Using multi-block analysis to select informative variables

Douglas N. Rutledge

Laboratoire de Chimie Analytique, AgroParisTech

16, rue Claude Bernard, 75005 Paris, France

rutledge@agroparistech.fr

Variable Selection

The quality of multivariate predictive models is increased by eliminating uninformative variables.

For discriminant models, pp-ANOVA is often used :

- test each variable separately
- varies more between groups than within groups ?

For regression analysis, many methods :

- Uninformative Variable Elimination-PLS [1]
- Genetic Algorithm-PLS [2]
- iPLS [3] ...

[1] V. Centner, D. L. Massart, O. E. deNoord, S. deJong, B. M. Vandeginste, C. Sterna, Elimination of uninformative variables for multivariate calibration.
Analytical Chemistry **1996, 68, 3851-3858**.
[2] A.S. Bangalore, R.E. Shaffer, G.W. Small, M.A. Arnold, Genetic algorithm-based method for selecting wavelengths and model size for use with partial least-squares regression: Application to near-infrared spectroscopy. ***Analytical Chemistry*** **1996, 68, 4200-4212**.
[3] L. Norgaard, A. Saudland, J. Wagner, J.P. Nielsen, L. Munck, S.B. Engelsen, Interval partial least-squares regression (iPLS): A comparative chemometric study with an example from near-infrared spectroscopy.
Applied Spectroscopy **2000, 54, 413-419**.

pp-ANOVA and iPLS

The most commonly used methods :

pp-ANOVA is intrinsically UNIVARIATE

iPLS applies PLS regression to ISOLATED BLOCKS

Better to use an intrinsically MULTIVARIATE, MULTIBLOCK method

Multi-block analysis

"Common Components and Specific Weights Analysis" - CCSWA [4]

Simultaneously study several matrices

- with different variables describing the same samples

Describe *m* data tables observed for the same *n* samples :

- a set of *m* data matrices (**X**) each with *n* rows,
- but not necessarily the same number columns

Determine a common space for all *m* data table,

- each matrix has a specific contribution ("salience") to the definition of each dimension of this common space

[4] E. Qannari, I. Wakeling, P. Courcoux, H.J.H MacFie,

Defining the underlying sensory dimensions. ***Food Quality and Preference*** 2000, 11, 151-154.

Multi-block analysis

Start with p matrices **Xi** of size $n \times ki$ ($i = 1$ to p)

Each **Xi** column-centered and scaled by dividing by matrix norm :

Xsi

For each **Xsi**, an $n \times n$ scalar product matrix **Wi** can be computed as :

$$\mathbf{Wi} = \mathbf{Xsi} \bullet \mathbf{Xsi}^{T}$$

Wi reflect the dispersion of the ***samples*** in the space of that table

The common dimensions of all the tables are computed iteratively
At each iteration, a weighted sum of the p **Wi** matrices is computed, resulting in a global $\mathbf{W_G}$ matrix

Multi-block analysis

For each successive Common Dimension, calculate a scores vector $\boldsymbol{q}$ (coordinates of the n samples along the common dimension)

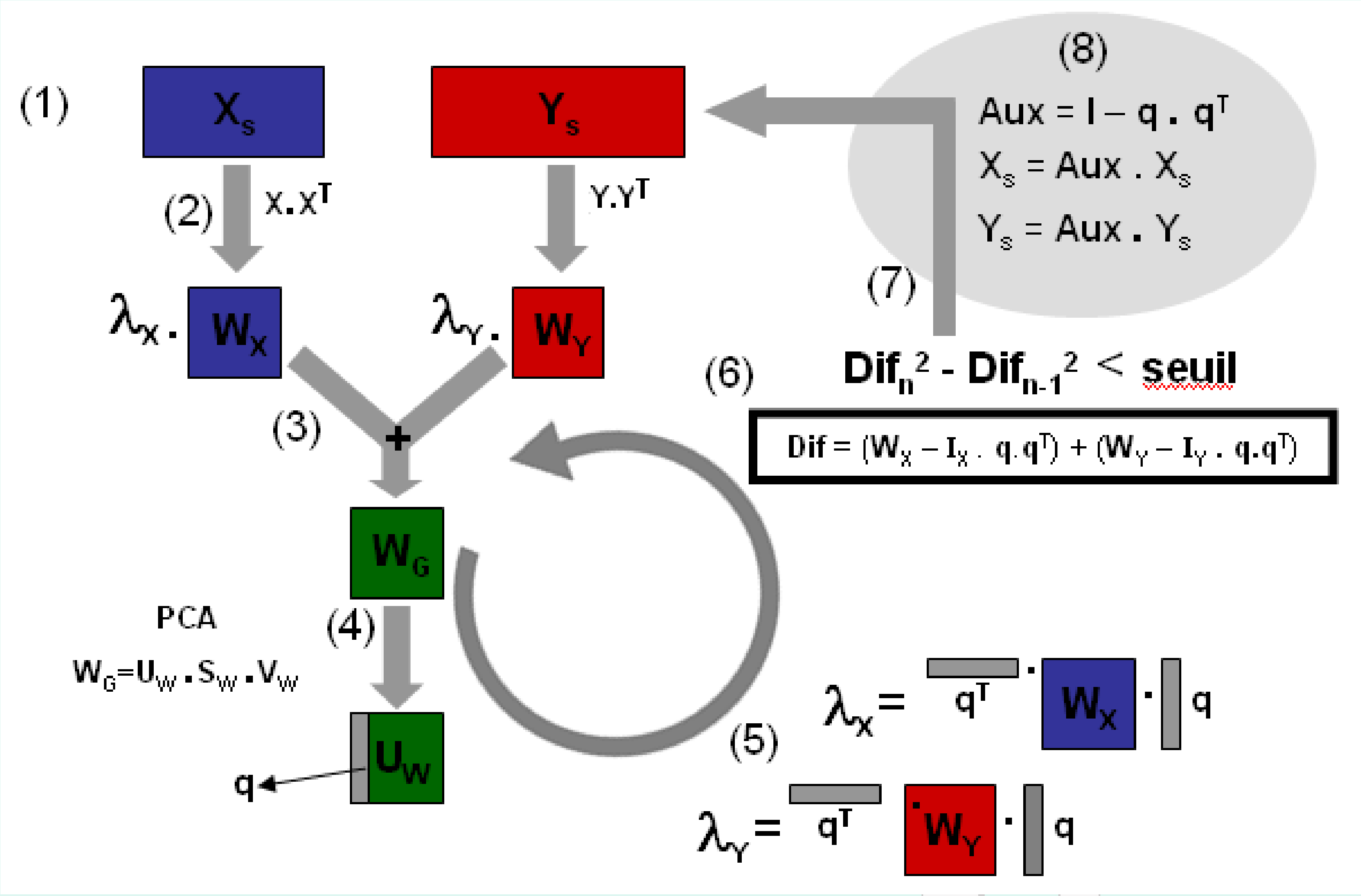
$$W_i = \sum_{j=1}^{j=n} \lambda_j^{(i)} q_j q_j^T$$

$\lambda_j^{(i)}$ is the ***specific weight*** ("salience") associated with the i^{th} table for the j^{th} Common Dimension generated by $\boldsymbol{q}_j$

Differences in the values of the ***specific weights*** for a dimension :
- information present in some tables but not others

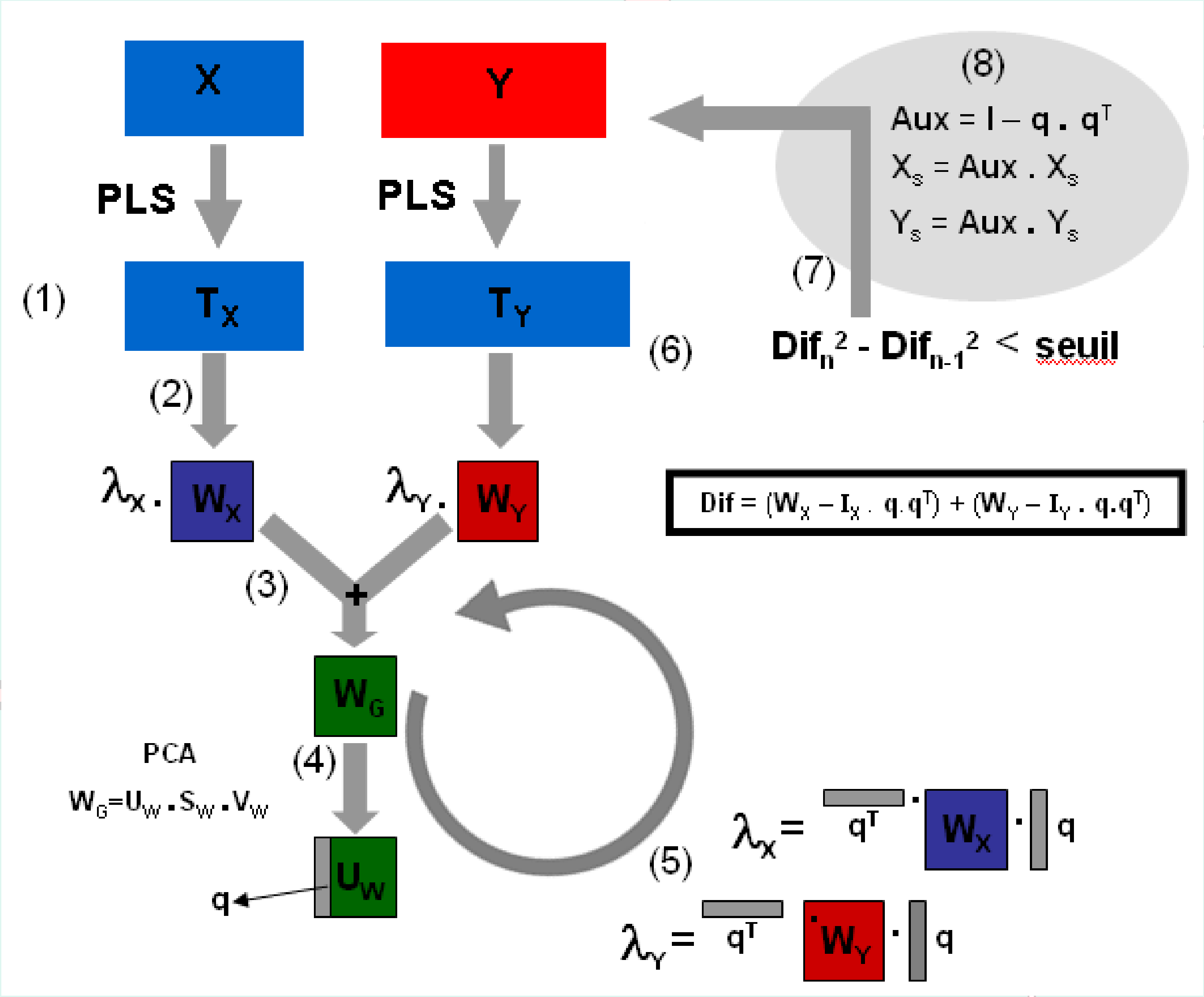
Subsequent components calculated after deflating the data tables

Classical ComDim



"ComDim" the implementation of CCSWA used here is part of the *SAISIR* toolbox
SAISIR (2008): Statistics Applied to the Interpretation of Spectra in the InfraRed
Dominique Bertrand (bertrand@nantes.inra.fr)

PLS-ComDim


X
Y
PLS
PLS
(8)
Aux = I – q . q^T
X_s = Aux . X_s
Y_s = Aux . Y_s
(7)
(1)
T_X
T_Y
(6)
Dif_n^2 - Dif_{n-1}^2 < seuil
(2)
λ_X . W_X
λ_Y . W_Y
Dif = (W_X – I_X . q.q^T) + (W_Y – I_Y . q.q^T)
(3)
+
W_G
PCA
W_G=U_W . S_W . V_W
(4)
U_W
q
(5)
λ_X= q^T . W_X . q
λ_Y= q^T . W_Y . q

1) Starch-Lignin mixtures

Samples

- 2 moisture contents :
  - High, Low
- 2 forms :
  - Cylinders, Films
- 5 Lignin contents :
  - 0, 5, 10, 15, 30 %
- 2 or 3 repetitions

