How to perform statistical analysis?

PCA analysis and (O)PLS(-DA) modelling

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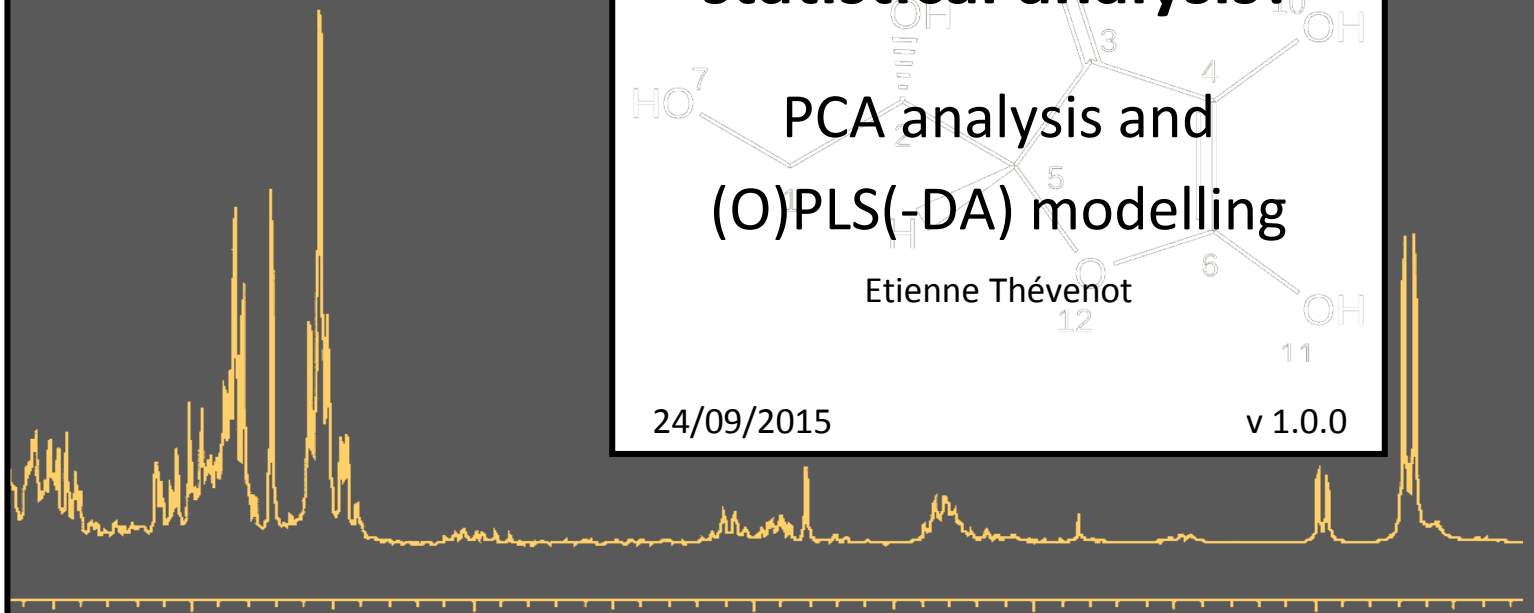
24/09/2015

v 1.0.0

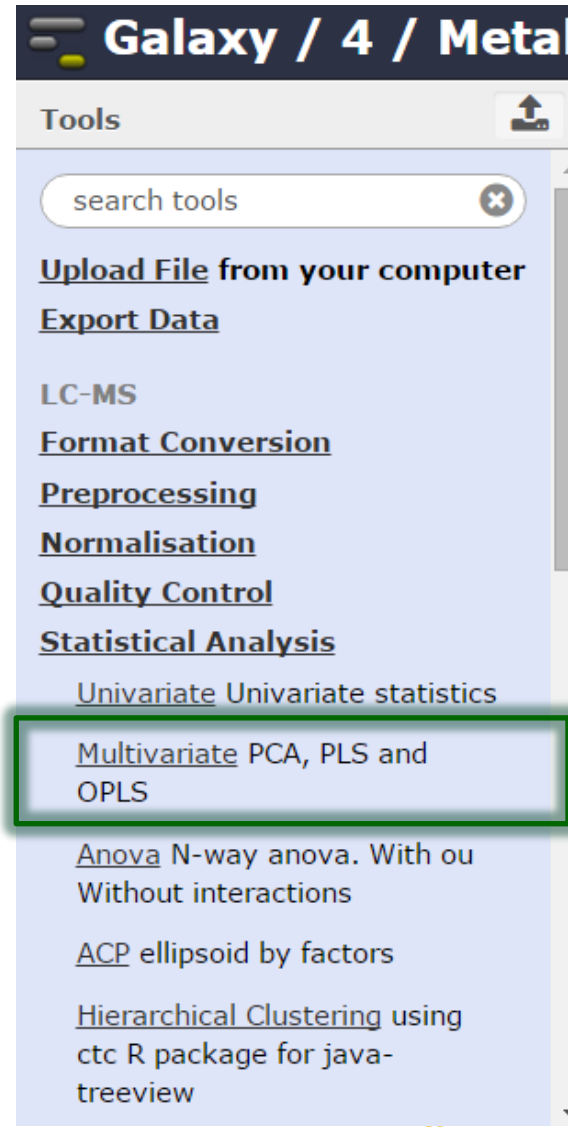


The "Multivariate" module

Multivariate

- The "**Multivariate**" module allows you to perform:
  - Principal Component Analysis (**PCA**)
  - Partial Least-Squares regression (**PLS**) and discriminant analysis (**PLS-DA**)
  - Orthogonal Partial Least-Squares regression (**OPLS**) and discriminant analysis (**OPLS-DA**)

- It is available in the "Statistical Analysis" sections of LC-MS, GC-MS, and NMR



The "Multivariate" module

Multivariate

- The Multivariate module uses internally the *ropls* R module from bioconductor

http://bioconductor.org/packages/ropls

  - implements the original, NIPALS based, algorithms for PCA, PLS and OPLS
  - diagnostics to detect outliers, overfitting
  - graphics (scores, loadings, predictions)
  - feature selection (VIP, regression coefficients)

Thévenot E.A., Roux A., Xu Y., Ezan E. and Junot C. (2015). Analysis of the human adult urinary metabolome variations with age, body mass index and gender by implementing a comprehensive workflow for univariate and OPLS statistical analyses. *Journal of Proteome Research,* **14:**3322-3335. http://dx.doi.org/10.1021/acs.jproteome.5b00354

Objectives

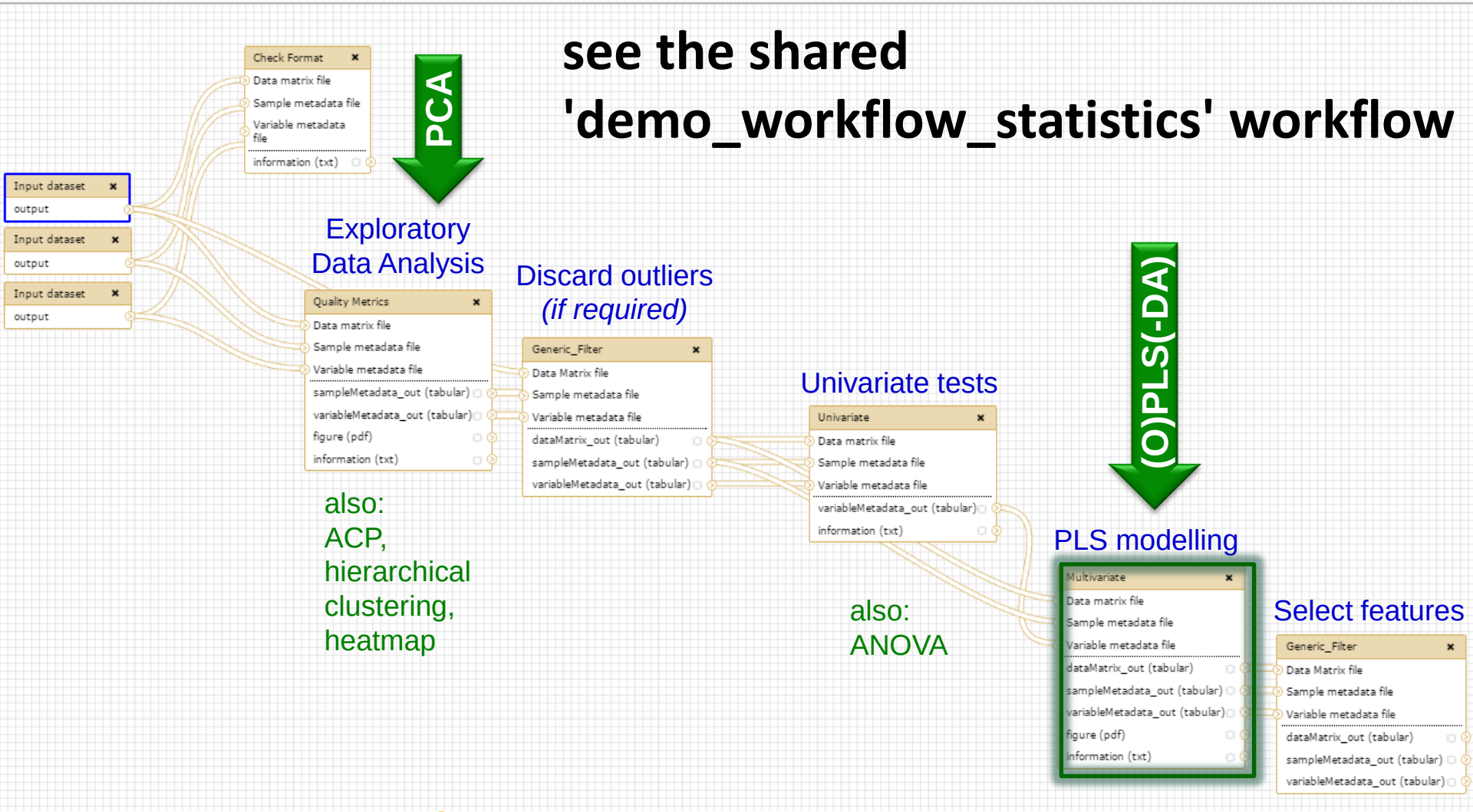
- Multivariate analysis:
  1. PCA [unsupervised]: Visualize the structure of the dataMatrix: $\mathbf{X}$
  2. (O)PLS(-DA) [supervised]: How can a factor of interest (response; column of sampleMetadata) be explained as a linear combination of **all** the variables (predictors) from dataMatrix: $\mathbf{y} = f(\mathbf{X})$
     a. when the response $\mathbf{y}$ is quantitative: (O)PLS regression
     b. when $\mathbf{y}$ is qualitative: (O)PLS(-DA) classification

     Complementary to univariate analysis (where variables are tested independently)

