

Multilevel Design

How to transform your dataMatrix



How to use Multilevel and Why

Experimental Design with:

- Repeated measurement on same subjects
 - Kinetic
 - Treatment (Before vs After)

Problem : inter-individual biological variability can be really high, sometime higher than the expected studied biological effect.

Experimental design; « cross-over » every individual is it own control

Variability is separated in 2 parts taking into account repeated measurments on each individuals

Data pairing= no independance

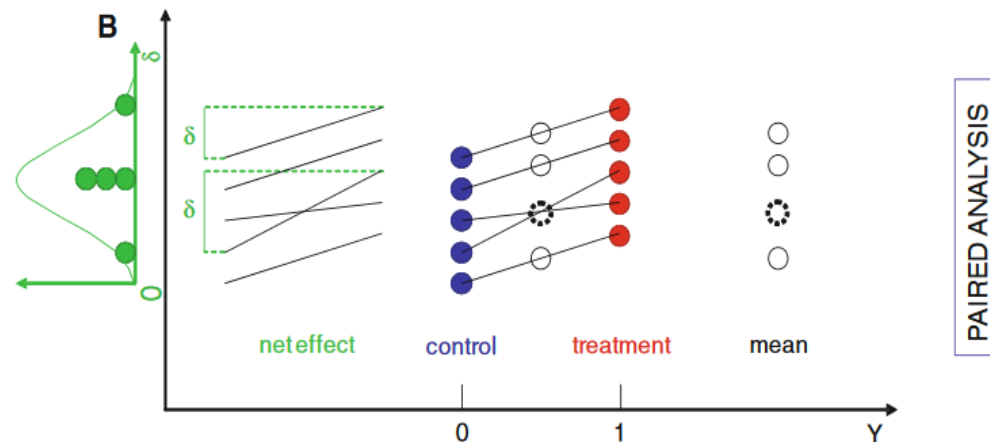
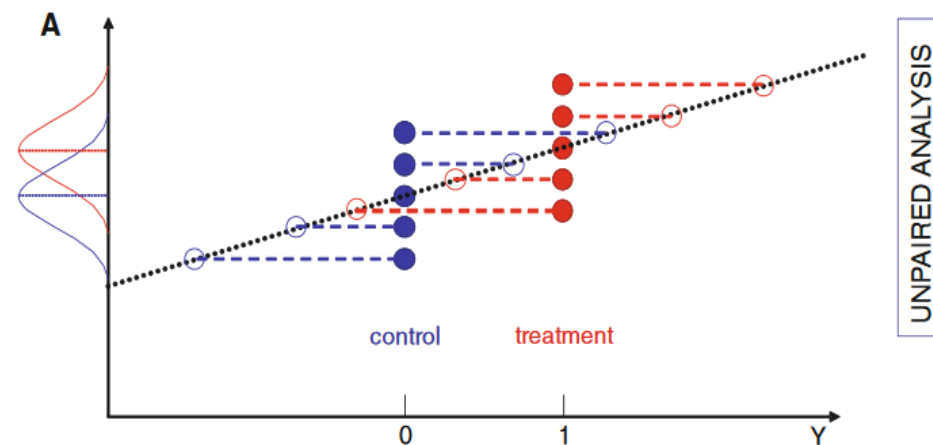
Not taken into account in usal Multivariates statistics



How to use Multilevel and Why

Experimental Design with:

- Repeated measurement on same subjects
- Kinetic
- Treatment (Before vs After)



Westerhuis, Johan A., Ewoud J. J. van Velzen, Huub C. J. Hoefsloot, and Age K. Smilde. 2010. 'Multivariate Paired Data Analysis: Multilevel PLSDA versus OPLSDA'. *Metabolomics* 6 (1): 119–28. doi:10.1007/s11306-009-0185-z.