Signals

- 58 x 258 point TD-NMR signals

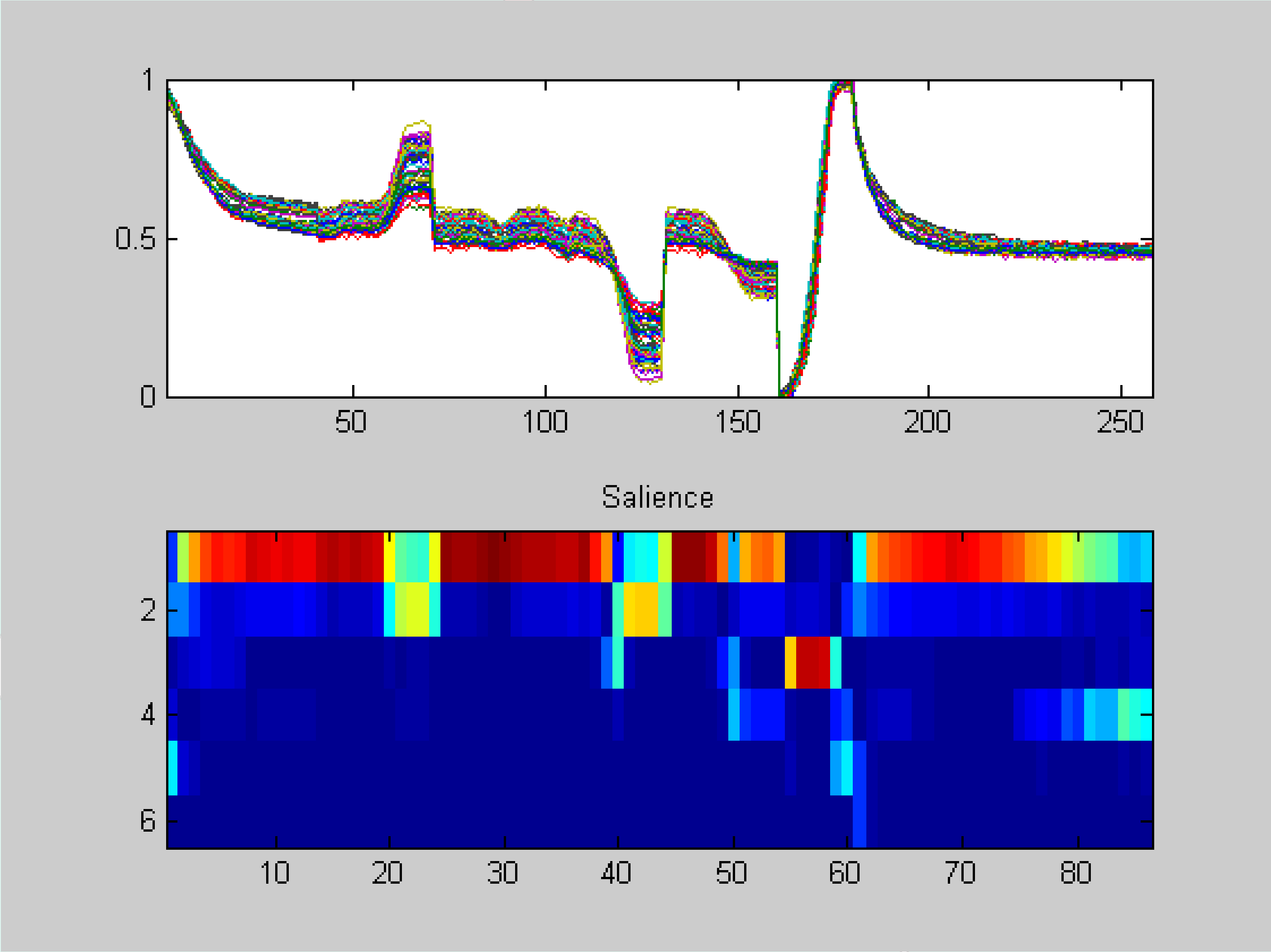
Tables

- 86 blocks of 3 variables
- 6 Common Dimensions

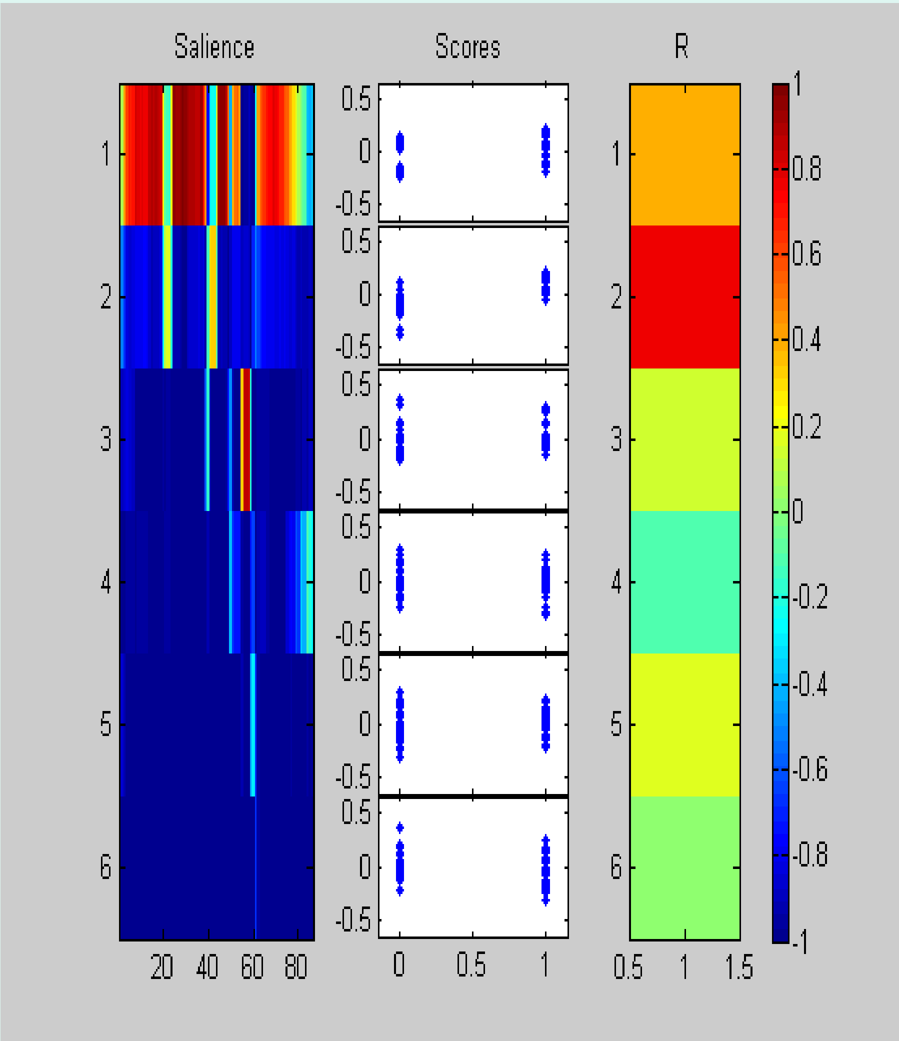
TD-NMR signals

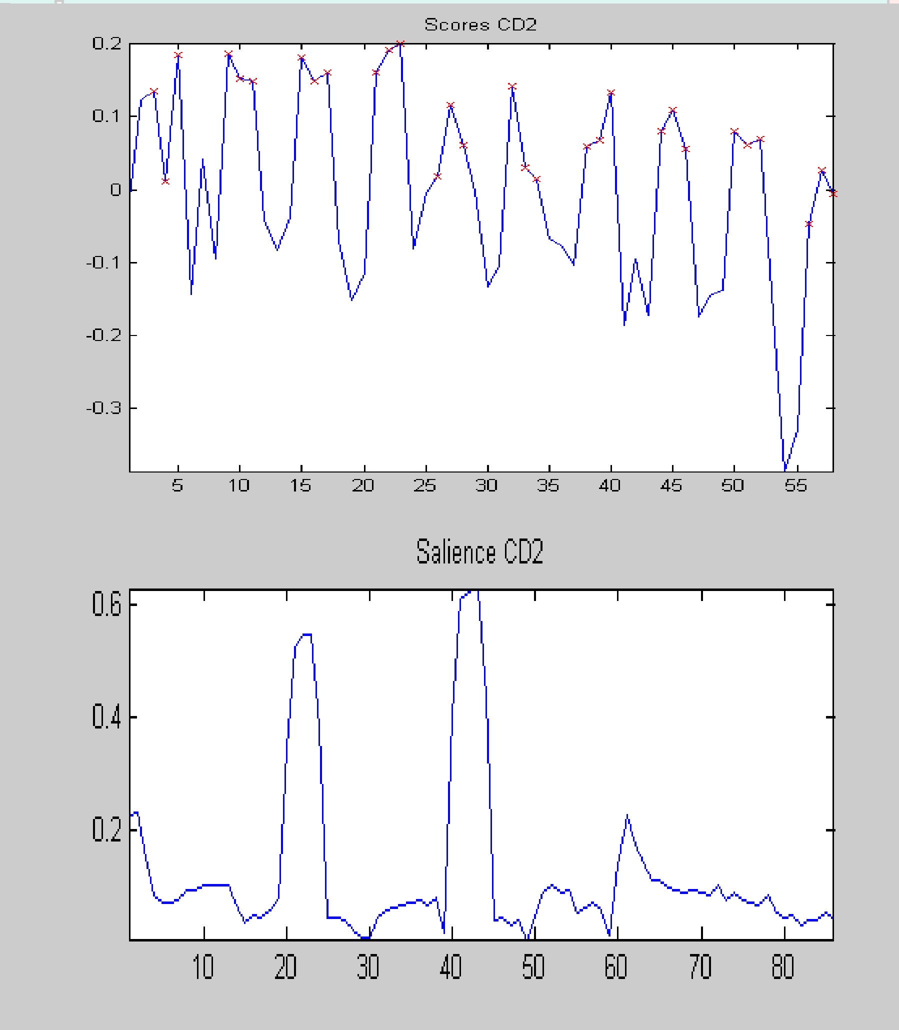
Spectra

ComDim Saliences

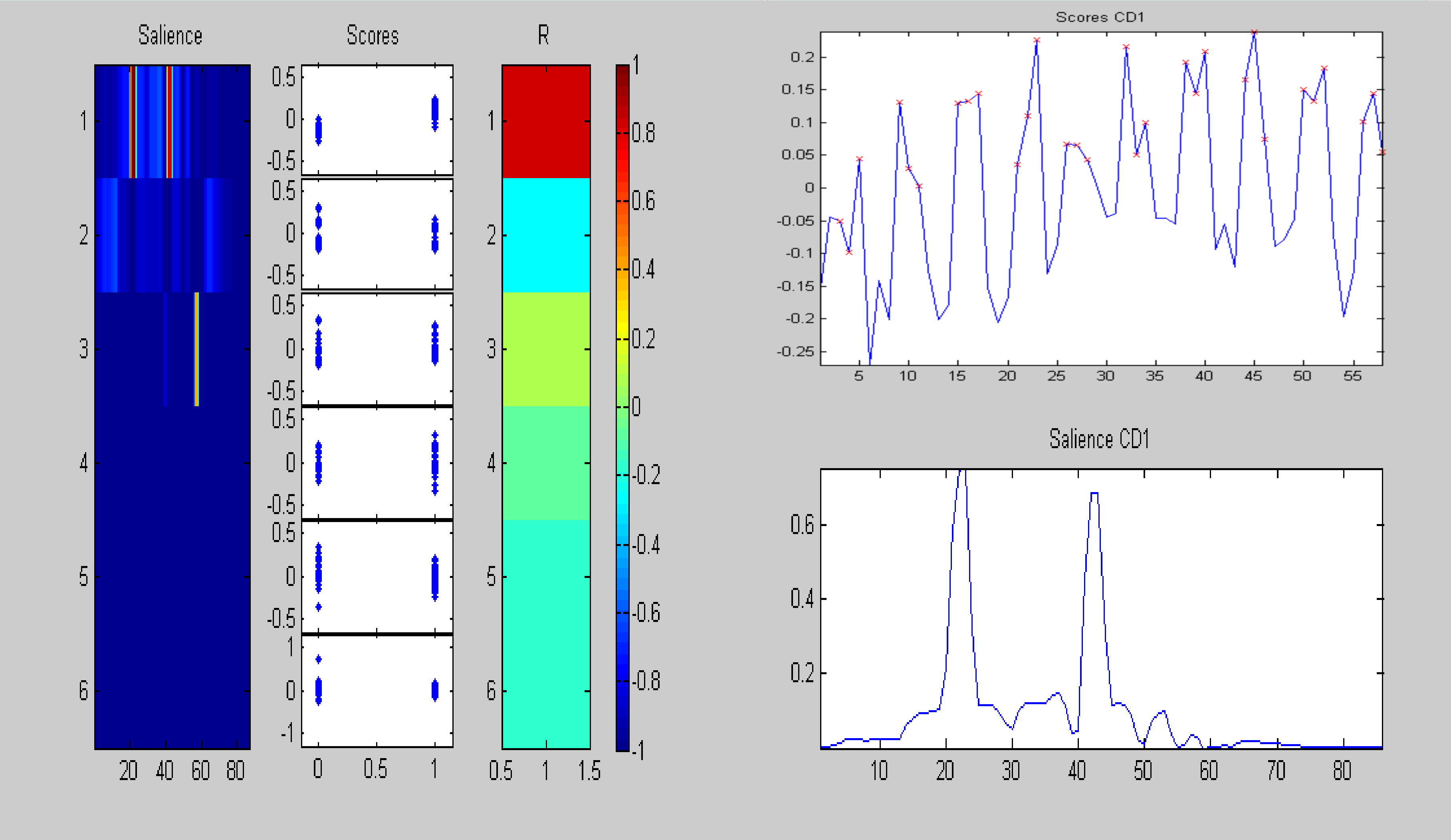


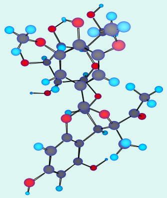
Correlation between ComDim Scores and "Form"





Correlation between PLS-ComDim Scores and "Form"