Latent variable methods

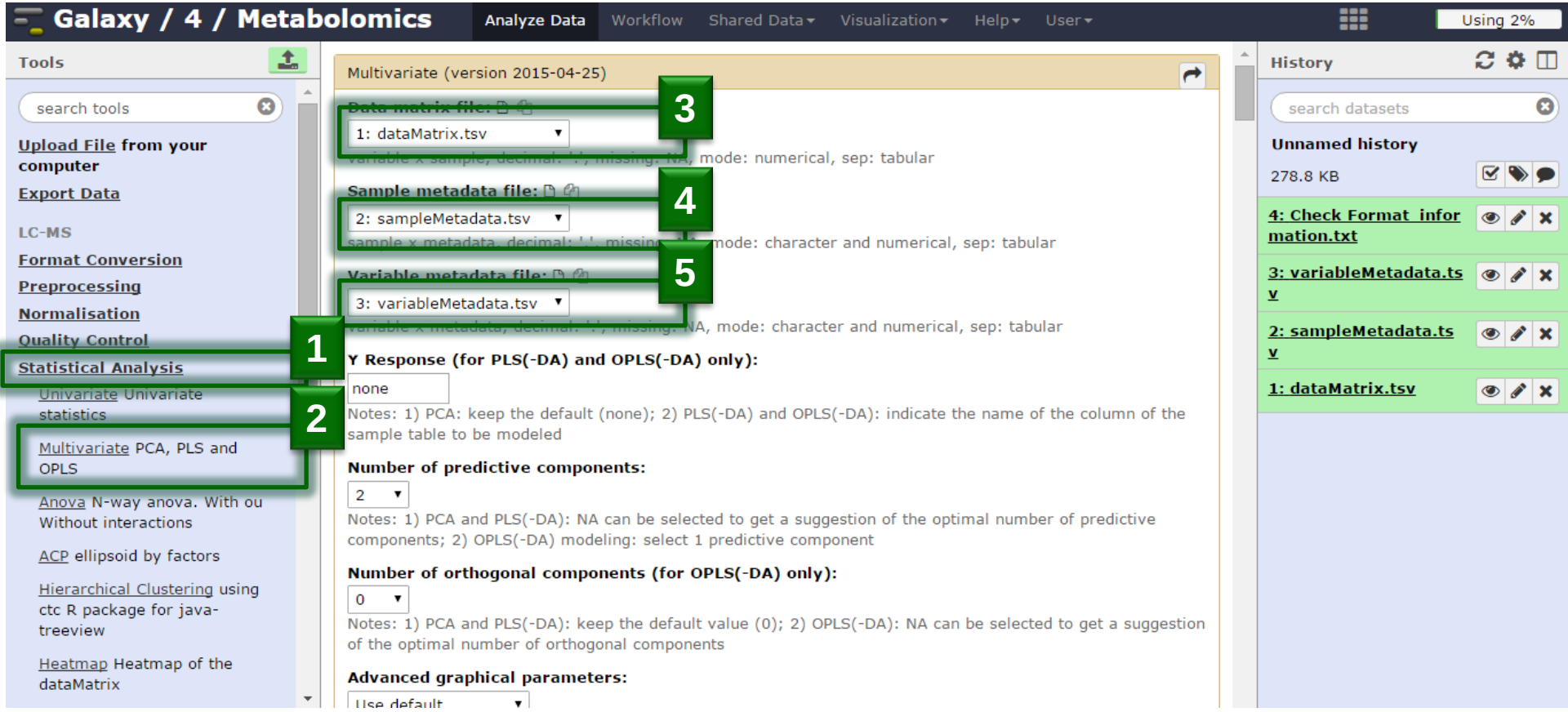
- PCA and (O)PLS(-DA) are **latent variable** methods: new components are computed as linear combinations of the original variables
- The assumption is that a few components can efficiently represent the whole dataset (PCA) or model the factor of interest (O)PLS(-DA)
- **Other powerful multivariate methods** exist for regression and classification (Support Vector Machine, Random Forest, etc.)
  - soon available on W4M

PCA and (O)PLS(-DA) steps in the analysis



Open the "Multivariate" module

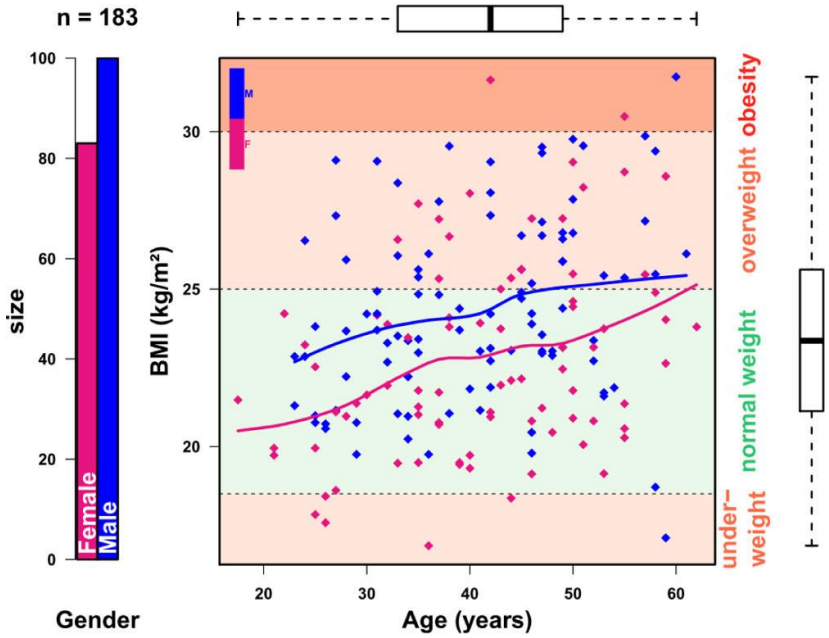
- and select your 3 files of interest:



- you are now ready to start your multivariate analyzes!

Sacurine dataset

- Objective: influence of age, body mass index and gender on metabolite concentrations in urine
- Cohort: 183 employees from the CEA institute
- Analytics: LTQ-Orbitrap (negative ionization mode)
- Annotation: 109 metabolites were identified or annotated at the MSI level 1 or 2.
- Pre-processing:
  - XCMS followed by Quan Browser
  - Signal drift and batch effect correction
  - Normalization to the osmolality
  - log10 transformation



Thévenot E.A., Roux A., Xu Y., Ezan E. and Junot C. (2015). Analysis of the human adult urinary metabolome variations with age, body mass index and gender by implementing a comprehensive workflow for univariate and OPLS statistical analyses. *Journal of Proteome Research,* **14:**3322-3335. http://dx.doi.org/10.1021/acs.jproteome.5b00354

PRINCIPAL COMPONENT ANALYSIS (PCA)

Objectives

- Visualize the dataMatrix
  - by selecting a few components which capture most of the spread (variance) of the cloud of samples
- Detect outliers
  - which may bias the computation of the component
- Detect clusters of samples
  - which may suggest an internal structuration of the data

Unsupervised analysis

***p* = 30 (quantitative) variables**

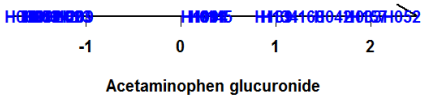
***n* = 20 samples**

	1,7-Dimethyluric acid	Dehydroepiandrosterone sulfate	Acetaminophen glucuronide	...
H011	2114	29025	44	
H023	43274	639	2	
H033	22386	325	1933	
H042	8185	13938	933	
H052	22385	357	5004	
H062	6380	292	1	
H073	10012	22781	1	
H083	30414	105	1	
H092	6637	35156	1	
H103	12100	2	1	
H114	33362	149041	46	
H124	11197	84536	1	
H134	18698	34053	254	
H145	14435	212398	52	
H157	31732	19317	2200	
H168	10221	78	475	
H180	22936	463	1	
H189	14423	1039	220	
H199	2888	12272	37	
H209	12563	100236	2	

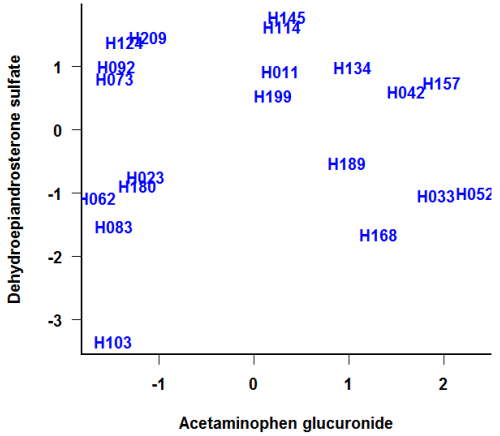
X

How to visualize multivariate observations?

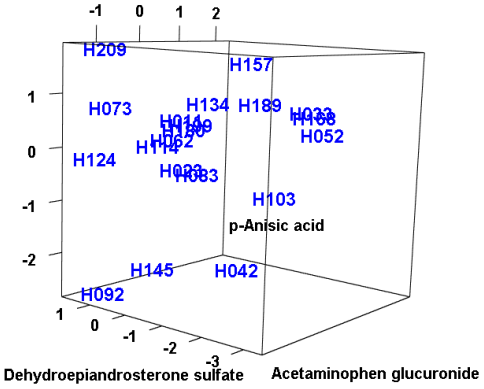
1 variable



2 variables



3 variables



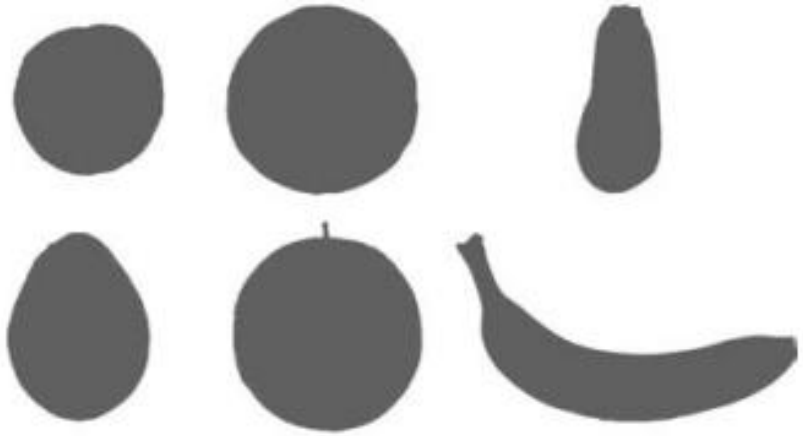
***p* variables**

?