How to use Multilevel and Why

Without data correction

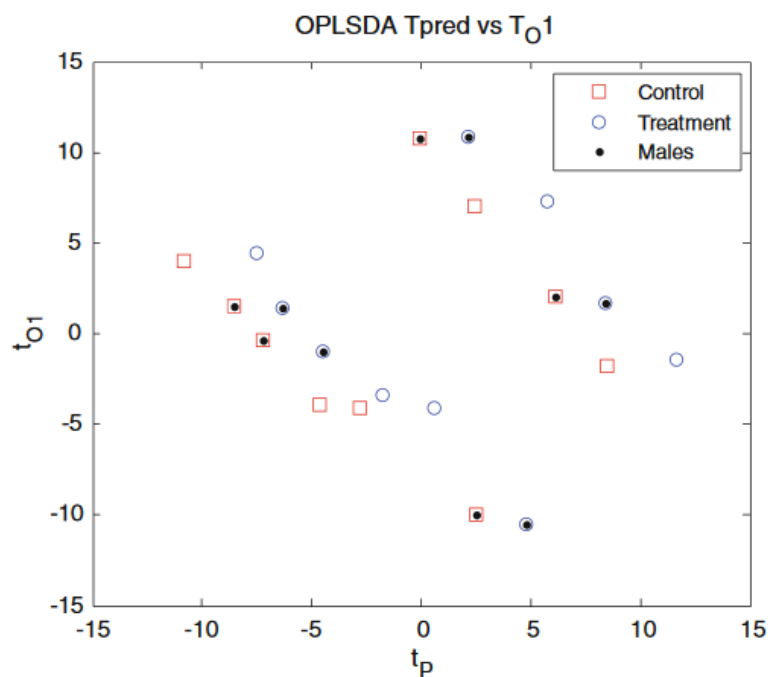


Fig. 2 Double cross validated OPLSDA score plot of simulated data.

With data correction

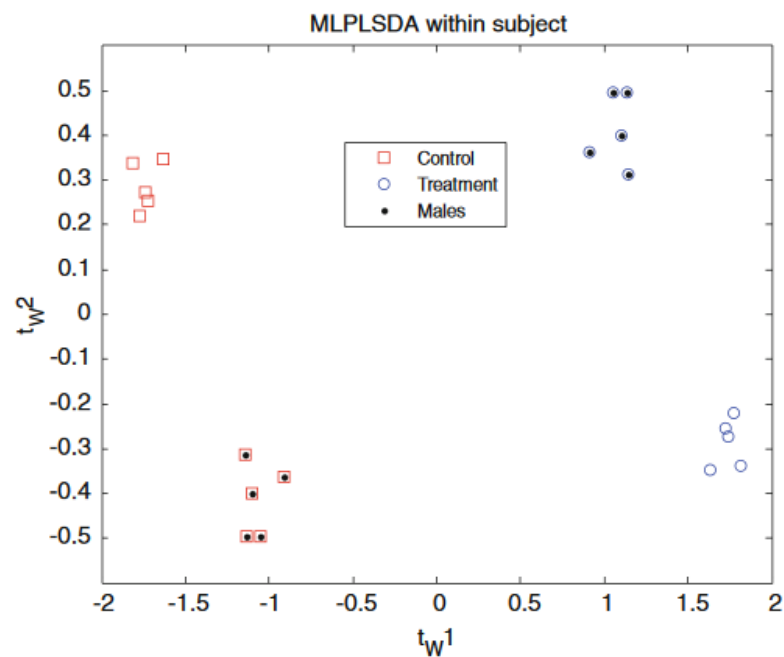


Fig. 3 The multilevel PLSDA scores (t_{w1} , t_{w2}) of the within subject

Westerhuis, Johan A., Ewoud J. J. van Velzen, Huub C. J. Hoefsloot, and Age K. Smilde. 2010. 'Multivariate Paired Data Analysis: Multilevel PLSDA versus OPLSDA'. *Metabolomics* 6 (1): 119–28. doi:10.1007/s11306-009-0185-z.

How to use Multilevel and Why

Normalisation

Normalization Normalization of (preprocessed) spectra

Multilevel Data transformation: Within matrix decomposition for repeated measurements (cross-over design) with mixOmics package

Determine batch correction to choose between linear, lowess and loess methods

Batch correction Corrects intensities for signal drift and batch-effects

Transformation Transforms the dataMatrix intensity values

Multilevel Data transformation: Within matrix decomposition for repeated measurements (cross-over design) with mixOmics package (Galaxy Version 0.5.0) Options

Data matrix file

18: dataMatrix.tsv

variable x sample, decimal: '.', missing: NA, mode: numerical, sep: tabular

Sample metadata file

18: dataMatrix.tsv

sample x metadata, decimal: '.', missing: NA, mode: character and numerical, sep: tabular

Repeated measurement label (Individual IDs, ...)

Indicate the column name of the sample table to be used as repeated measurement factor

Select number of levels¹

Level name (as in sampleMetadata)

Indicate the column name of the sample table to be used as factor

Add transformation to dataMatrix before withinVariation

Author(s) Benoit Liquet, Kim-Anh Le Cao, Benoit Gautier, Ignacio Gonzalez.

Galaxy wrapper and scripts developers for W4M integration Guillon Yann LABERCA yann.quitton@oniris-nantes.fr