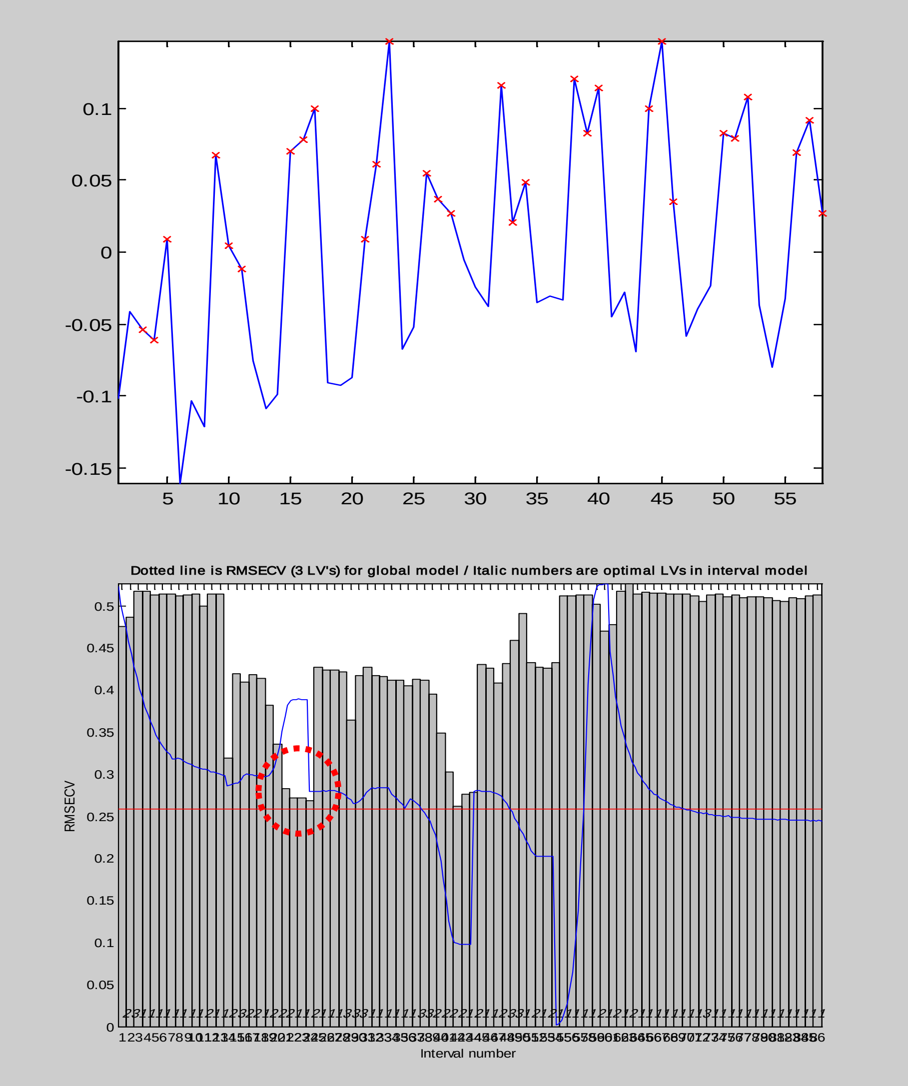




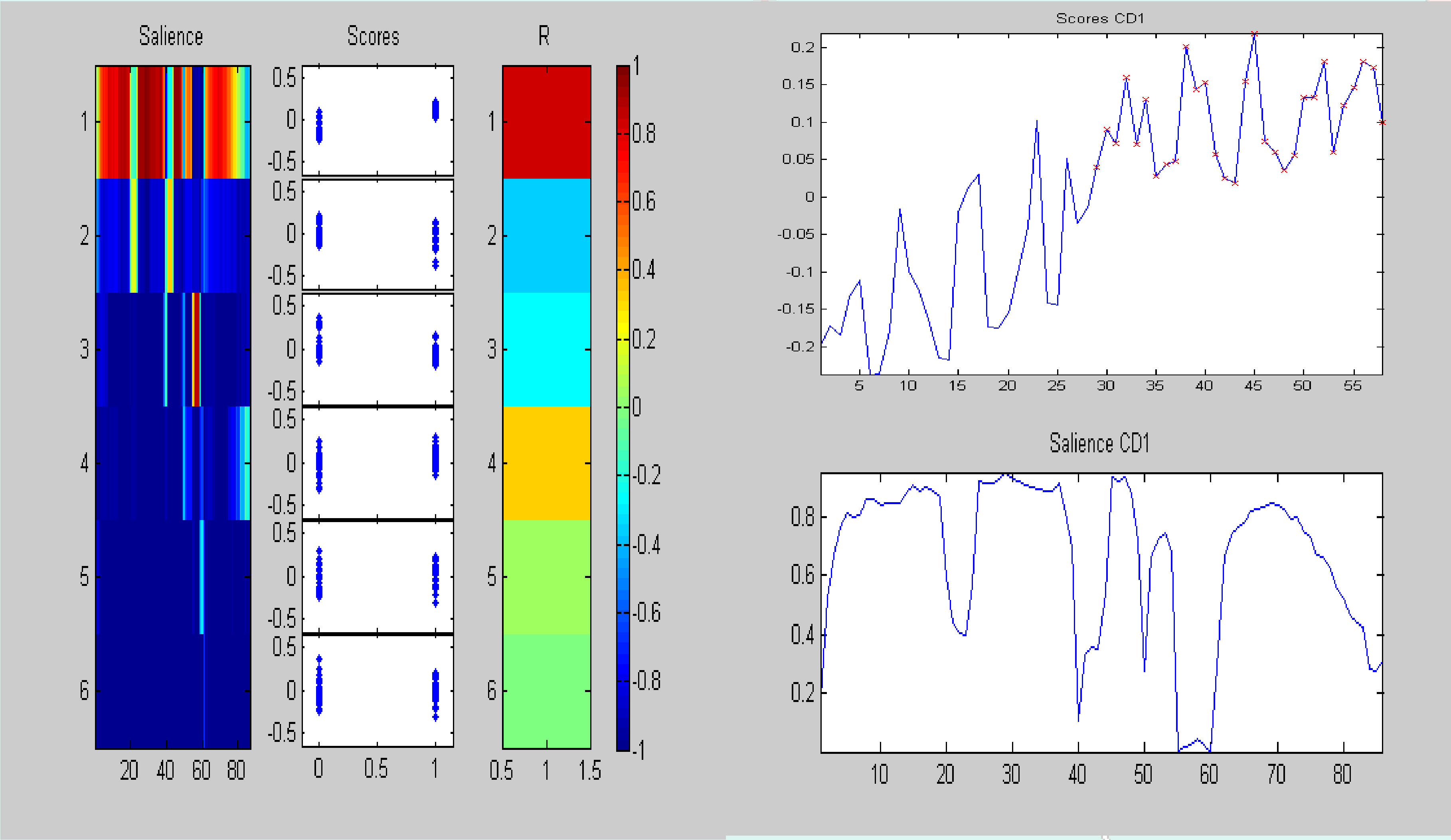
i-PLS between NIR and "Form"

- Blocks = 86
- Mean centred
- Max LVs = 3
- CV = Full

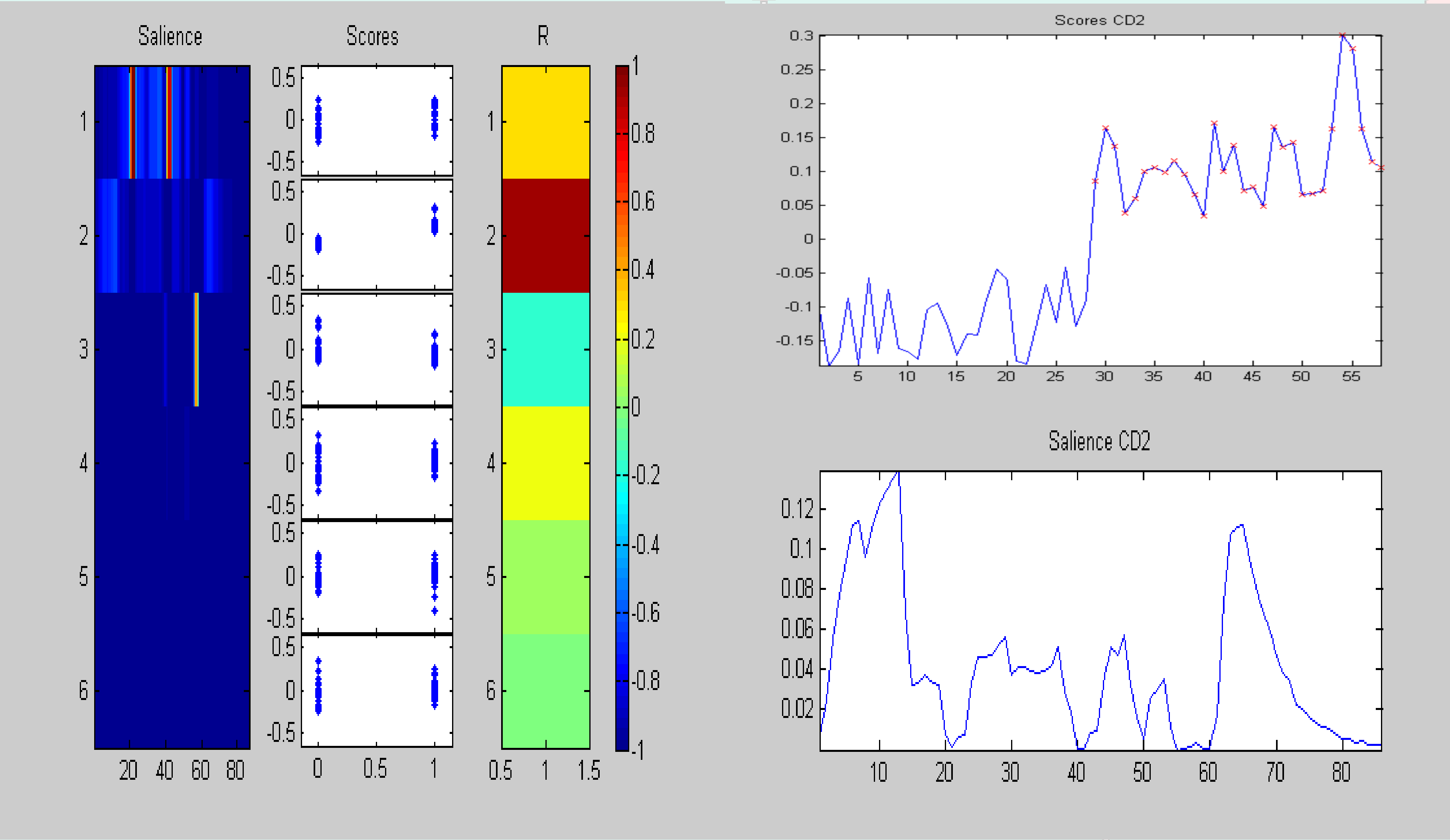
- Scores on LV1
  for Block 24



Correlation between ComDim Scores and "H2O"



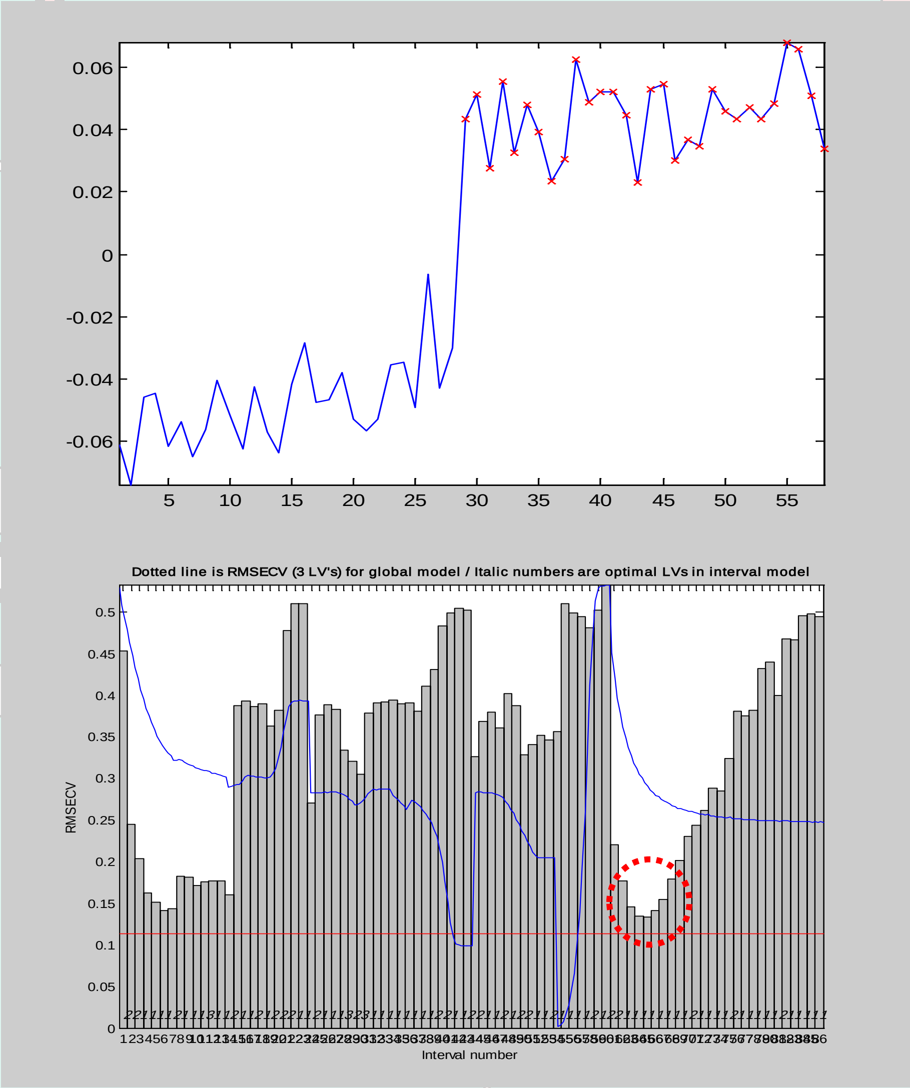
Correlation between PLS-ComDim Scores and "H2O"



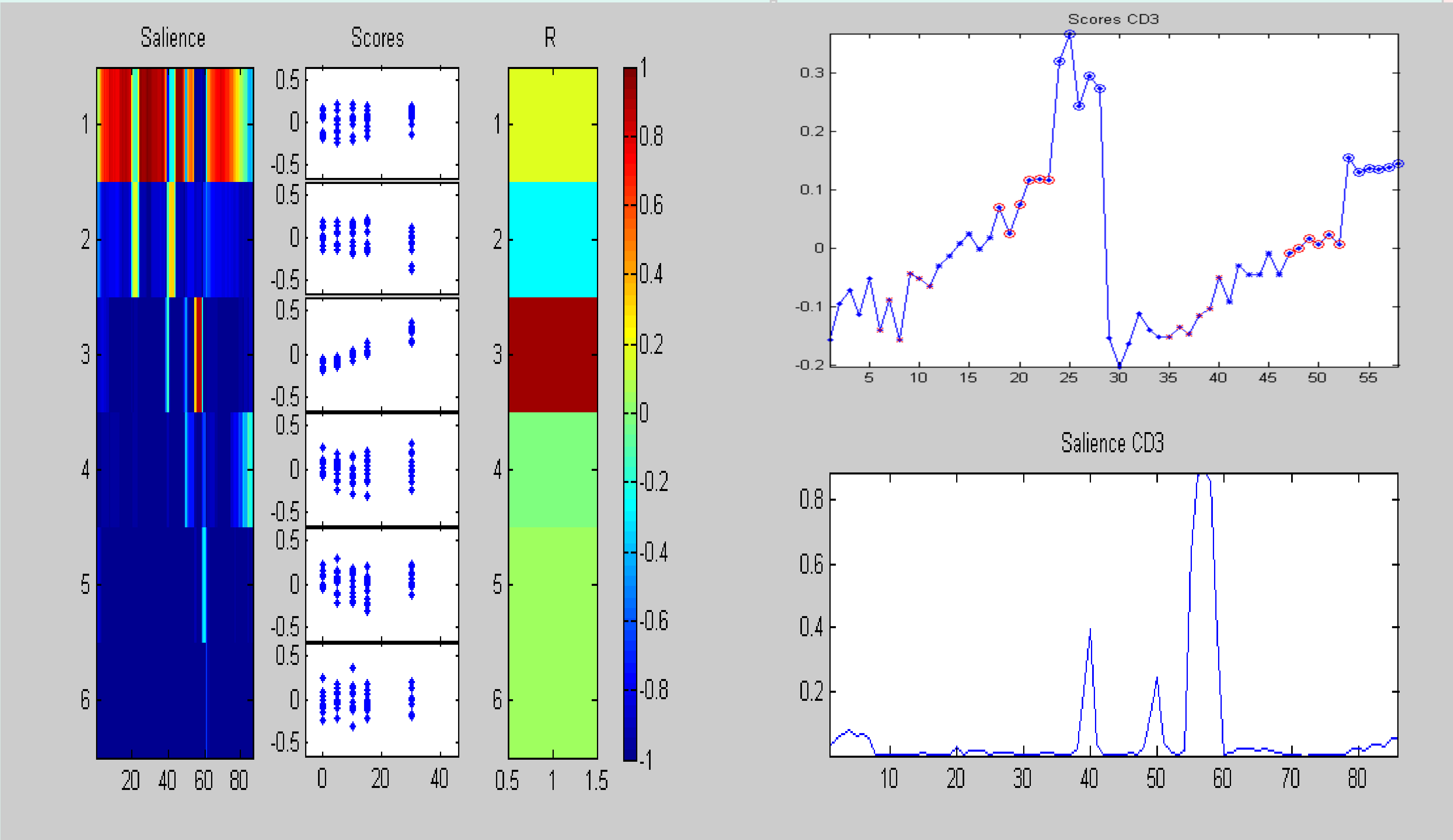
i-PLS between NIR and "H2O"