=> Dimension reduction

Projection

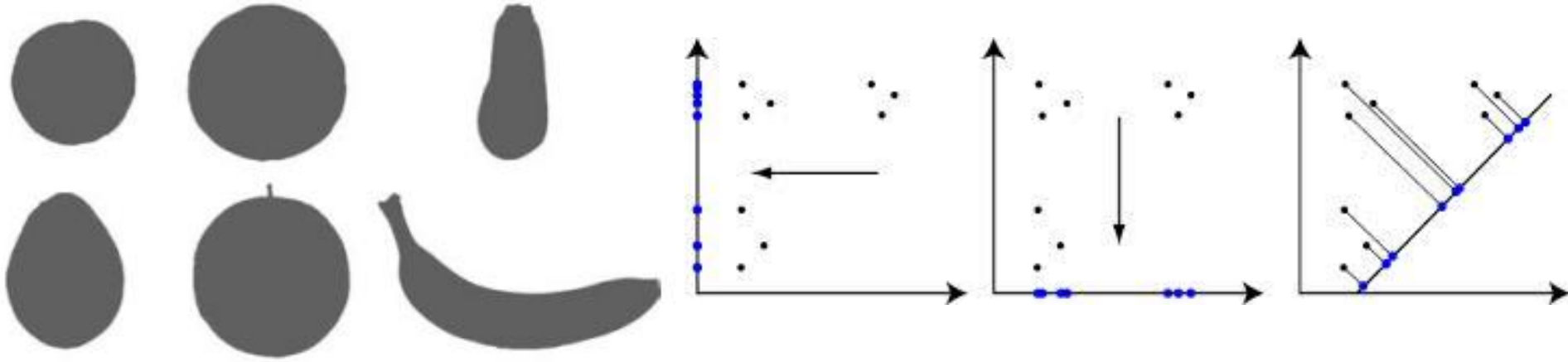
- Projected distances as high as possible



Husson and Pages (2011). Exploratory multivariate analysis by example using R. Chapman & Hall/CRC

Projection on latent variables

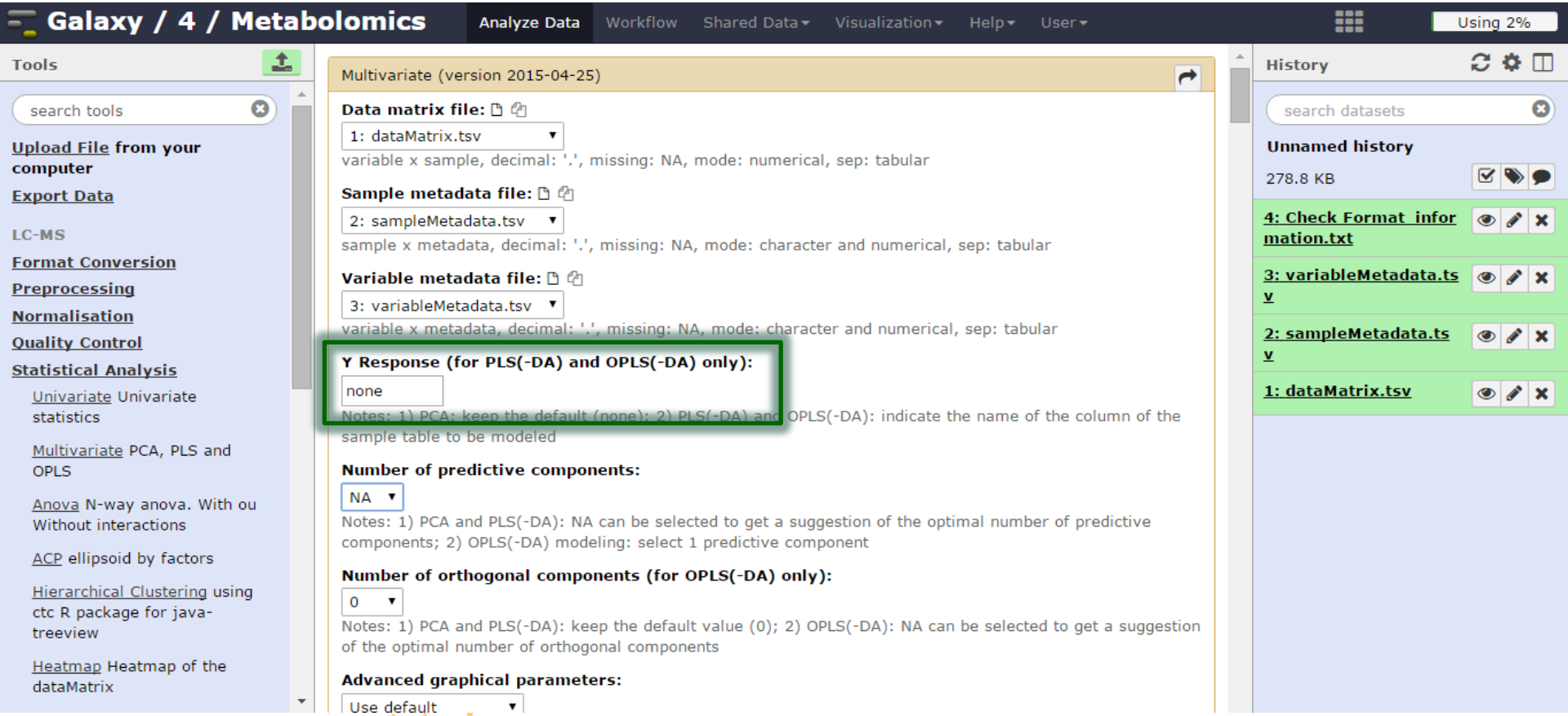
- Projected distances as high as possible
- Define new variables as linear combination of original ones



Husson and Pages (2011). Exploratory multivariate analysis by example using R. Chapman & Hall/CRC

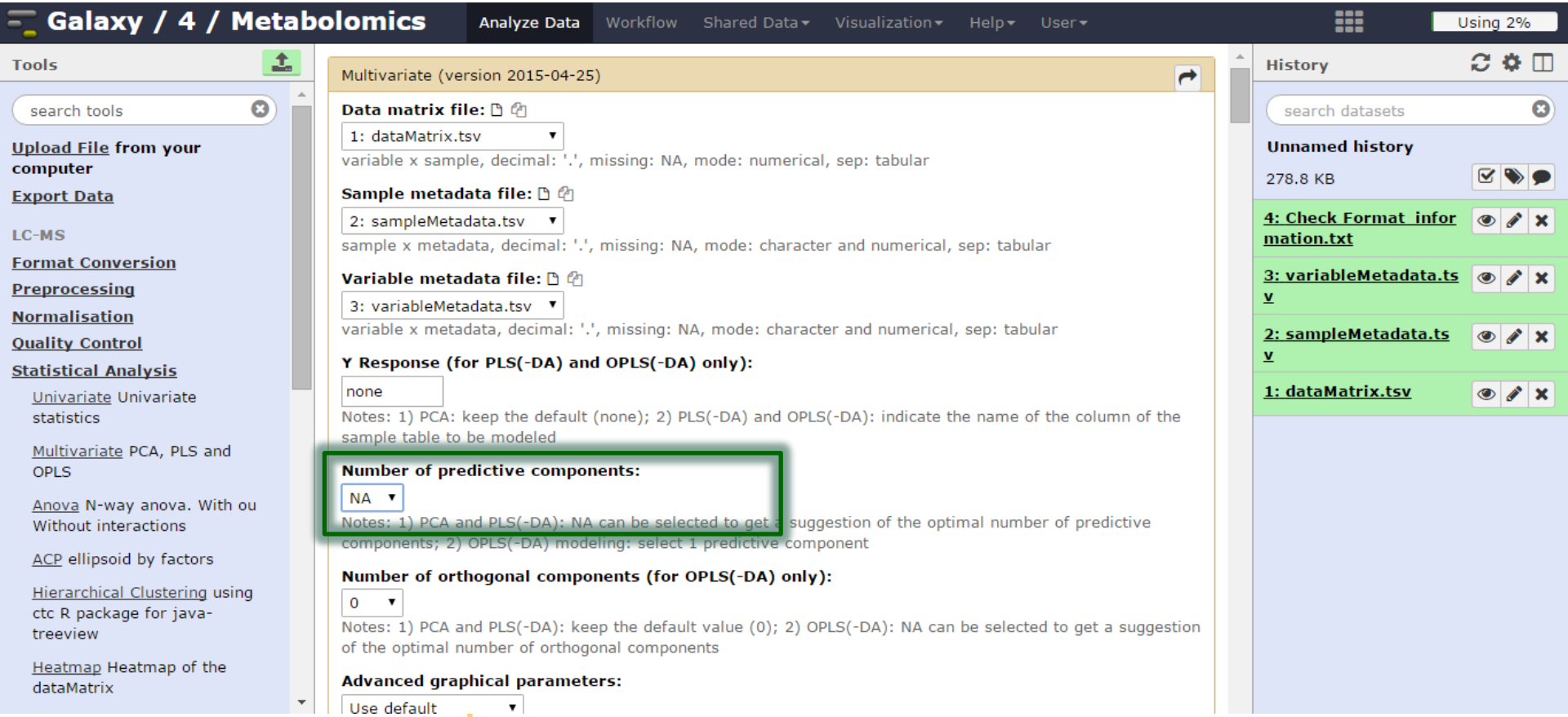
Selection of PCA as the type of analysis

- Keep the "Y response" to 'none' for PCA (unsupervised analysis)



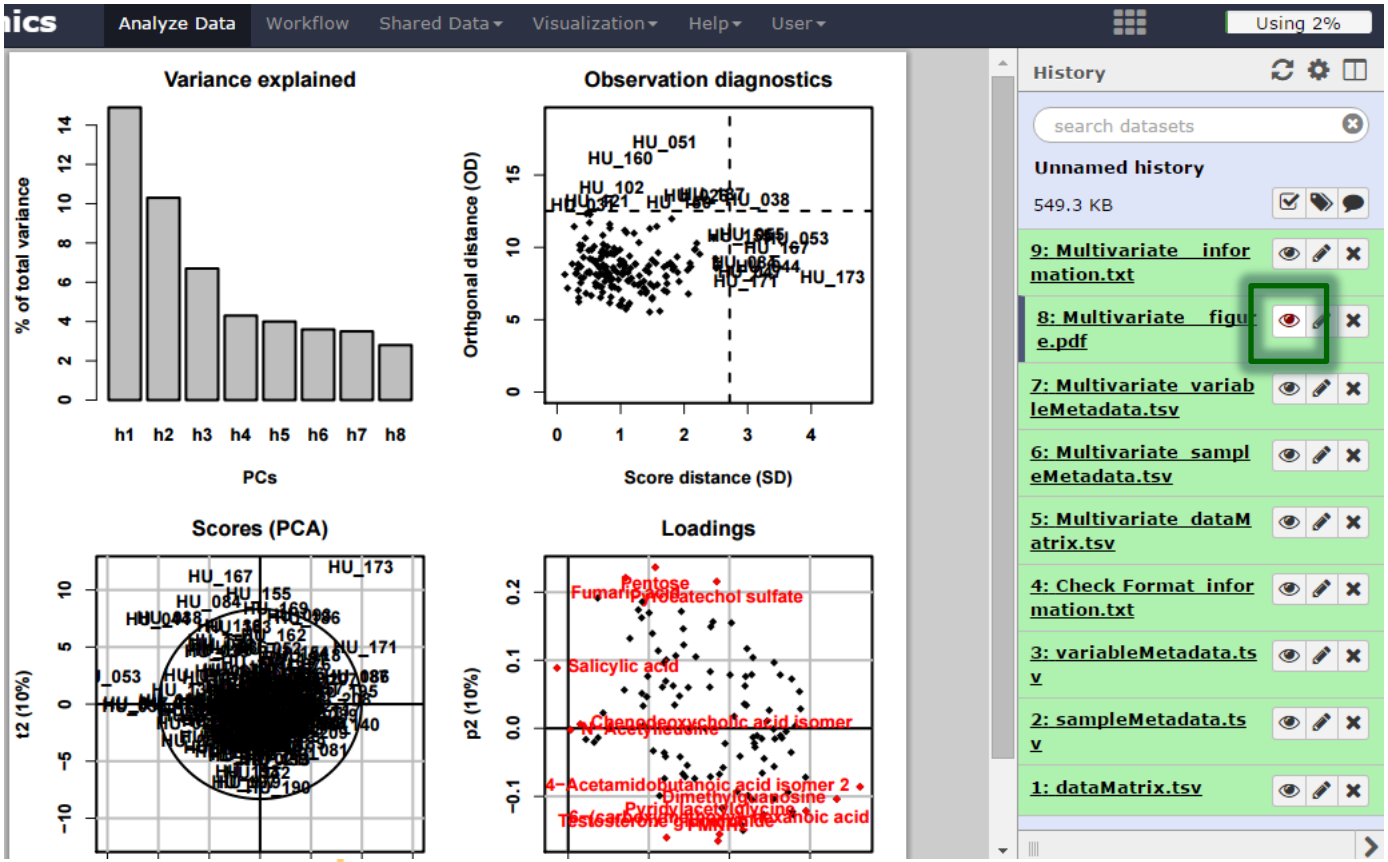
Automatic selection of the number of components

