


DTU

Partial Least Squares Regression analysis

Course 27411
Chemometrics and Biological Data Analysis

Thanks to Jens Christian Frisvad for some of the slides.

Per Bruun Brockhoff
Building 324
Technical University of Denmark
2800 Kgs. Lyngby – Denmark
E-mail: perbb@dtu.dk



DTU Compute
Department of Applied Mathematics and Computer Science

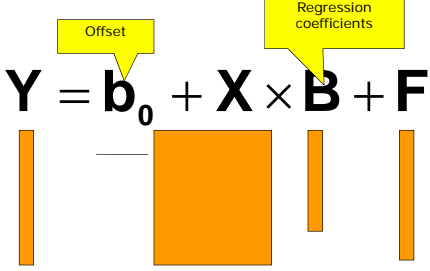
DTU

Symbolics, One Ys

$$Y = b_0 + X \times B + F$$

Offset (pointing to b_0)

Regression coefficients (pointing to B)



4 DTU Compute, Technical University of Denmark 09/03/2015

DTU

Principal component analysis

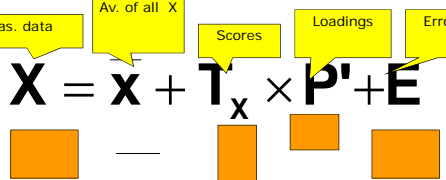
Meas. data (pointing to X)

Av. of all X (pointing to \bar{X})

Scores (pointing to T_X)

Loadings (pointing to P')

Errors (pointing to E)

$$X = \bar{X} + T_X \times P' + E$$


2 DTU Compute, Technical University of Denmark 09/03/2015

DTU

PLS1: Symbolics

Scores (pointing to t_1)

Loadings (pointing to p_1)

Errors (pointing to E_1)

Meas. data (pointing to X)

Av. of all X (pointing to \bar{X})

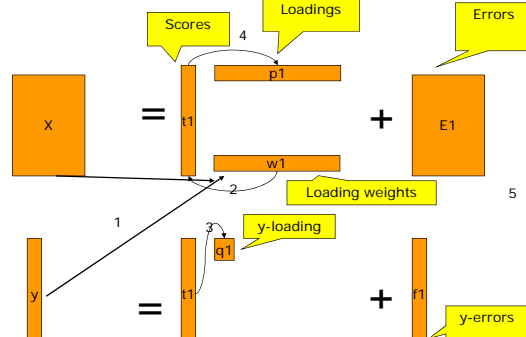
Y (pointing to y)

Loadings weights (pointing to w_1)

y-loading (pointing to q_1)

y-errors (pointing to f_1)

$$X = \bar{X} + t_1 p_1 + E_1$$

$$y = \bar{y} + t_1 q_1 + f_1$$


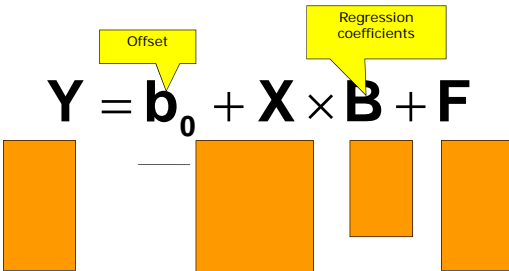
5 DTU Compute, Technical University of Denmark 09/03/2015

DTU

Symbolics, Many Ys

Offset (pointing to b_0)

Regression coefficients (pointing to B)

$$Y = b_0 + X \times B + F$$


3 DTU Compute, Technical University of Denmark 09/03/2015

DTU

PLS1: Symbolics

Scores (pointing to t_2)

Loadings (pointing to p_2)

Errors (pointing to E_2)

Meas. data (pointing to X)

Av. of all X (pointing to \bar{X})

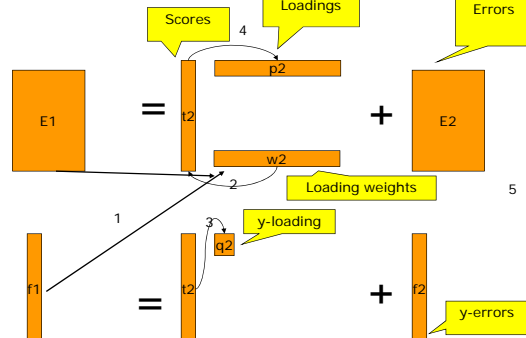
Y (pointing to y)

Loadings weights (pointing to w_2)

y-loading (pointing to q_2)

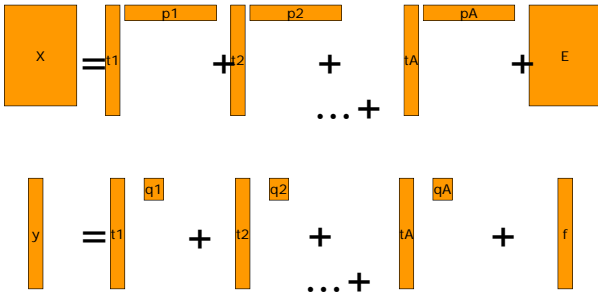
y-errors (pointing to f_2)

$$X = \bar{X} + t_2 p_2 + E_2$$

$$y = \bar{y} + t_2 q_2 + f_2$$


6 DTU Compute, Technical University of Denmark 09/03/2015

PLS1: Symbolics



7 DTU Compute, Technical University of Denmark

09/03/2015

PLS in perspective



- Other extensions:
 - N-PLS (Multiblock data: X,Y,Z)
 - L-PLS (For consumer preference mapping)
 -
 -
 -

10 DTU Compute, Technical University of Denmark

09/03/2015

PLS2 Intuition (=“PCR2”)



PCA of X: $X = \bar{x} + T \times P' + E$

PCA of Y: $Y = \bar{y} + U \times Q' + F$

Let the X-components describe the Y-components:

$$T \longrightarrow U$$

In PLS2: The X and Y decompositions are NOT chosen independently from each other

(In classical text books: Canonical Correlation analysis)

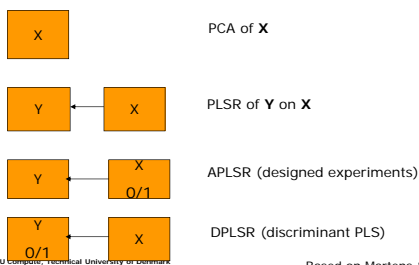
8 DTU Compute, Technical University of Denmark

09/03/2015

PLS in perspective



- Two matrices X and Y are compared



9 DTU Compute, Technical University of Denmark

Based on Martens & Martens¹⁵