- Blocks = 86
- Mean centred
- Max LVs = 3
- CV = Full

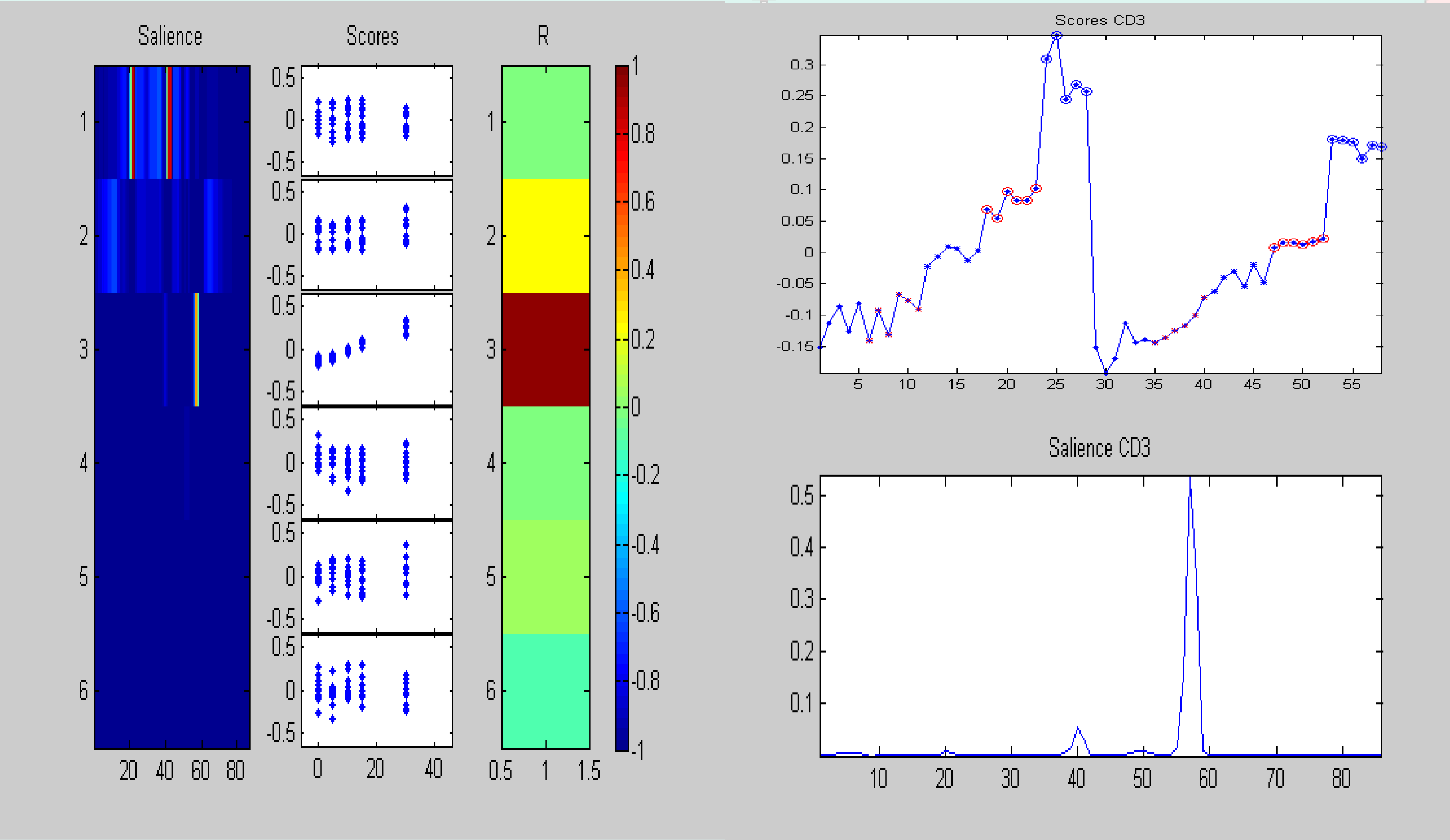
- Scores on LV1
  for Block 64



Correlation between ComDim Scores and "Lignin"



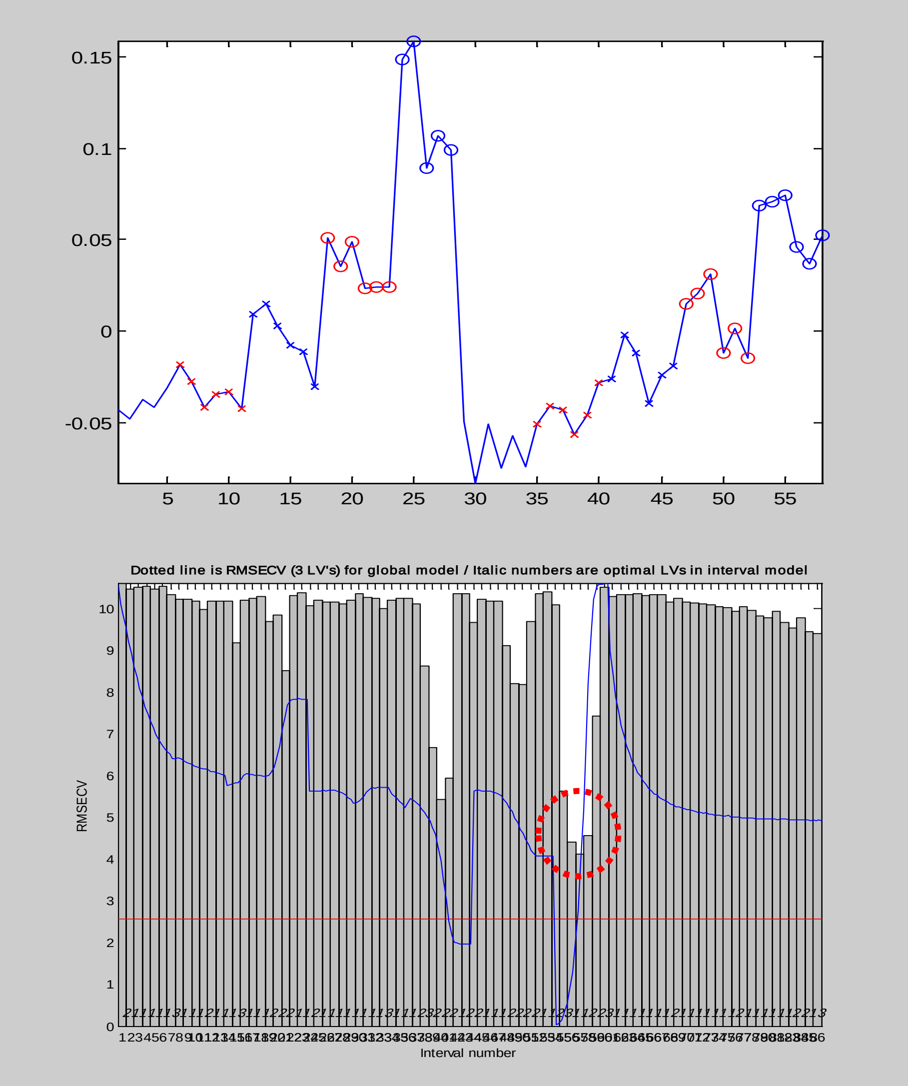
Correlation between PLS-ComDim Scores and "Lignin"



i-PLS between NIR and "Lignin"

- Blocks = 86
- Mean centred
- Max LVs = 3
- CV = Full

- Scores on LV1
  for Block 56



2) NIR on apples

Samples

- 2 Varieties :
  - Cox, Jonagold
- 2 Faces :
  - Red, Green
- 3 Maturity levels :
  - fresh, ripe, over-ripe
- 8 different apples