- Until the variance is less than the mean variance of all components



Graphical results

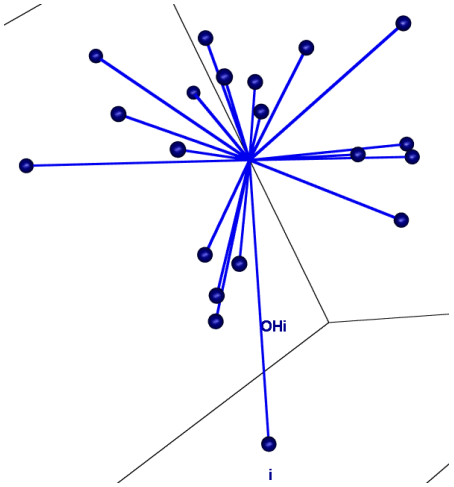
- scree plot, outliers, and the loading and score plots



Diagnostics R2X: How much of the original inertia is still reflected by the model?

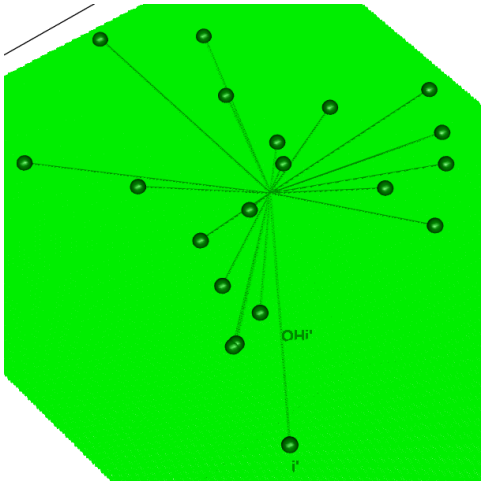
Total

$$TSS = \sum_{i=1}^{n} OH_i{}^2$$



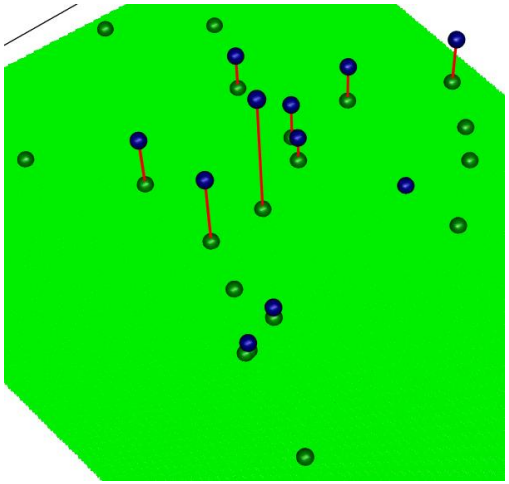
Explained

$$ESS = \sum_{i=1}^{n} OH'_i{}^2$$



Residual

$$RSS = \sum_{i=1}^{n} HH'_i{}^2 = TSS - ESS$$



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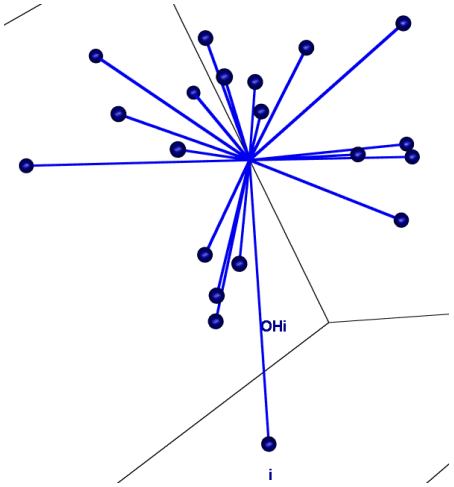

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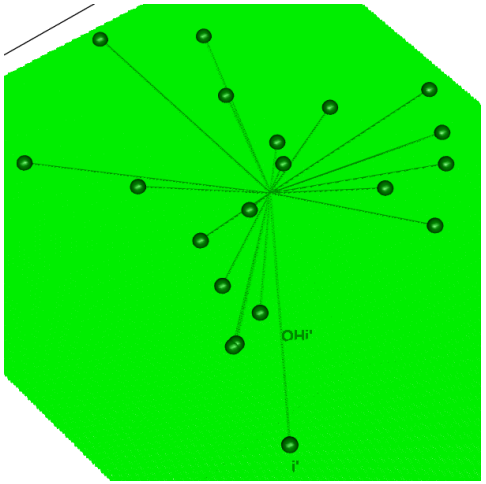
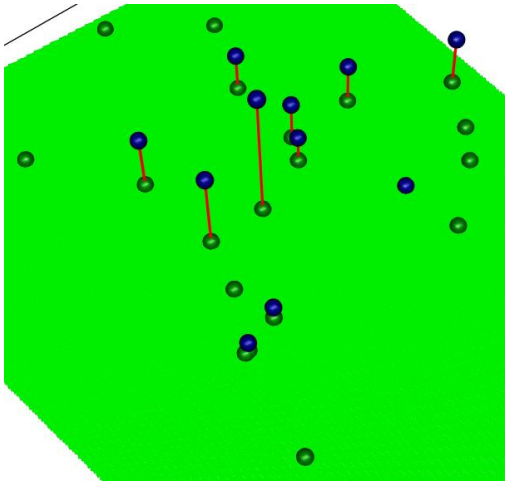


Residual

$$RSS = \sum_{i=1}^{n} HH'_i{}^2 = TSS - ESS$$

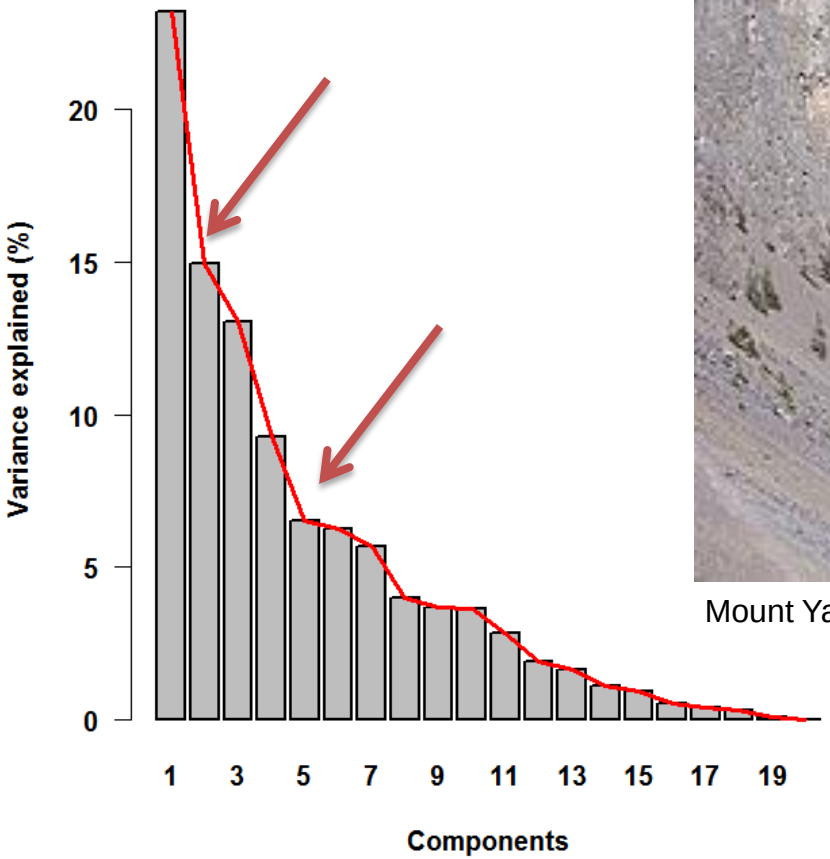


$$R2X = \frac{ESS}{TSS} = 1 - \frac{RSS}{TSS} \qquad 0 \leq R2X \leq 1$$

- R2X increases with the number of components in the model
- For a given number of components, the higher the R2X, the more inertia is captured by the model (projection)

Scree plot

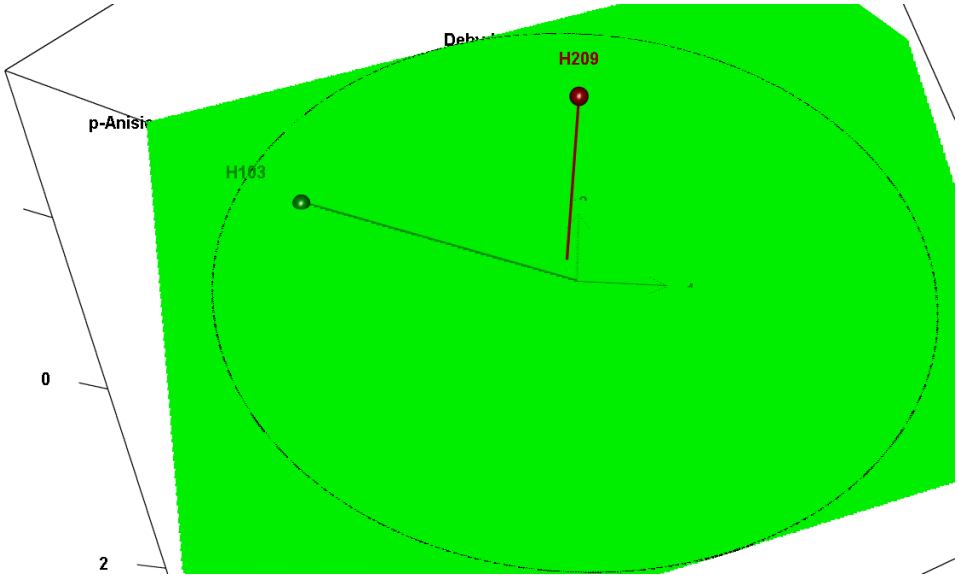
- Check that the first components capture most of the variance

