaboration d'un modèle de maturité du cépage Mourvèdre.

2005 - Hospital of Aversa (Italy): Evaluation of patient satisfaction in health services.

2004 - Oeneo group (France): Identifying the main influential processing factors on the permeability and the mechanical properties of the Altec cork.

2003 - INRA-CIRAD : Modeling the parasitic attacks of the coffee tree roots in Costa-Rica.

2002 - ITV France : Models of the vintage quality in the Bordeaux area.

2000 - DANONE group - TEPRAL research center : Sensorial analyses of orange juices.

Short Bibliography :

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Wold, H. (1984), "PLS Regression", Encyclopaedia of Statistical Sciences. N. Johnson and S. Kotz eds. John Wiley, New York, Vol. 6, 58 -591.

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