Spectra

- 94 x 200 points

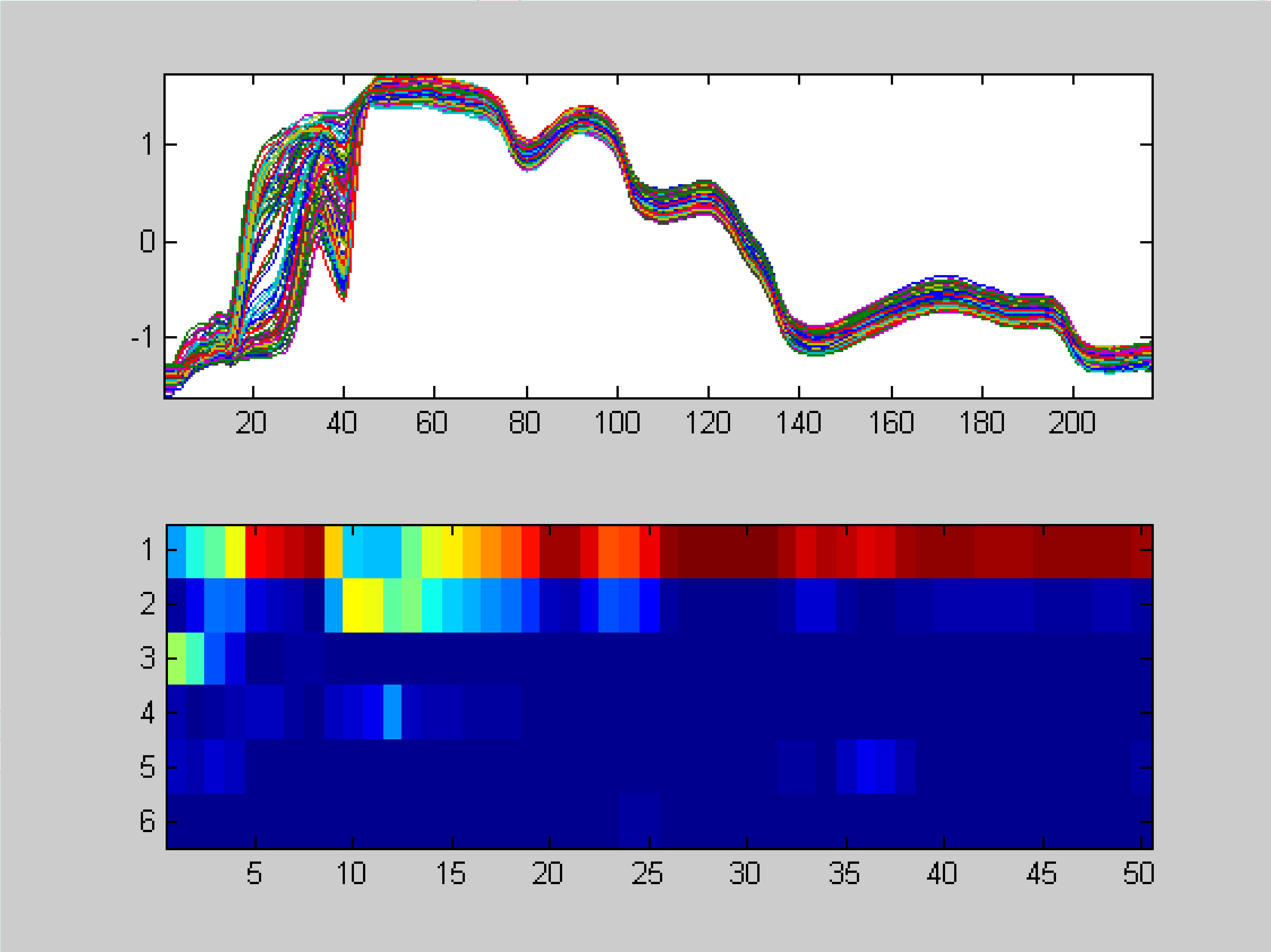
Tables

- 50 blocks of 4 variables
- 6 Common Dimensions

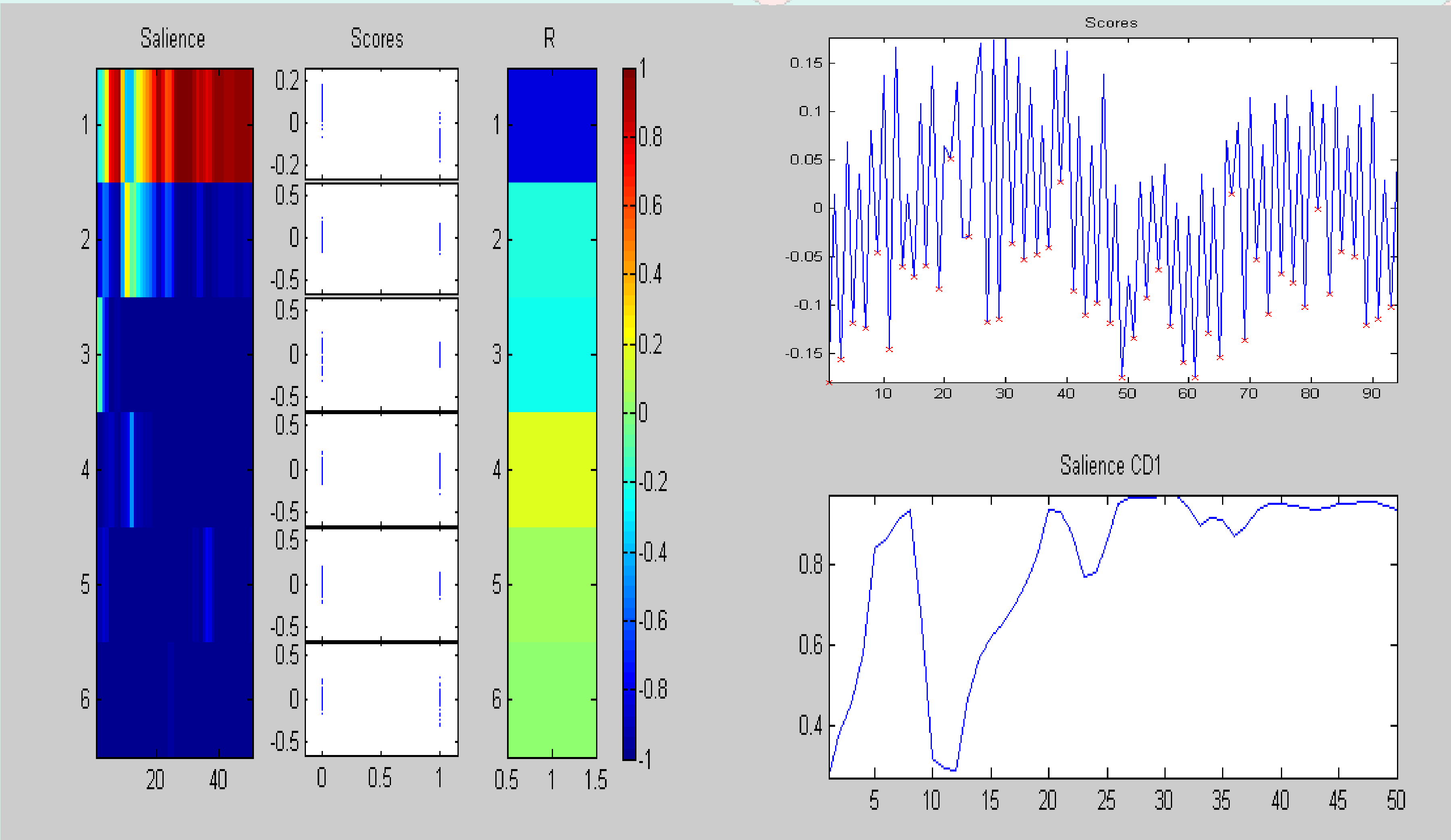
NIR Spectra

Spectra

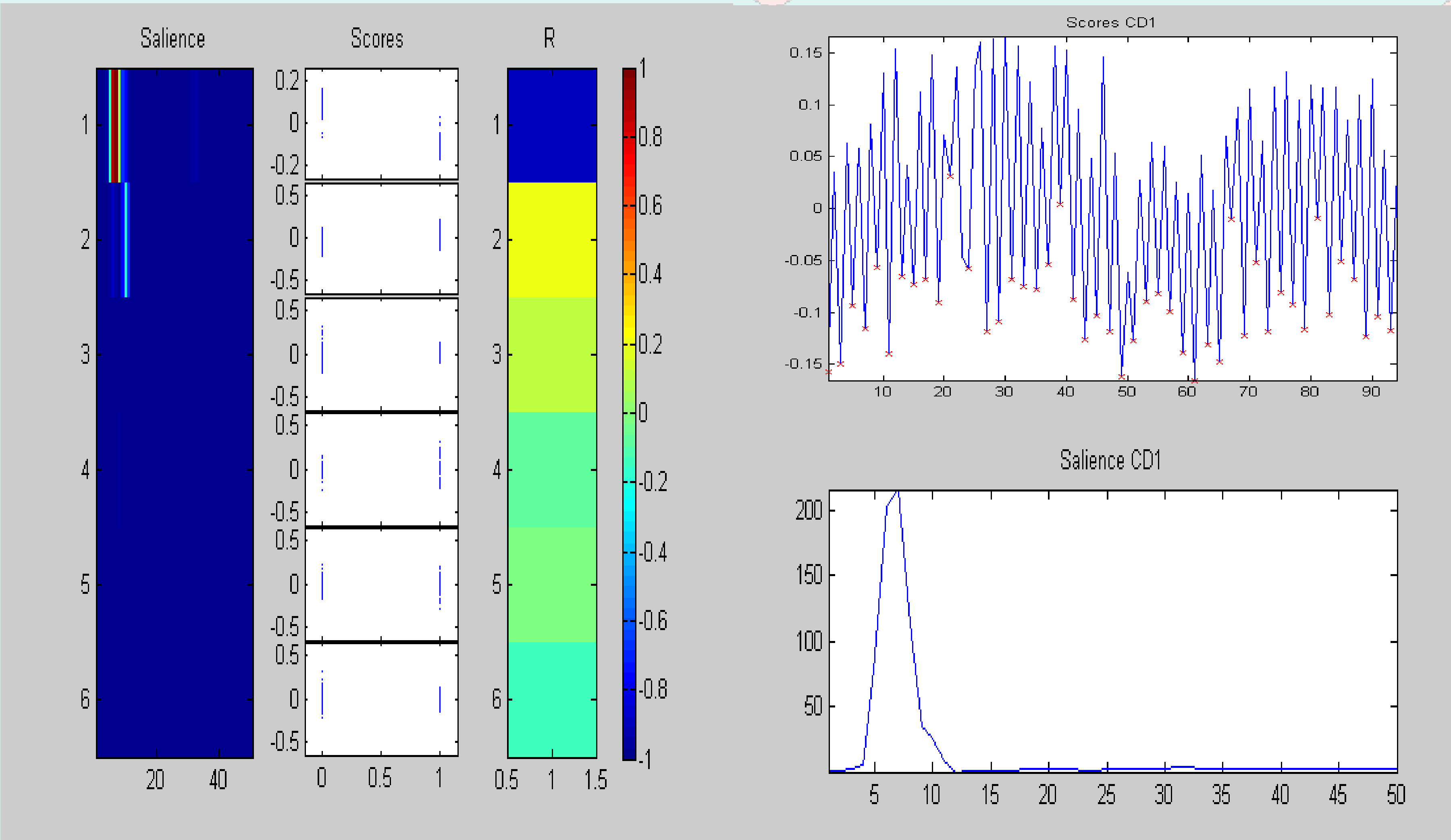
ComDim Saliences



Correlation between ComDim Scores and "Face"



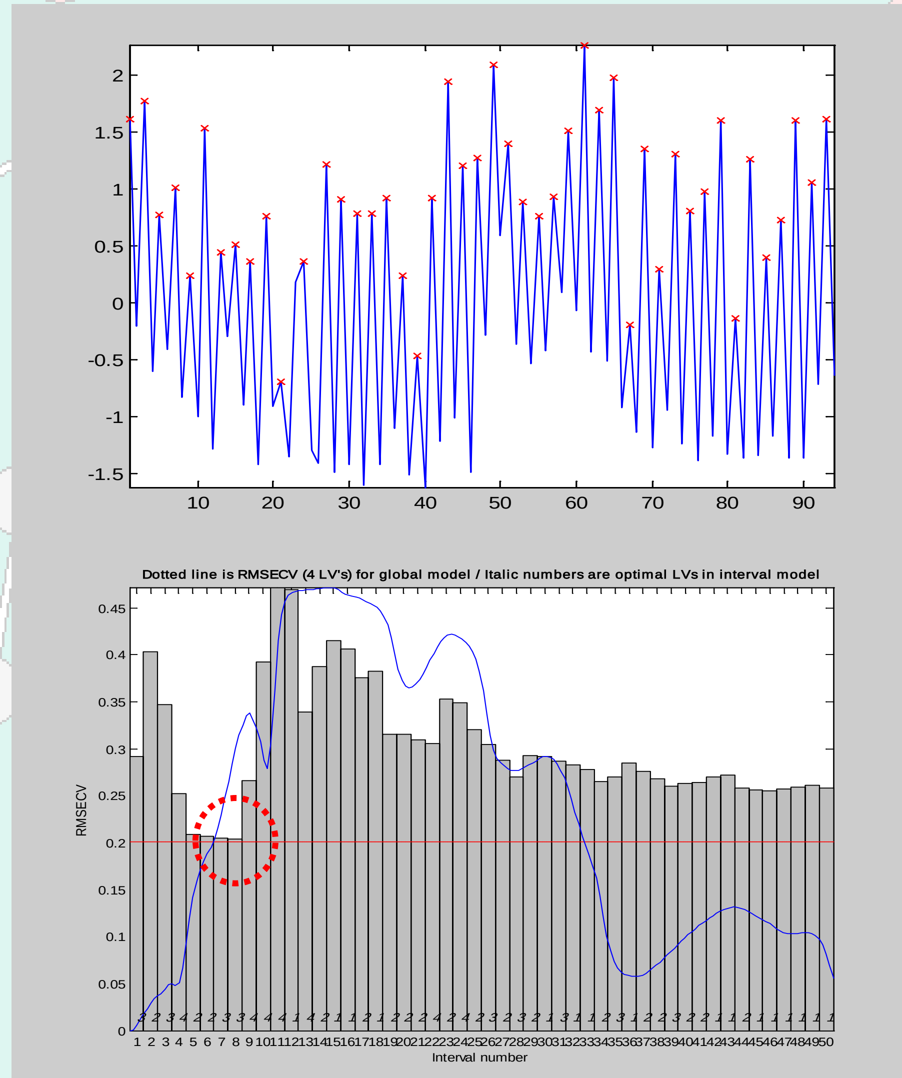
Correlation between PLS-ComDim Scores and "Face"



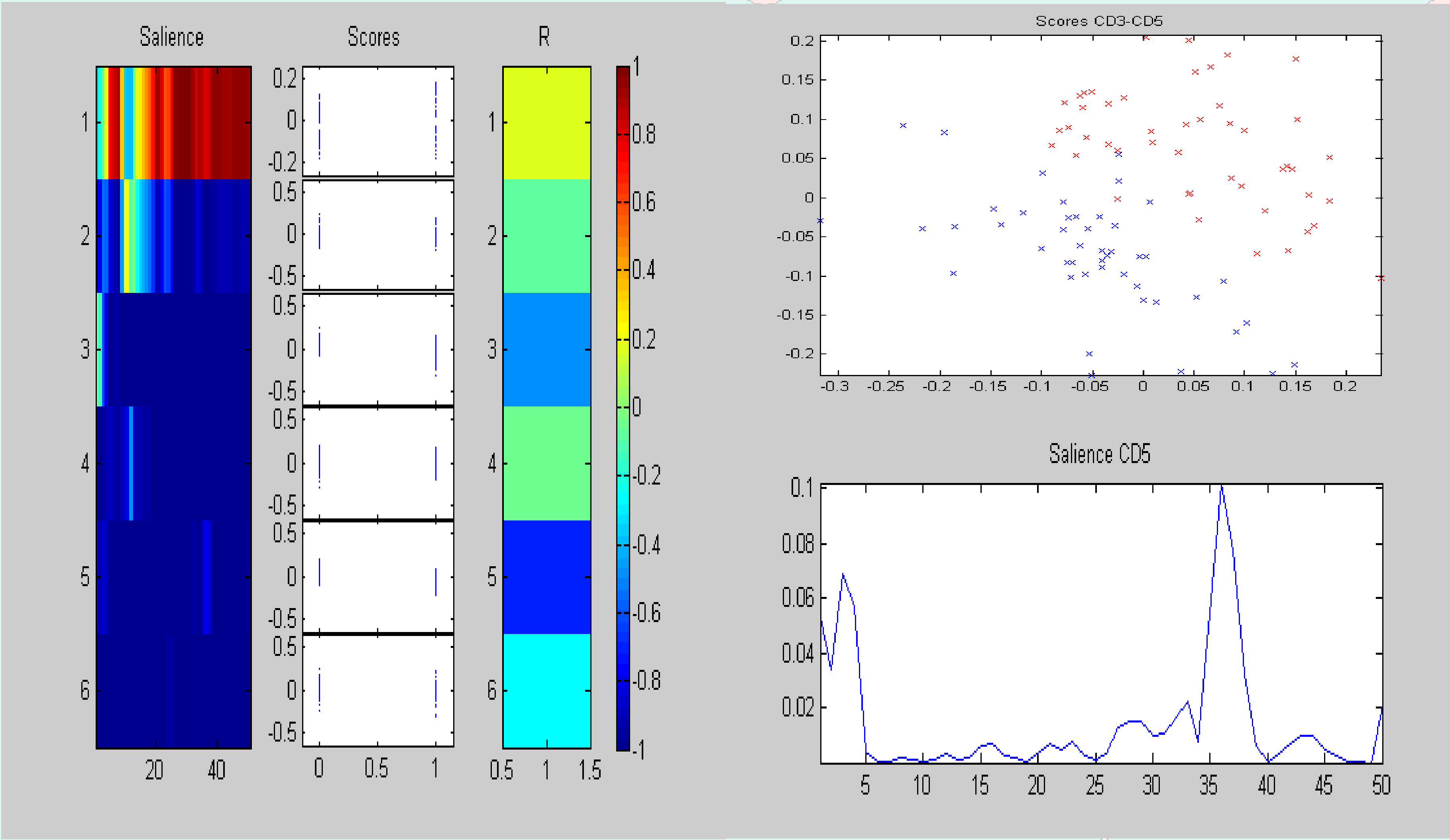
i-PLS between NIR and "Face"

- Blocks = 50
- Mean centred
- Max LVs = 4
- CV = Full

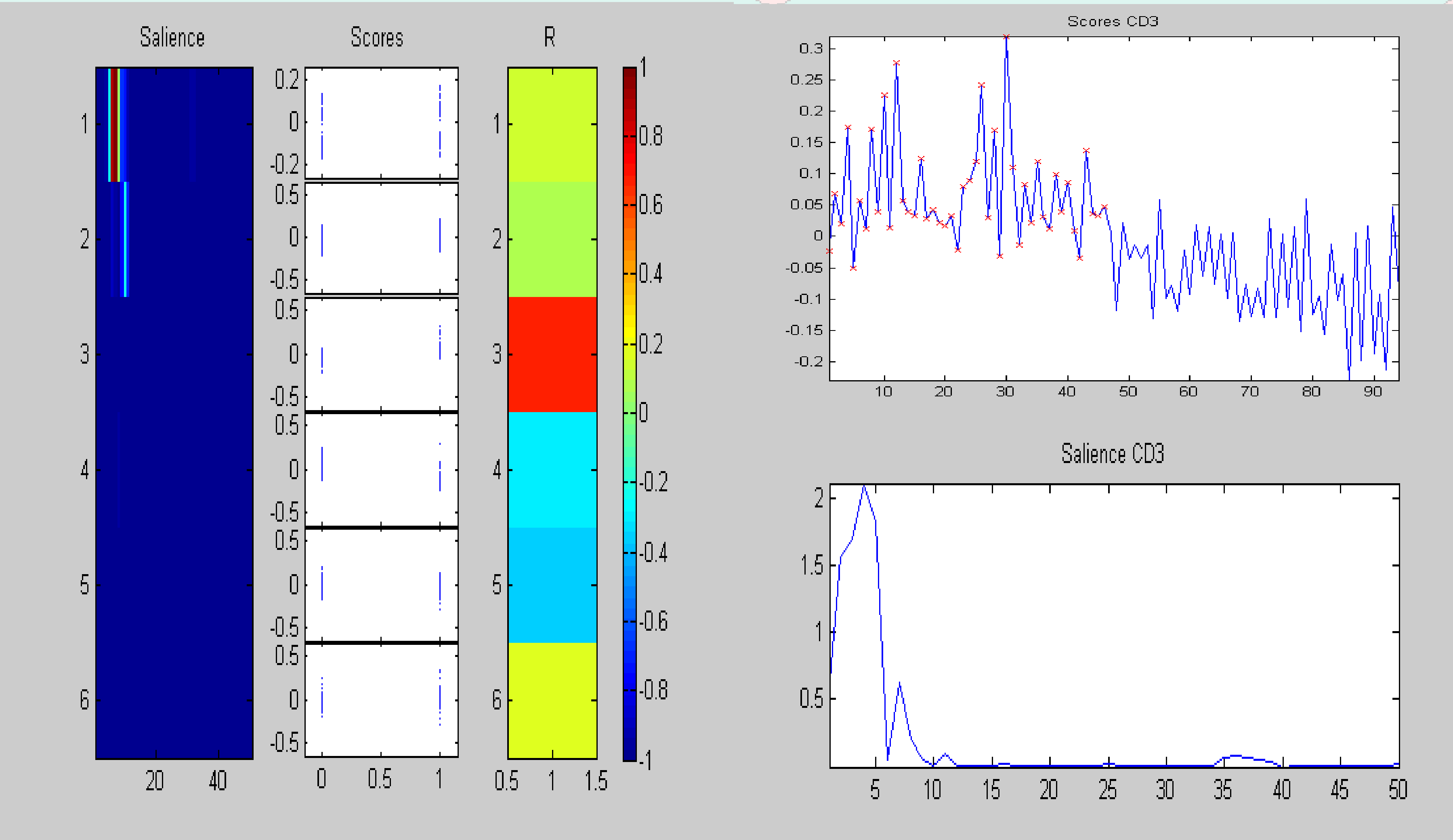
- Scores on LV1
  for Block 8



Correlation between ComDim Scores and "Variety"