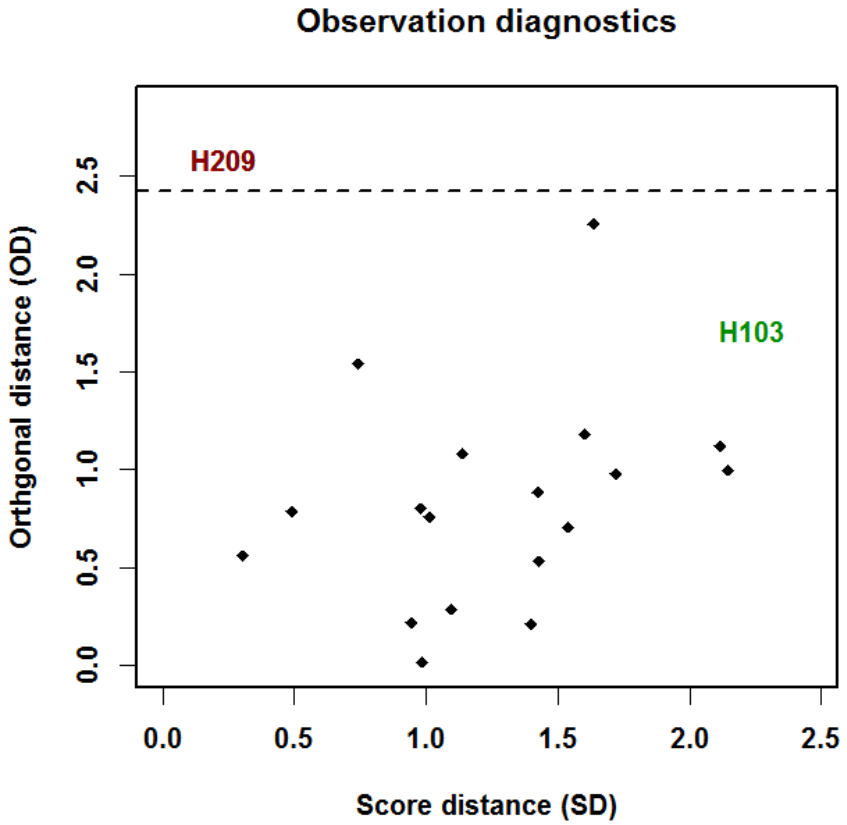


Mount Yamnuska, Alberta. Wikipedia

Observation diagnostics

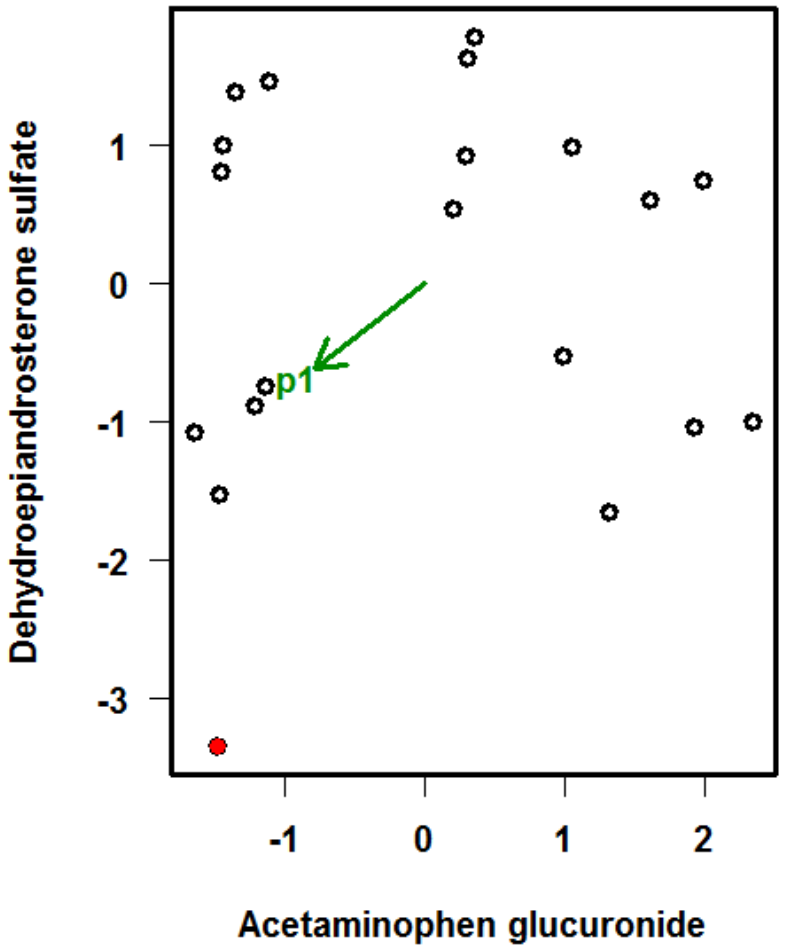
- Samples which may bias the PCA computation and/or may not be faithfully visualized by the score plot

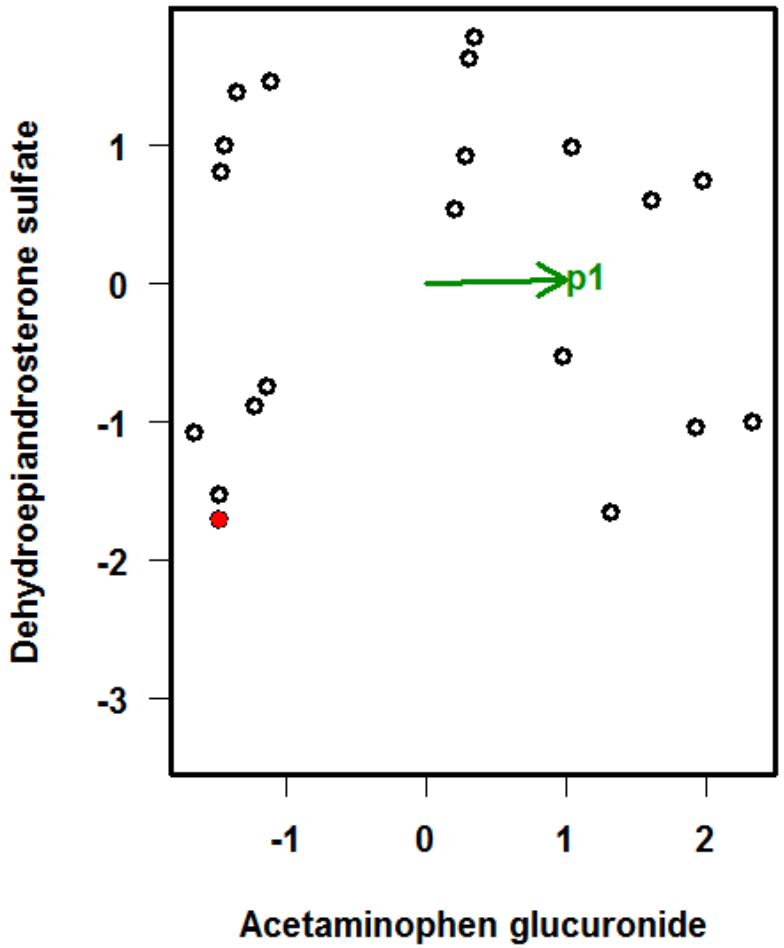




Hubert M., Rousseeuw P. and Vanden Branden K. (2005). ROBPCA: a new approach to robust principal component analysis. *Technometrics,* **47:**64-79. DOI: 10.1198/004017004000000563