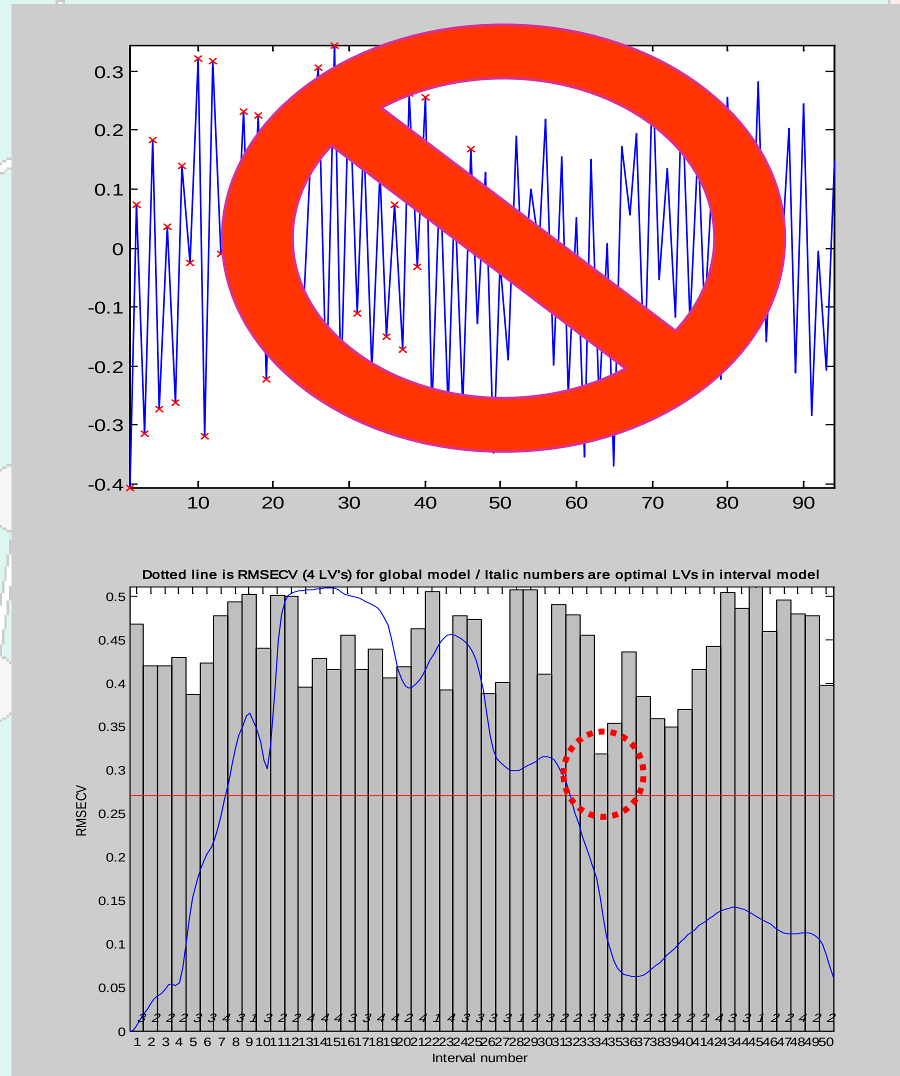
Correlation between PLS-ComDim Scores and "Variety"



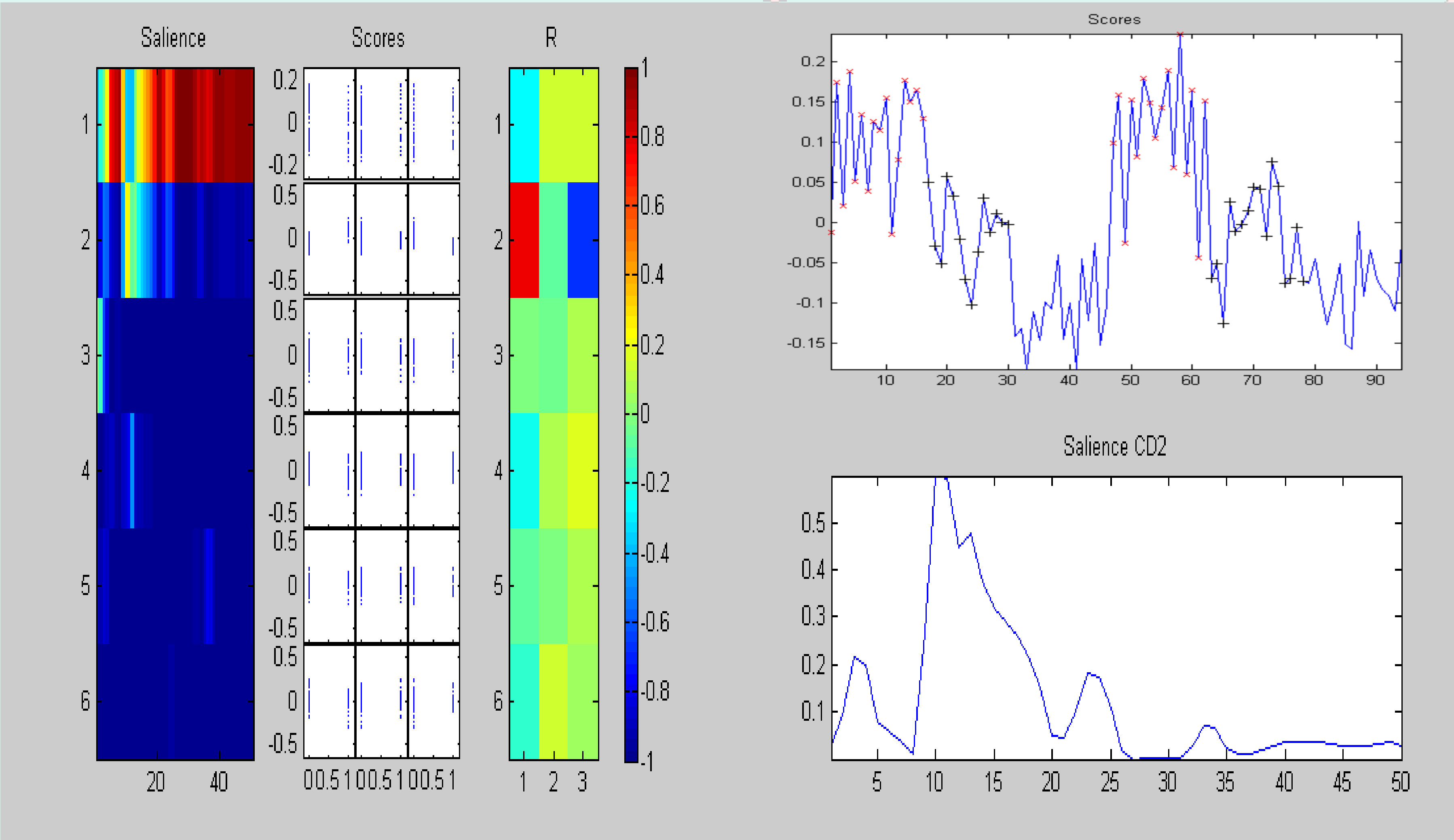
i-PLS between NIR and "Variety"

- Blocks = 50
- Mean centred
- Max LVs = 4
- CV = Full

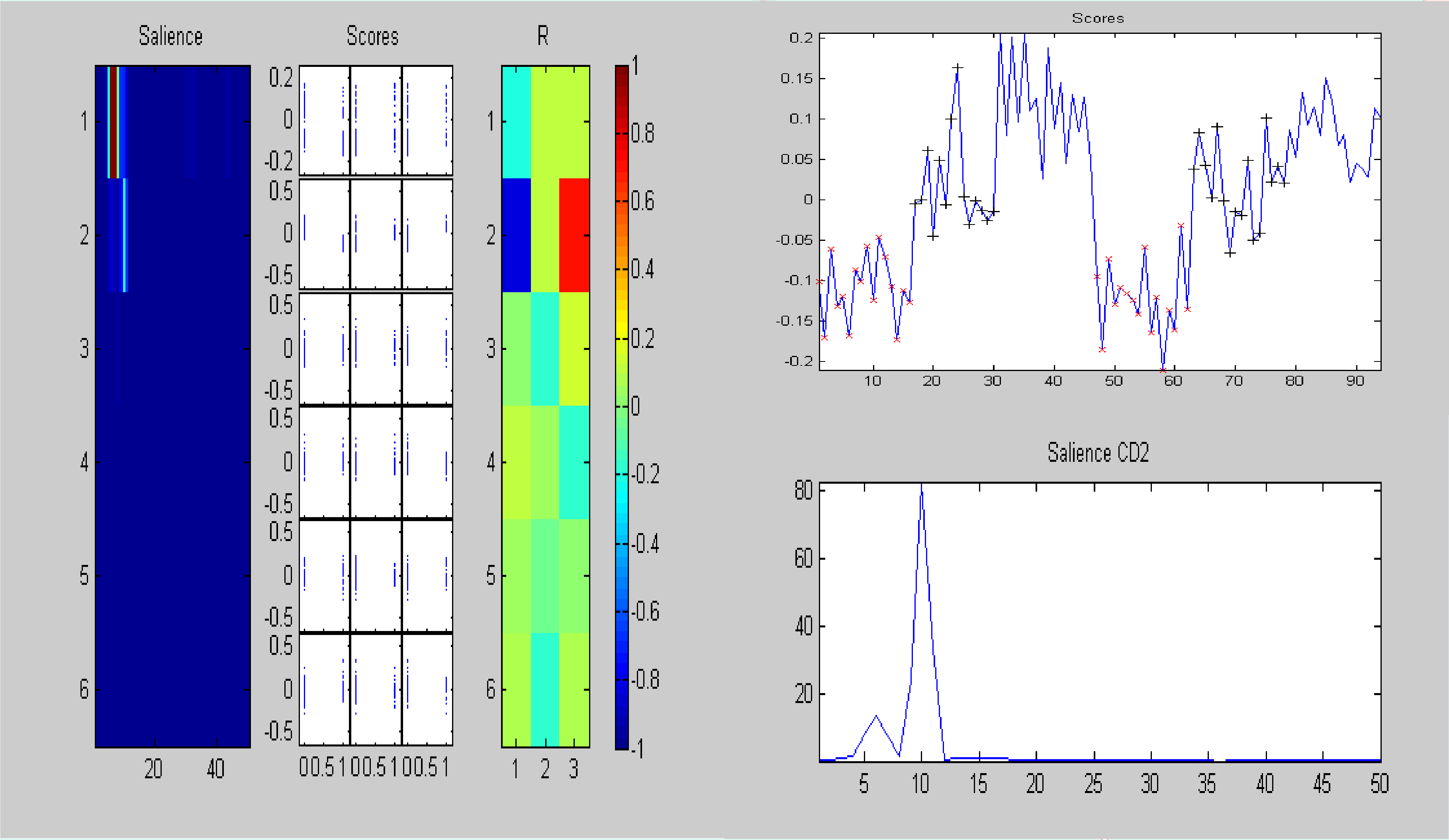
- Scores on LV1
  for Block 33



Correlation between ComDim Scores and "Maturity"



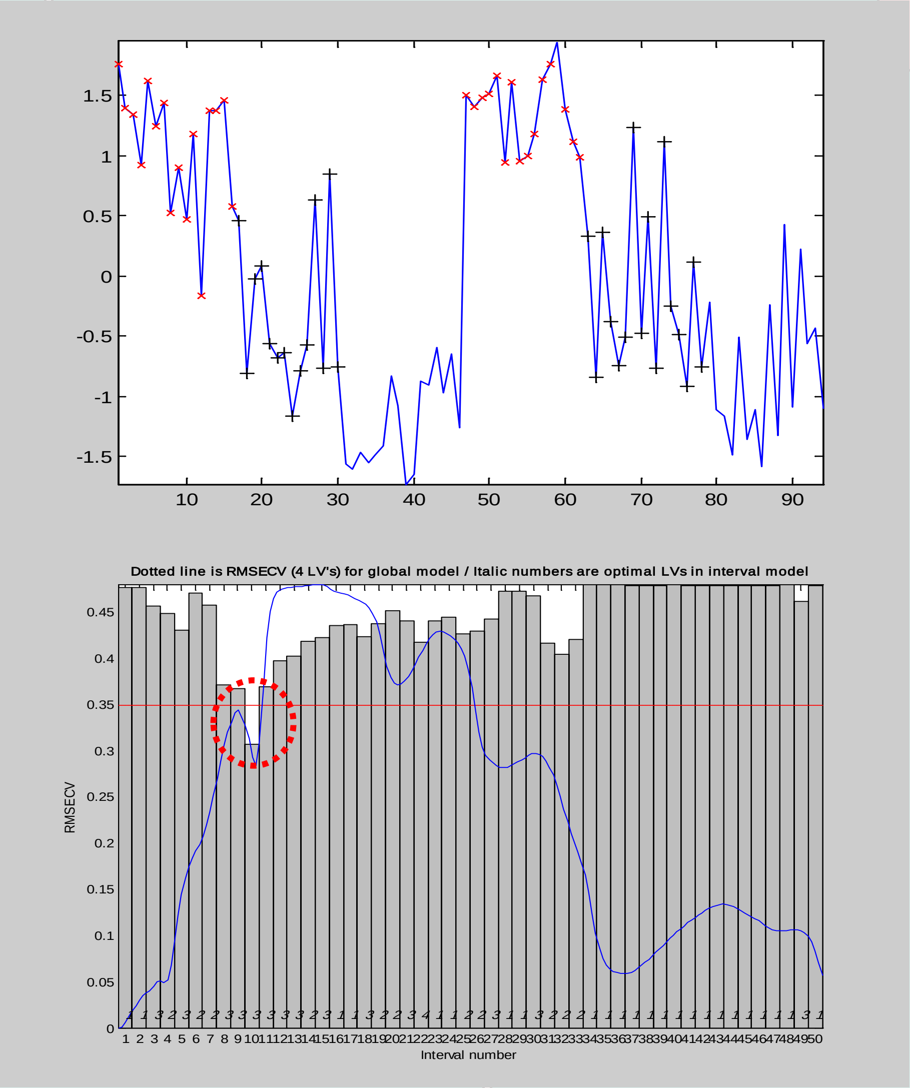
Correlation between PLS-ComDim Scores and "Maturity"



i-PLS between NIR and "Maturity"

- Blocks = 50
- Mean centred
- Max LVs = 4
- CV = Full

- Scores on LV1
  for Block 10



3) 2D-Fluorescence on wines

Samples

- Vintage :
  - 2004, 2005, 2006
- Micro-oxygenation :
  - Yes, No
- Oak chips :
  - Yes, No
- 3 repetitions

Signals

- 37 x 100*45 points 2D-Fluorescence spectra

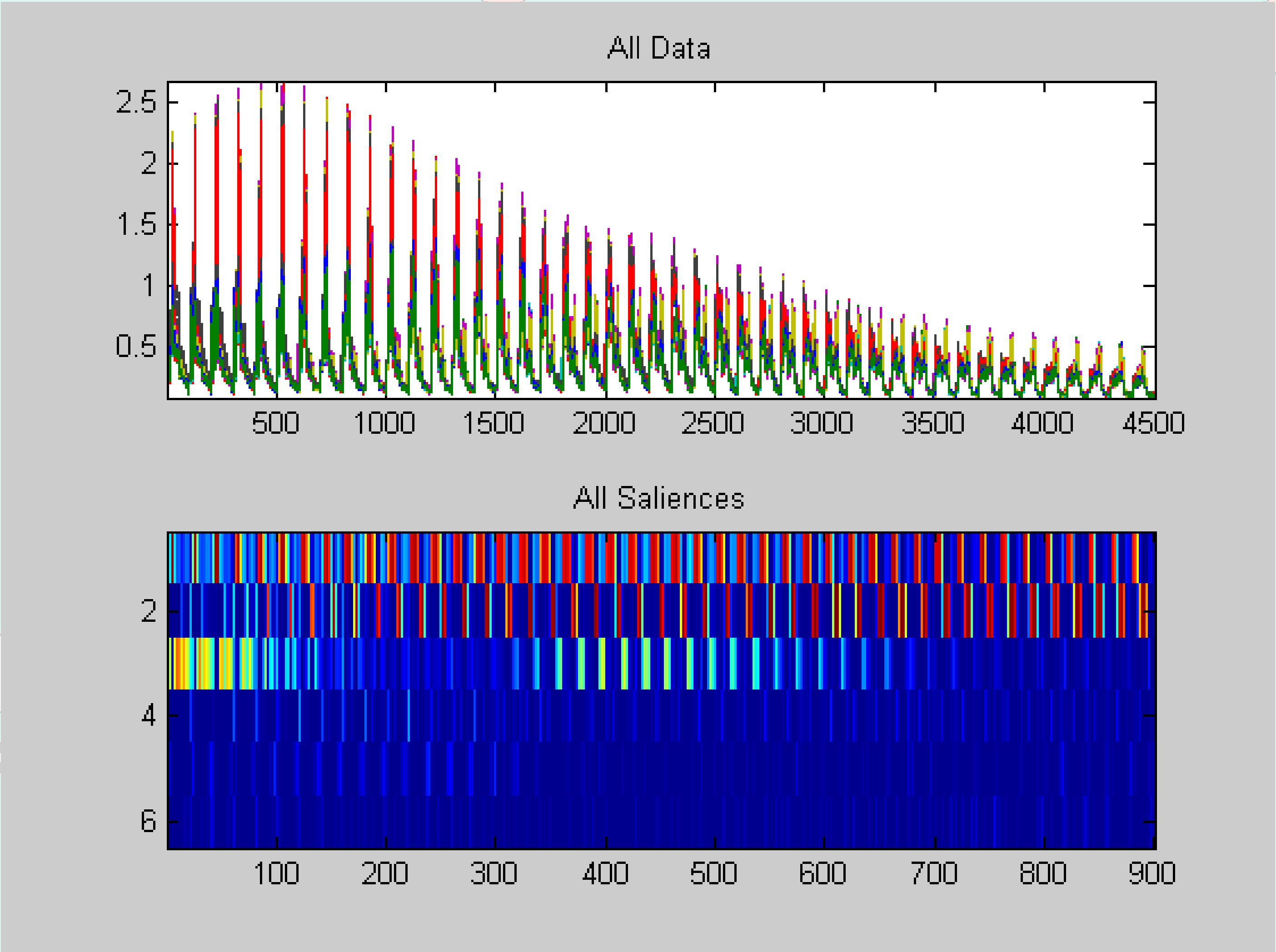
Tables

- 900 blocks of 5 variables
- 6 Common Dimensions

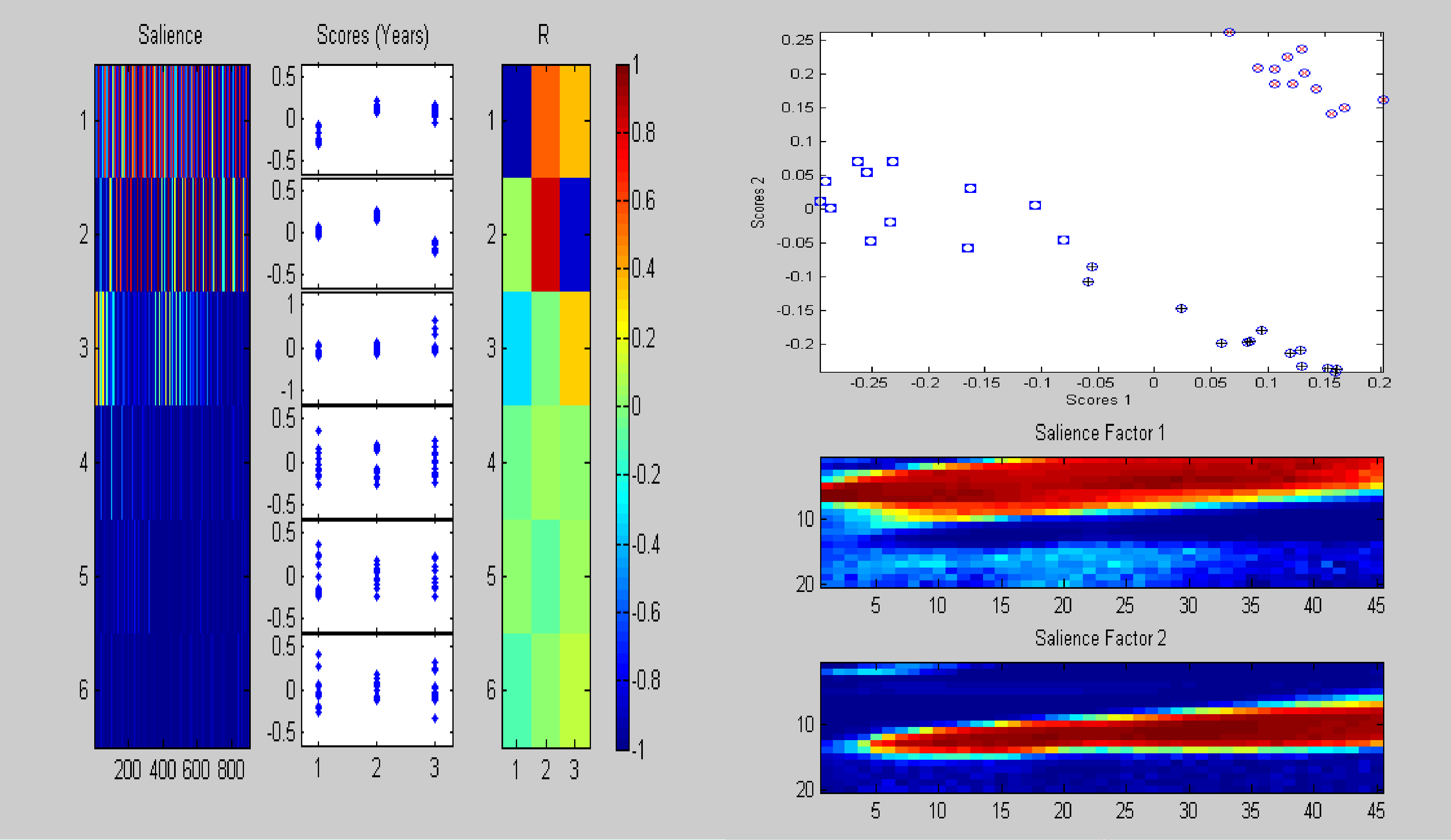
Unfolded 3D-Fluorescence Spectra

Spectra

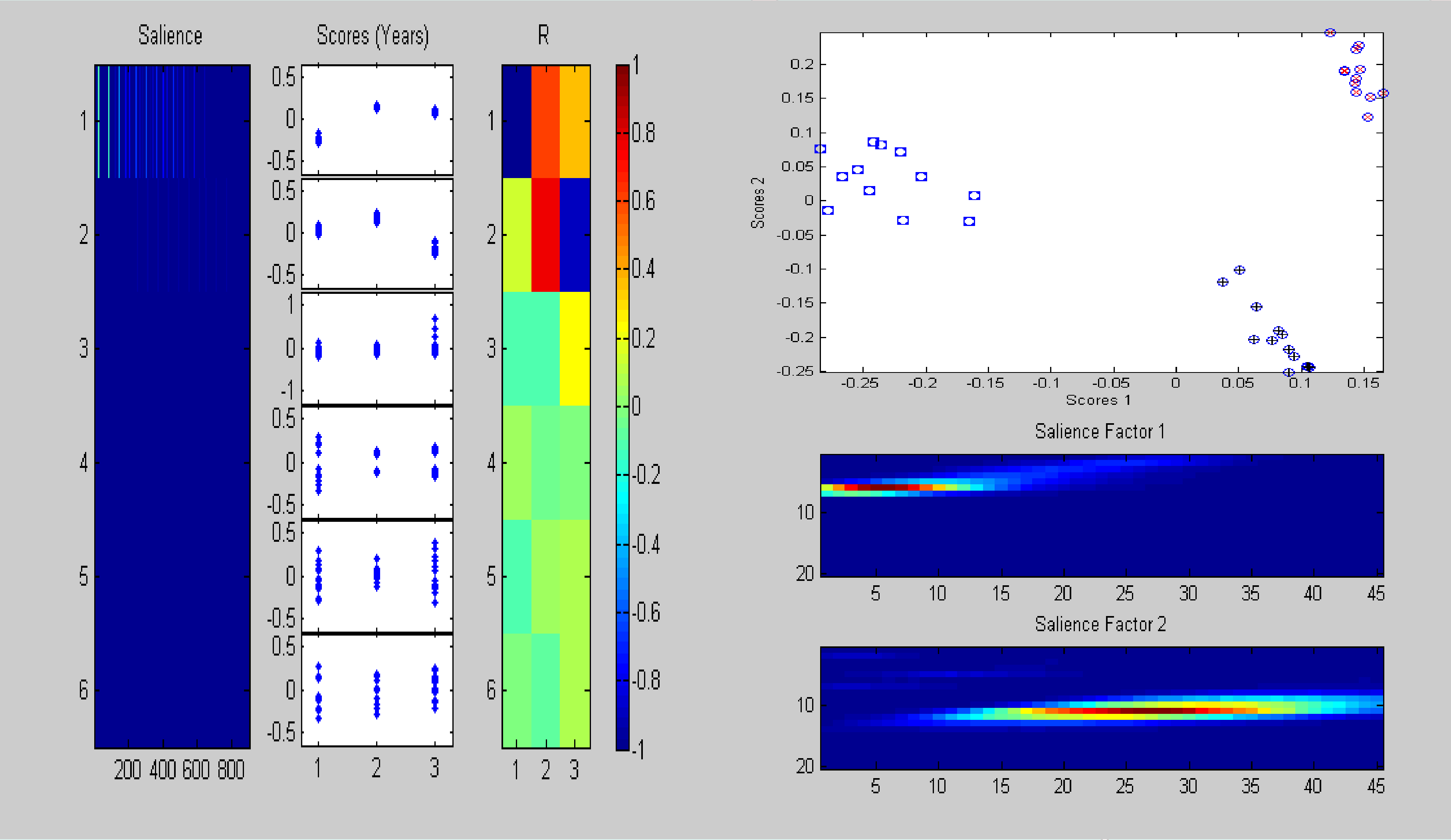
ComDim Saliences



Correlation between ComDim Scores and "Year"



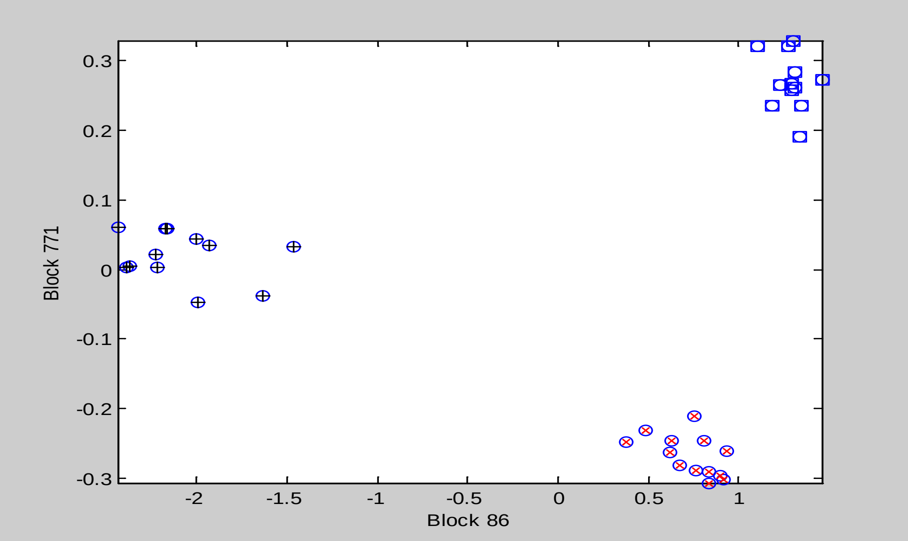
Correlation between PLS-ComDim Scores and "Year"



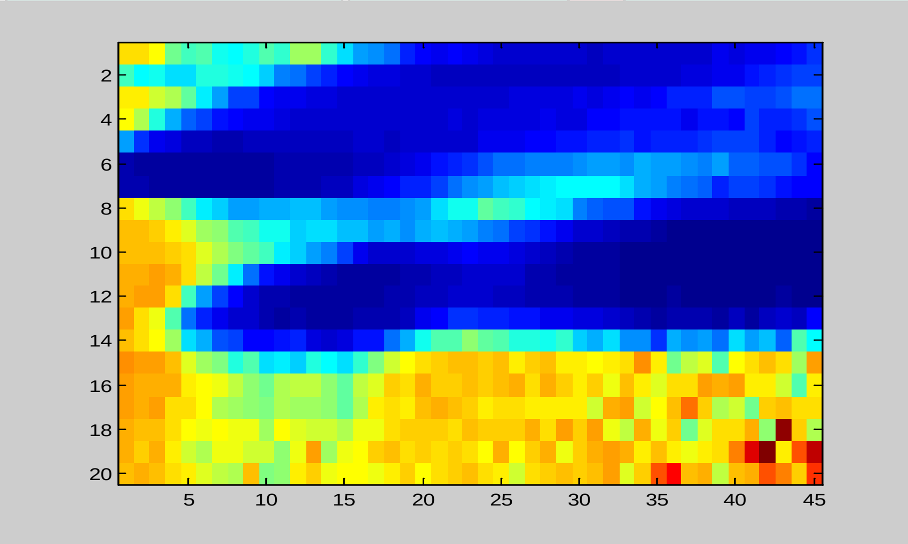
i-PLS between NIR and "Year"