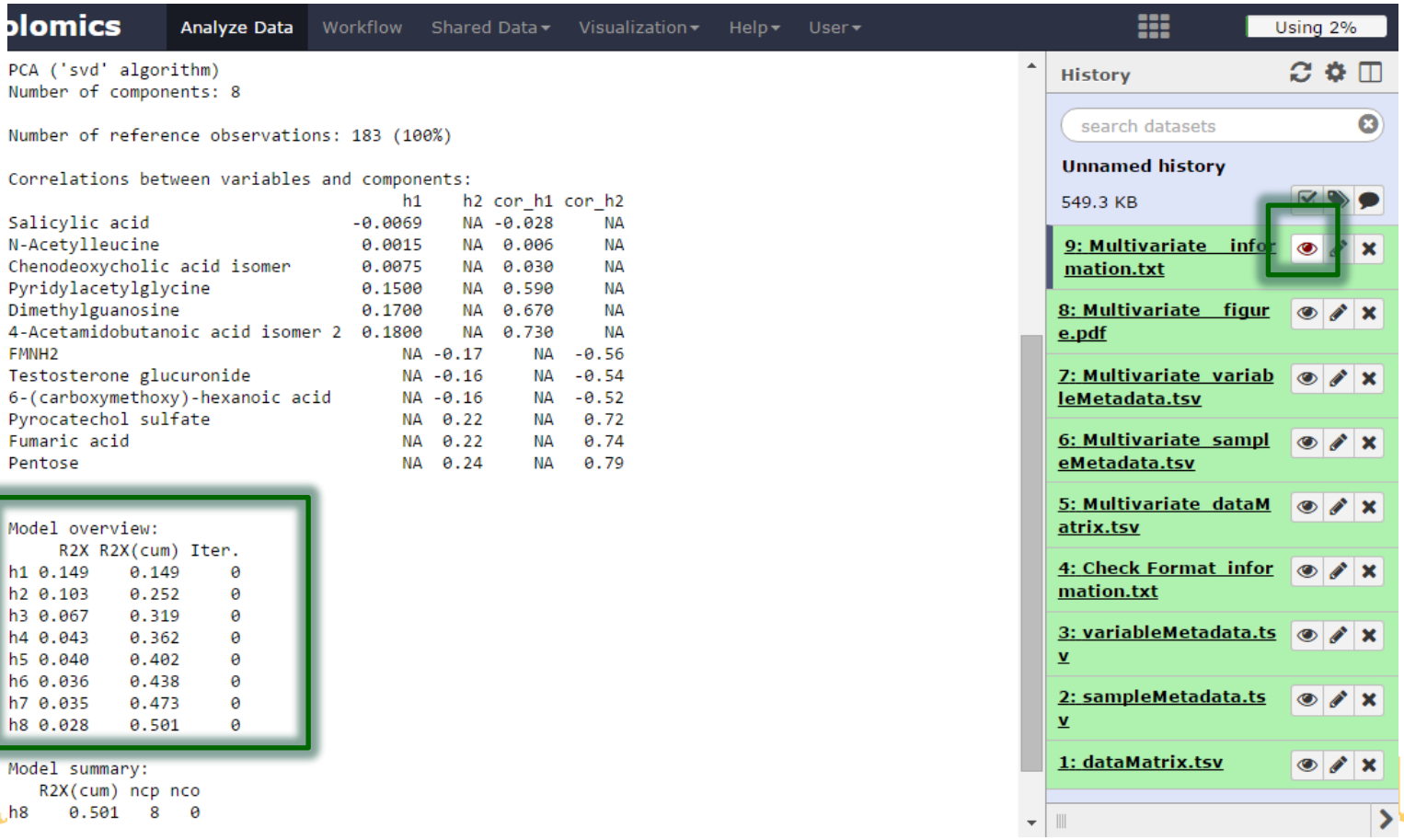
Sensitivity to outliers





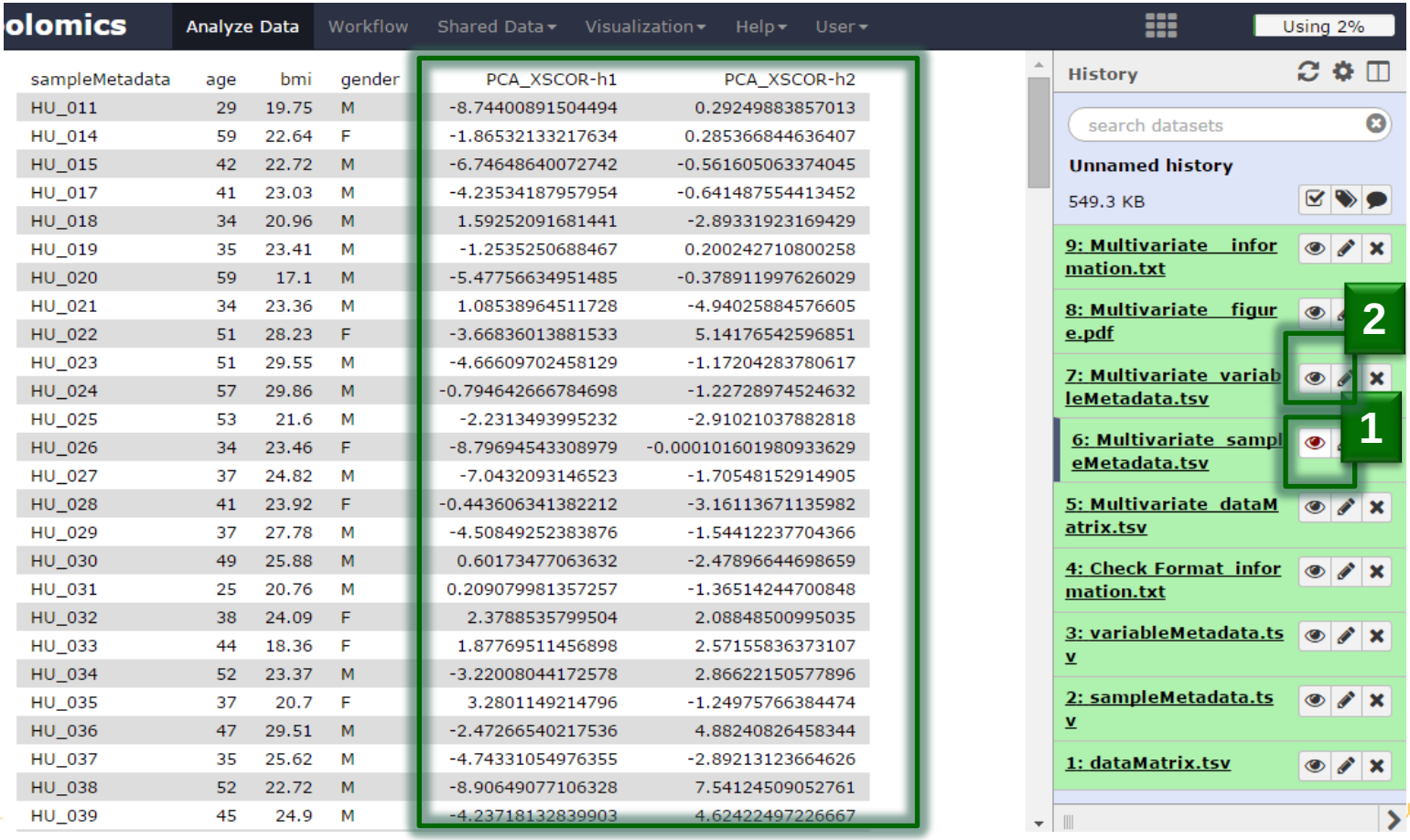
Numerical results

- Numerical results (including the percentage of explained inertia) can be viewed in the "information.txt" file



Score and loading values

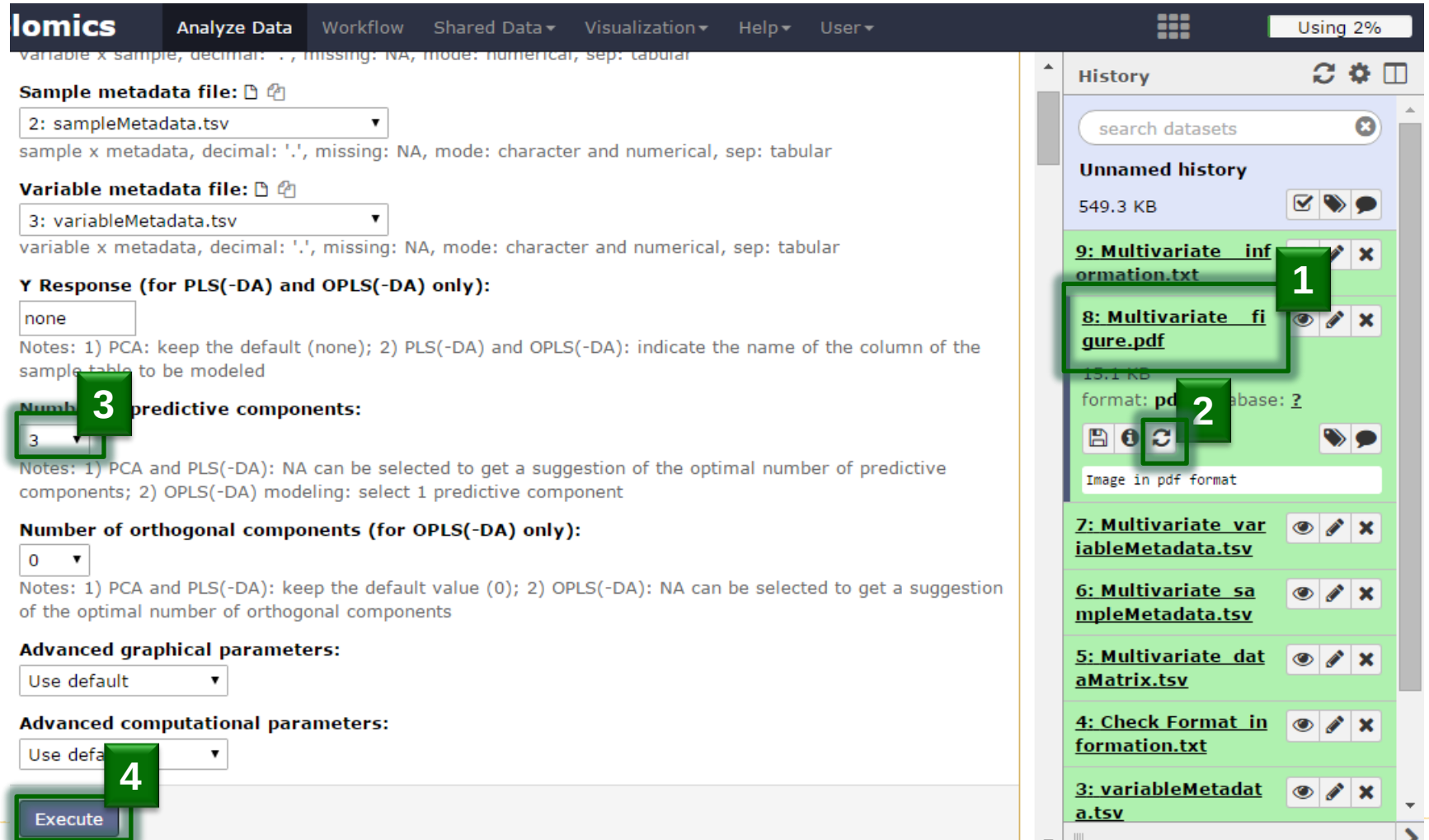
- The score (resp. loading) values of the selected components have been added as columns in the sampleMetadata (resp. variableMetadata) files



sampleMetadata	age	bmi	gender	PCA_XSCOR-h1	PCA_XSCOR-h2
HU_011	29	19.75	M	-8.74400891504494	0.29249883857013
HU_014	59	22.64	F	-1.86532133217634	0.285366844636407
HU_015	42	22.72	M	-6.74648640072742	-0.561605063374045
HU_017	41	23.03	M	-4.23534187957954	-0.641487554413452
HU_018	34	20.96	M	1.59252091681441	-2.89331923169429
HU_019	35	23.41	M	-1.2535250688467	0.200242710800258
HU_020	59	17.1	M	-5.47756634951485	-0.378911997626029
HU_021	34	23.36	M	1.08538964511728	-4.94025884576605
HU_022	51	28.23	F	-3.66836013881533	5.14176542596851
HU_023	51	29.55	M	-4.66609702458129	-1.17204283780617
HU_024	57	29.86	M	-0.794642666784698	-1.22728974524632
HU_025	53	21.6	M	-2.2313493995232	-2.91021037882818
HU_026	34	23.46	F	-8.79694543308979	-0.000101601980933629
HU_027	37	24.82	M	-7.0432093146523	-1.70548152914905
HU_028	41	23.92	F	-0.443606341382212	-3.16113671135982
HU_029	37	27.78	M	-4.50849252383876	-1.54412237704366
HU_030	49	25.88	M	0.60173477063632	-2.47896644698659
HU_031	25	20.76	M	0.209079981357257	-1.36514244700848
HU_032	38	24.09	F	2.3788535799504	2.08848500995035
HU_033	44	18.36	F	1.87769511456898	2.57155836373107
HU_034	52	23.37	M	-3.22008044172578	2.86622150577896
HU_035	37	20.7	F	3.2801149214796	-1.24975766384474
HU_036	47	29.51	M	-2.47266540217536	4.88240826458344
HU_037	35	25.62	M	-4.74331054976355	-2.89213123664626
HU_038	52	22.72	M	-8.90649077106328	7.54124509052761
HU_039	45	24.9	M	-4.23718132839903	4.62422497226667

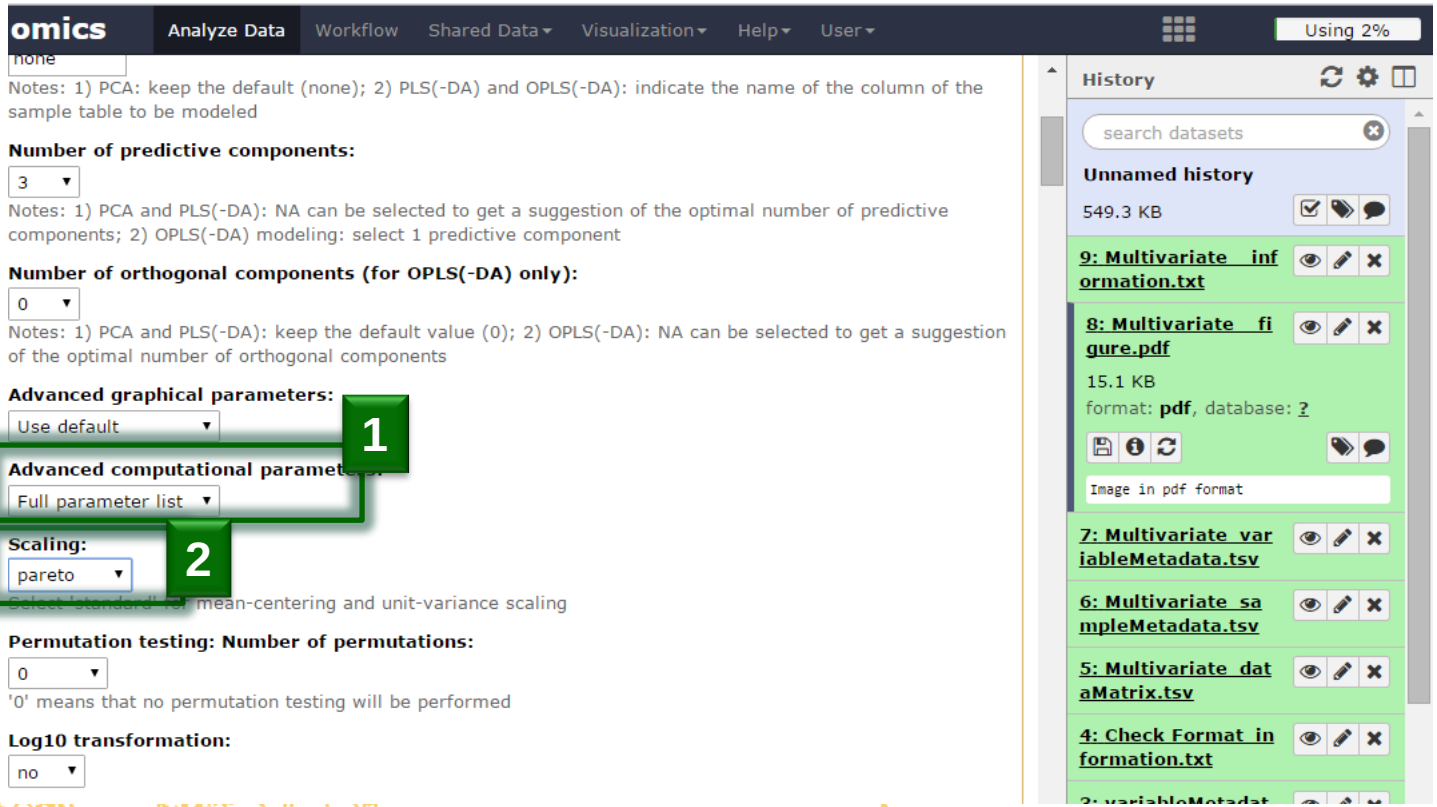
Tuning the parameters

- You can recall the page with your parameters, modify them, and restart the analysis



Advanced parameters: Scaling

- Variables are mean-centered for PCA
- By default, they are also unit-variance scaled
  - absence of variance scaling or changing to Pareto scaling can be selected in the advanced computational parameters



Advanced parameters: Ellipses

- Indicate the column name of sampleMetadata to be used

olomics | Analyze Data | Workflow | Shared Data | Visualization | Help | User

Variable metadata file:

3: variableMetadata.tsv

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

Y Response (for PLS(-DA) and OPLS(-DA) only):

none

Notes: 1) PCA: keep the default (none); 2) PLS(-DA) and OPLS(-DA): indicate the name of the column of the sample table to be modeled

Number of predictive components:

3

Notes: 1) PCA and PLS(-DA): NA can be selected to get a suggestion of the optimal number of predictive components; 2) OPLS(-DA) modeling: select 1 predictive component

Number of orthogonal components (for OPLS(-DA) only):

0

Notes: 1) PCA and PLS(-DA): keep th lt value (0); 2) OPLS(-DA): NA can be selected to get a suggestion of the optimal number of orthogonal ents

1

Advanced graphical parameters:

Full parameter list

Graphic:

x-score

2

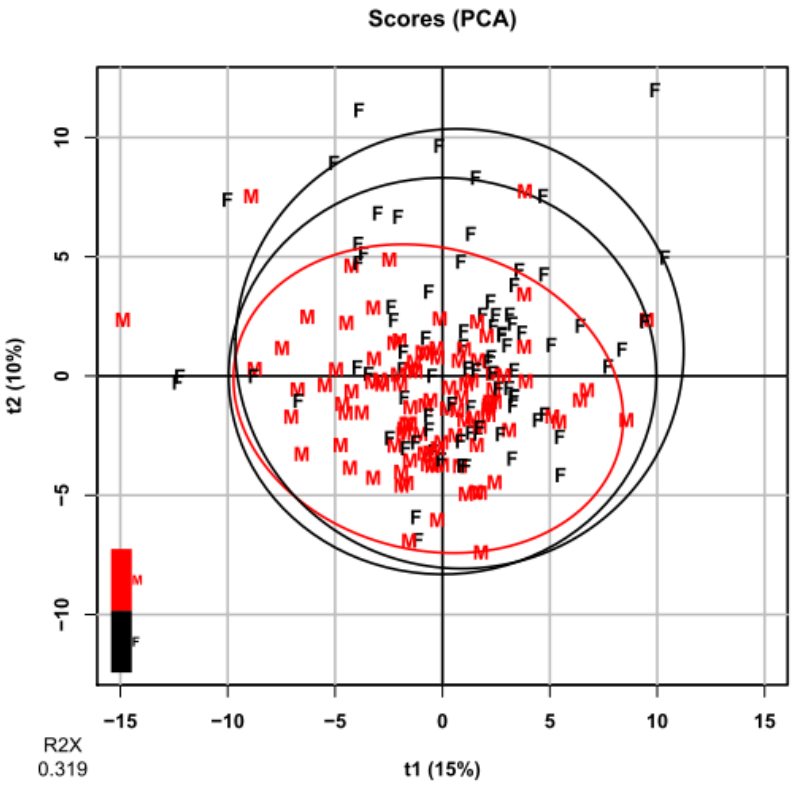
Mahalanobis ellipses:

gender

data column with the classes to be used for drawing ellipses (for (O)PLS-DA: indicate the same name as the 'Response' argument above); If you do not want ellipses, keep the default, none

Sample colors:

none

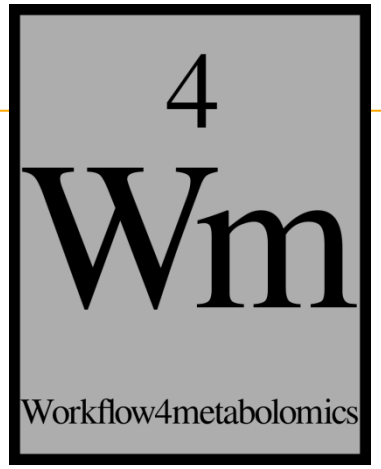


References

- Husson F., Le S. and Pages J. (2011). Exploratory multivariate analysis by example using R. *Chapman & Hall/CRC*

- Ringner M. (2008). What is principal component analysis? *Nature Biotechnology*, **26**:303-304. http://dx.doi.org/10.1038/nbt0308-303

- Baccini A. (2010). Statistique descriptive multidimensionnelle (pour les nuls). www.math.univ-toulouse.fr/~baccini/zpedago/asdm.pdf



PARTIAL LEAST SQUARES REGRESSION (PLS) AND DISCRIMINANT ANALYSIS (PLS-DA)

PLS(-DA) modelling

- Powerful regression method when

$$n_{samples} < p_{variables}$$

- **Complementary to univariate hypothesis testing** (where variables are tested independantly)

- **Risk of overfitting**: i.e., building a model whose (apparently) good performances result from chance only

Supervised analysis (i.e. with labels)

1 response

p = 30 (quantitative) variables

n = 20 samples

	bmi
H011	19.8
H023	29.6
H033	18.4
H042	19.8
H052	20.1
H062	22.2
H073	25.4
H083	29.8
H092	21.8
H103	26.8
H114	29.4
H124	22.2
H134	22.9
H145	29.1
H157	22.0
H168	20.8
H180	23.7
H189	19.4
H199	21.0
H209	21.5

	1,7-Dimethyluric acid	Dehydroepiandrosterone sulfate
H011	3.33	4.46
H023	4.64	2.81
H033	4.35	2.51
H042	3.91	4.14
H052	4.35	2.55
H062	3.80	2.47
H073	4.00	4.36
H083	4.48	2.02
H092	3.82	4.55
H103	4.08	0.21
H114	4.52	5.17
H124	4.05	4.93
H134	4.27	4.53
H145	4.16	5.33
H157	4.50	4.29
H168	4.01	1.89
H180	4.36	2.67
H189	4.16	3.02
H199	3.46	4.09
H209	4.10	5.00

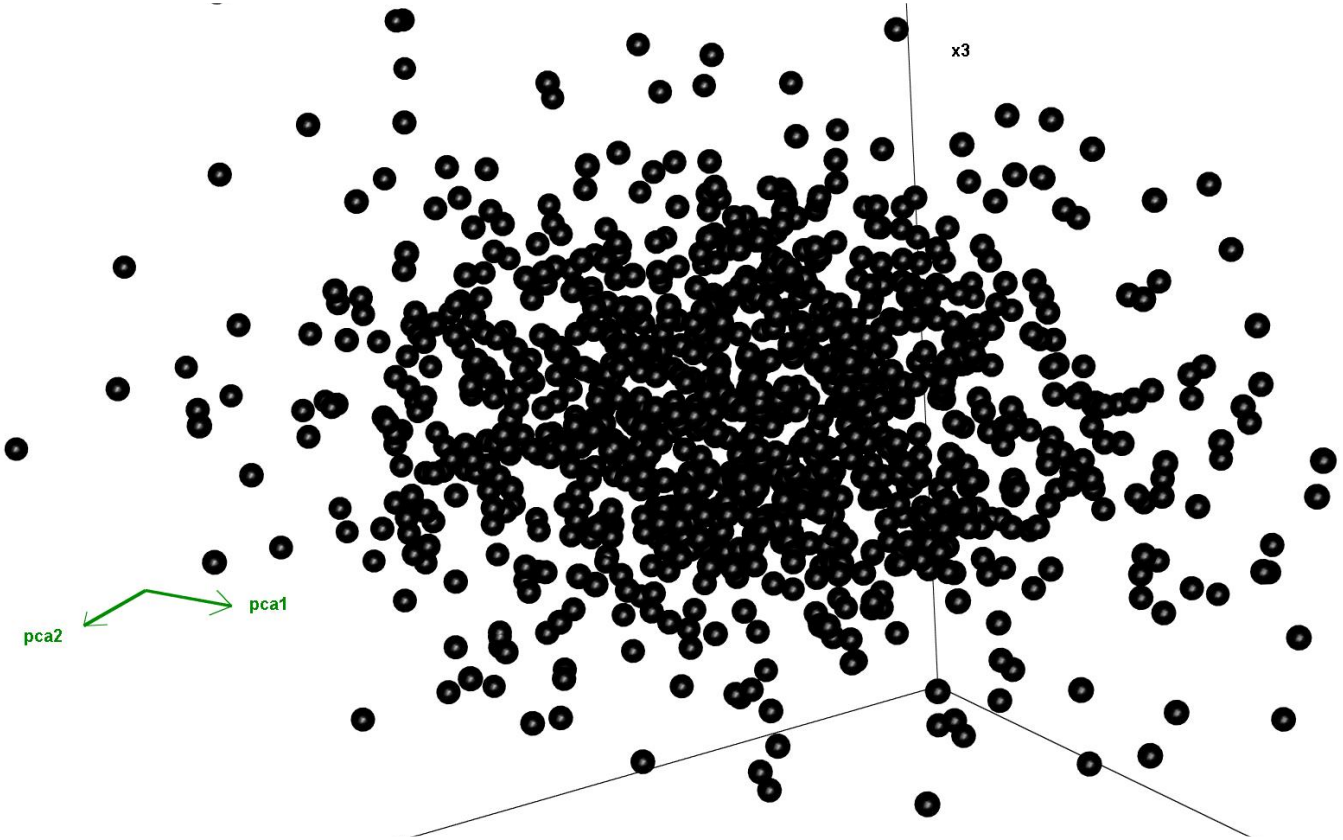
...