- Blocks = 900
- Mean centred
- Max LVs = 4
- CV = Full

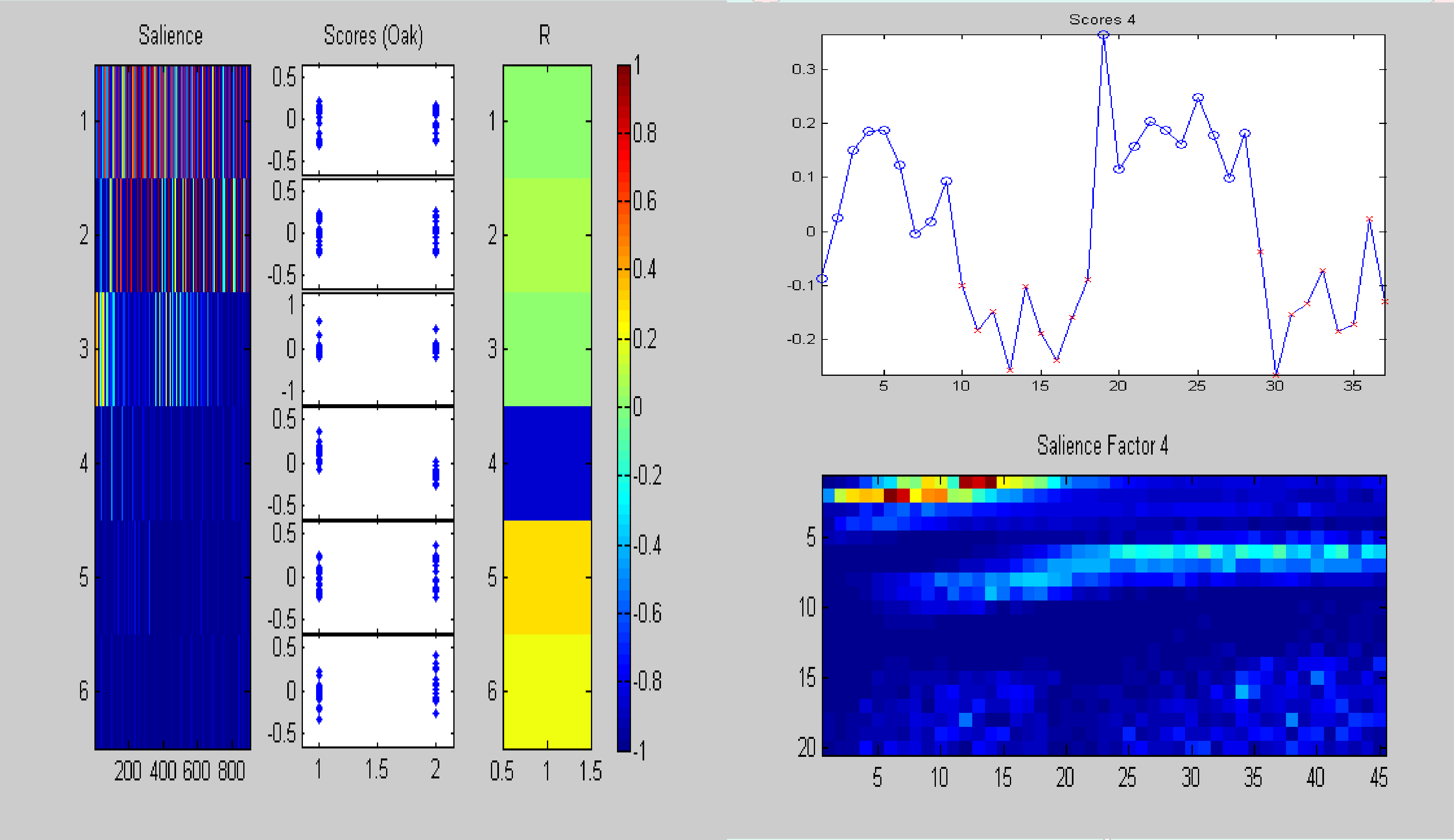
- Scores on LV1
  for Blocks 86 & 771



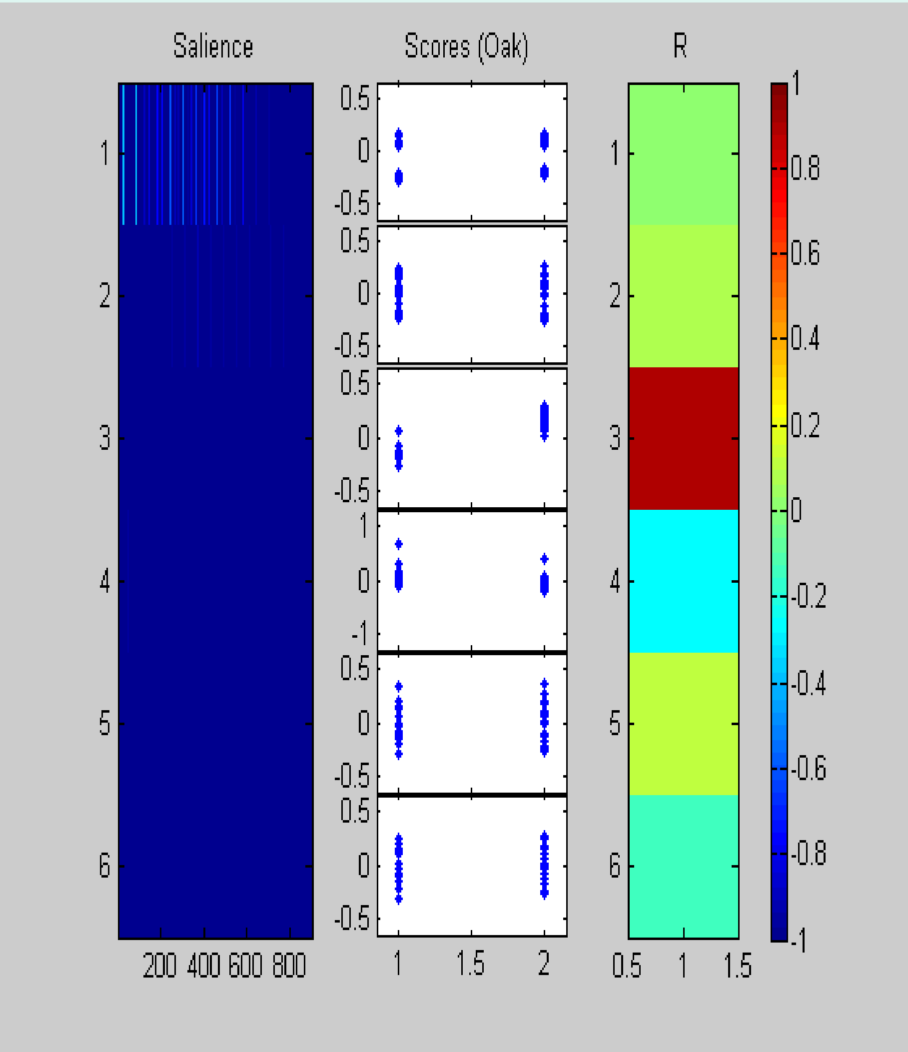
- RMSE for 1 LV

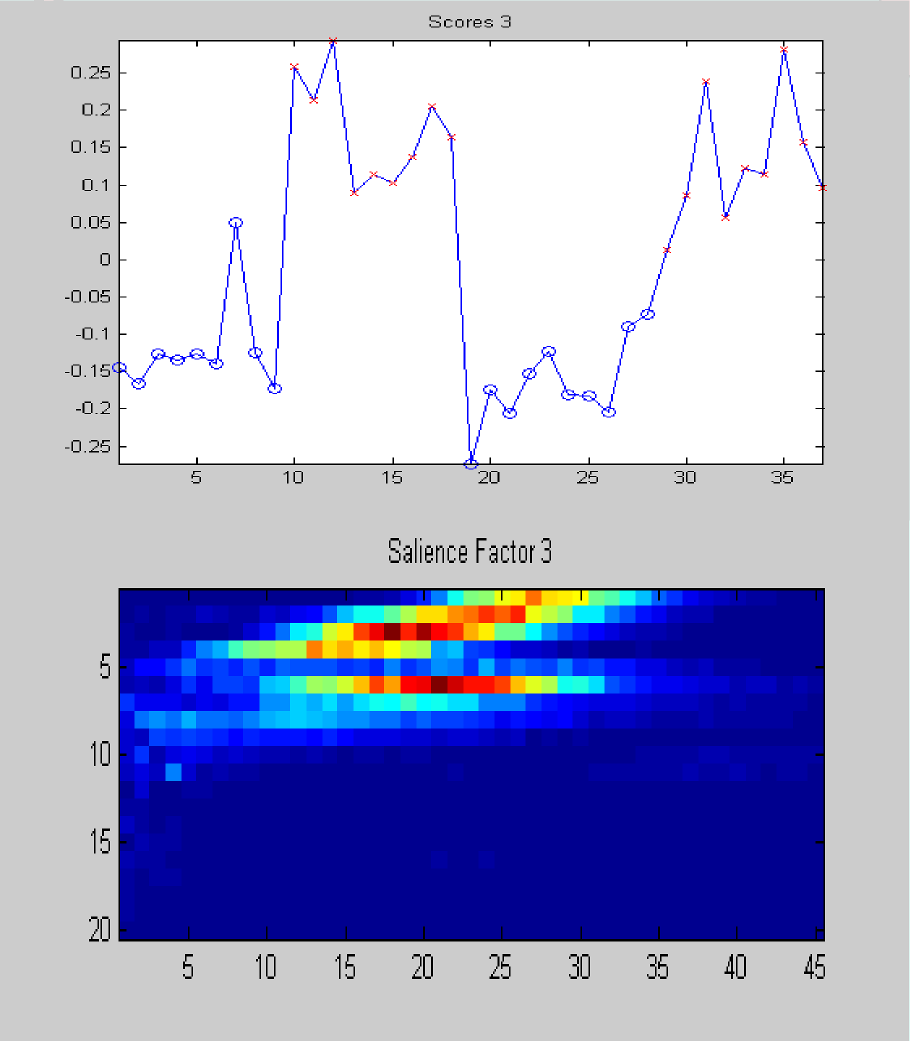


Correlation between ComDim Scores and "Oak"



Correlation between PLS-ComDim Scores and "Oak"

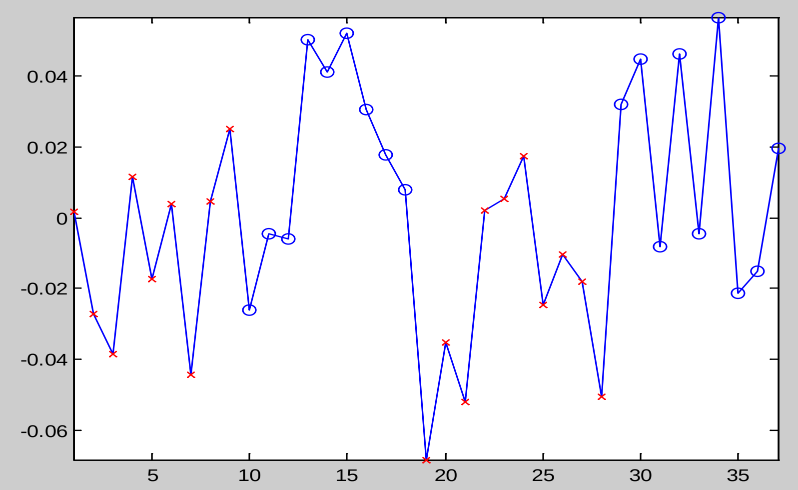




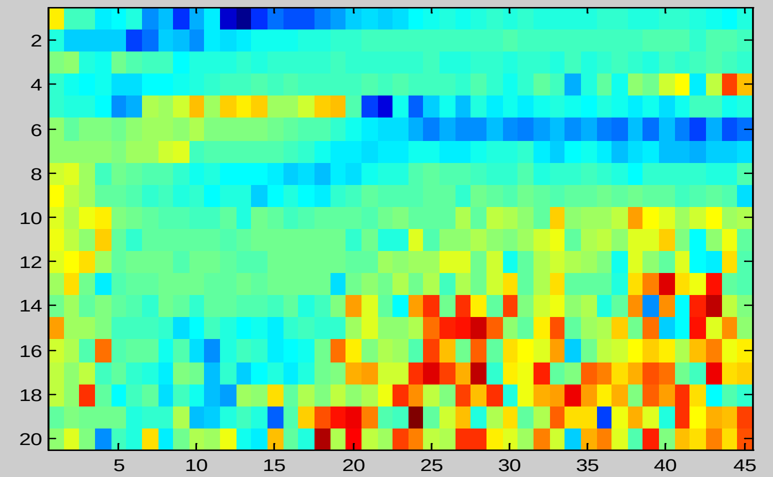
i-PLS between NIR and "Oak"

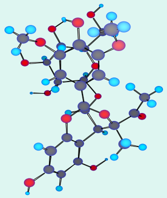
- Blocks = 900
- Mean centred
- Max LVs = 4
- CV = Full

- Scores on LV1
  for Block 798



- RMSE for 1 LV

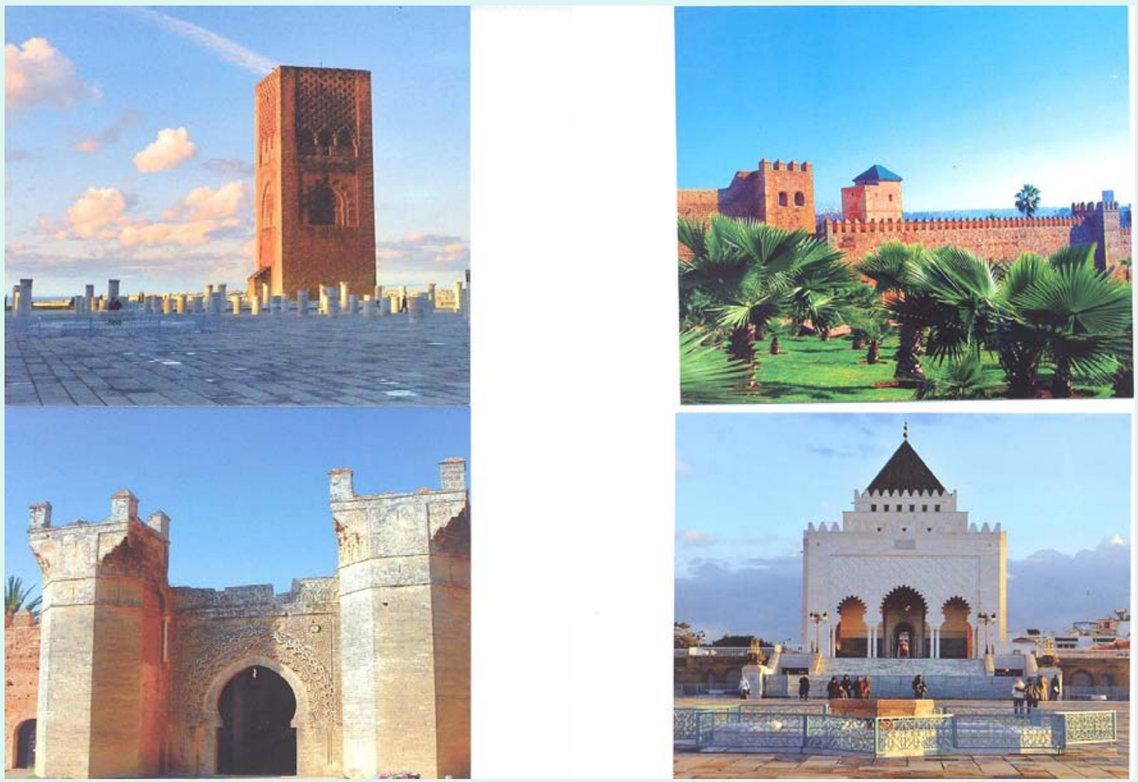




First African-European Conference on Chemometrics

Mining School of Rabat

Morocco, 20^{th} to 24^{th} of September 2010



www.afrodata.org