y

X

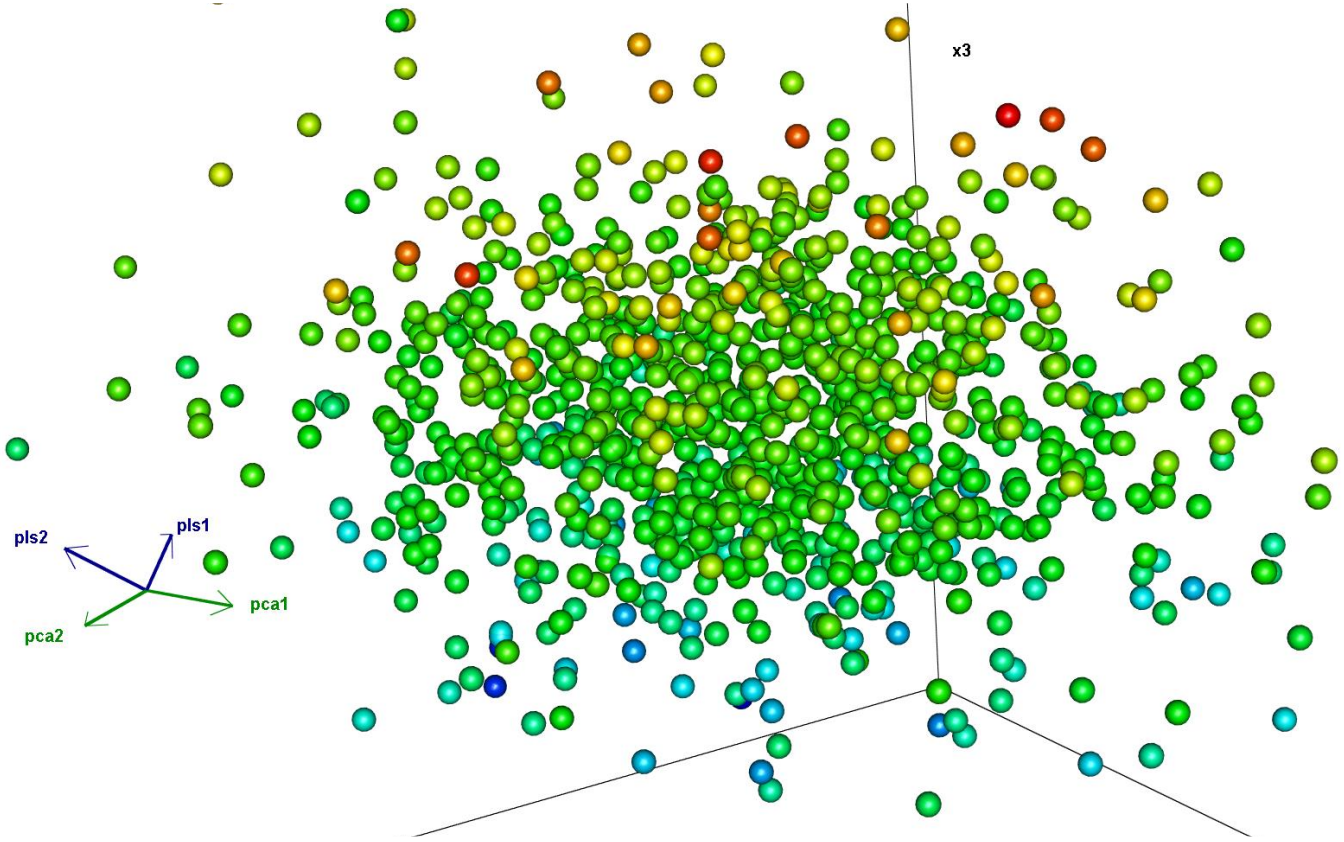
PLS vs PCA

- PCA finds the directions of maximum variance



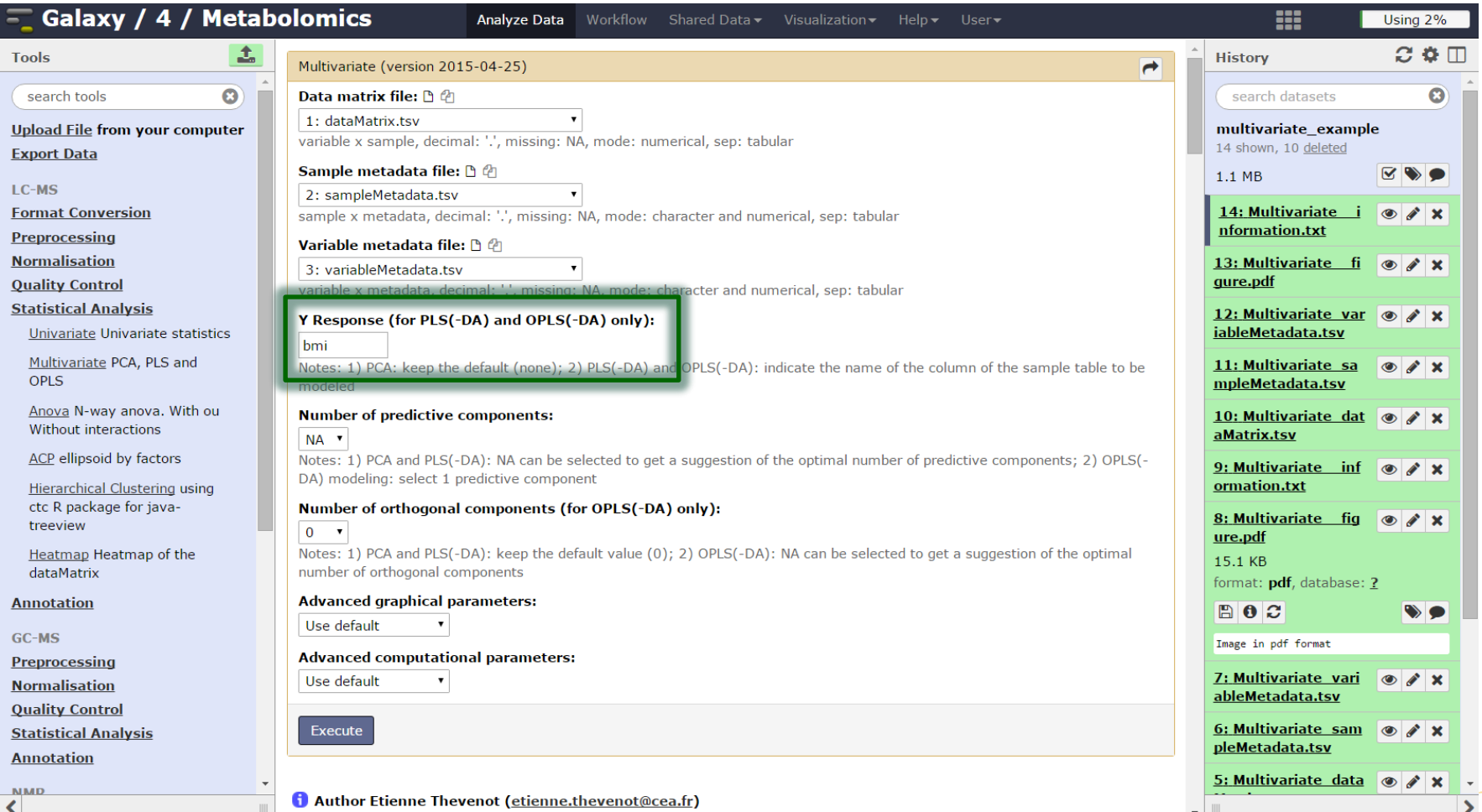
PLS vs PCA

- PLS includes the labels into the model



Selection of PLS(-DA) as the type of analysis

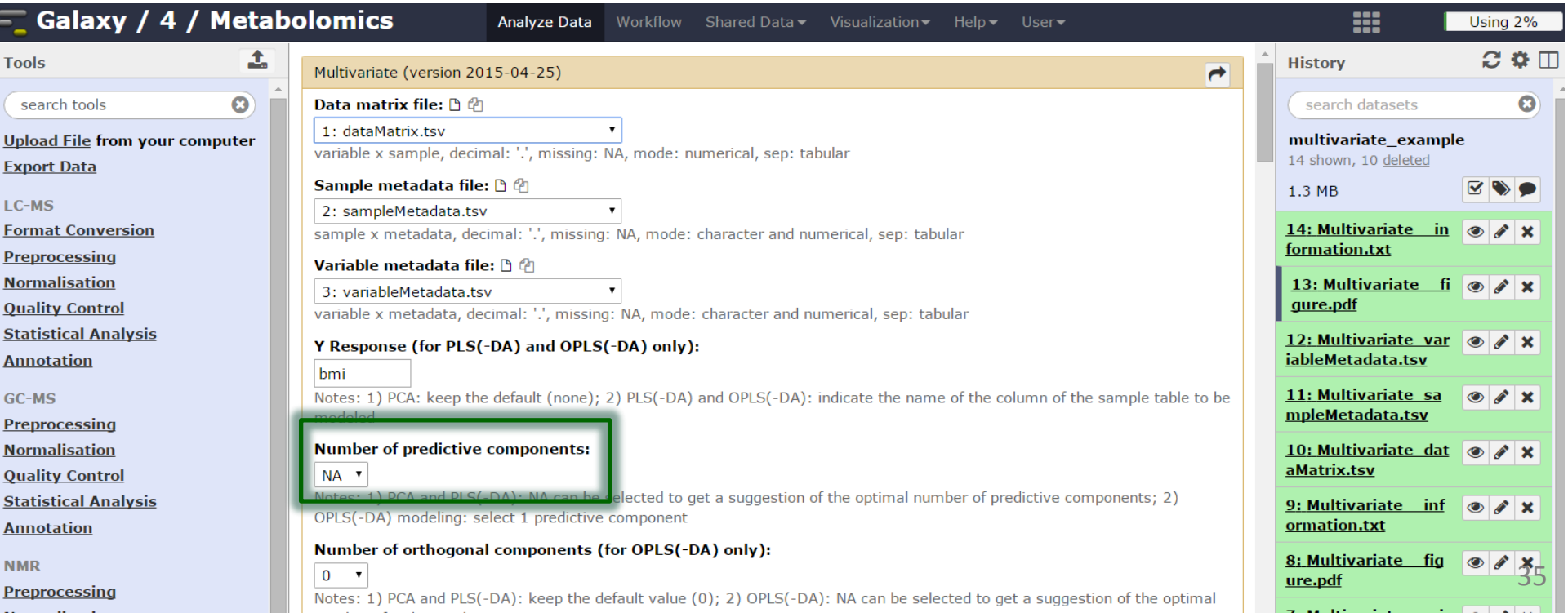
- Select the "Y response" to be modelled (column of sampleMetadata):
  - column of numbers (age, bmi): **PLS** regression
  - column of characters ('M'/'F', 'patient'/'control'): **PLS-DA** classification



Automatic selection of the number of components

- A new component *h* is added to the model if:
  - $R2Y_h \geq 1\%$
  - $Q2Y_h \geq 0 \left(\text{or } 5\% \text{ if } n_{samples} \leq 100\right)$

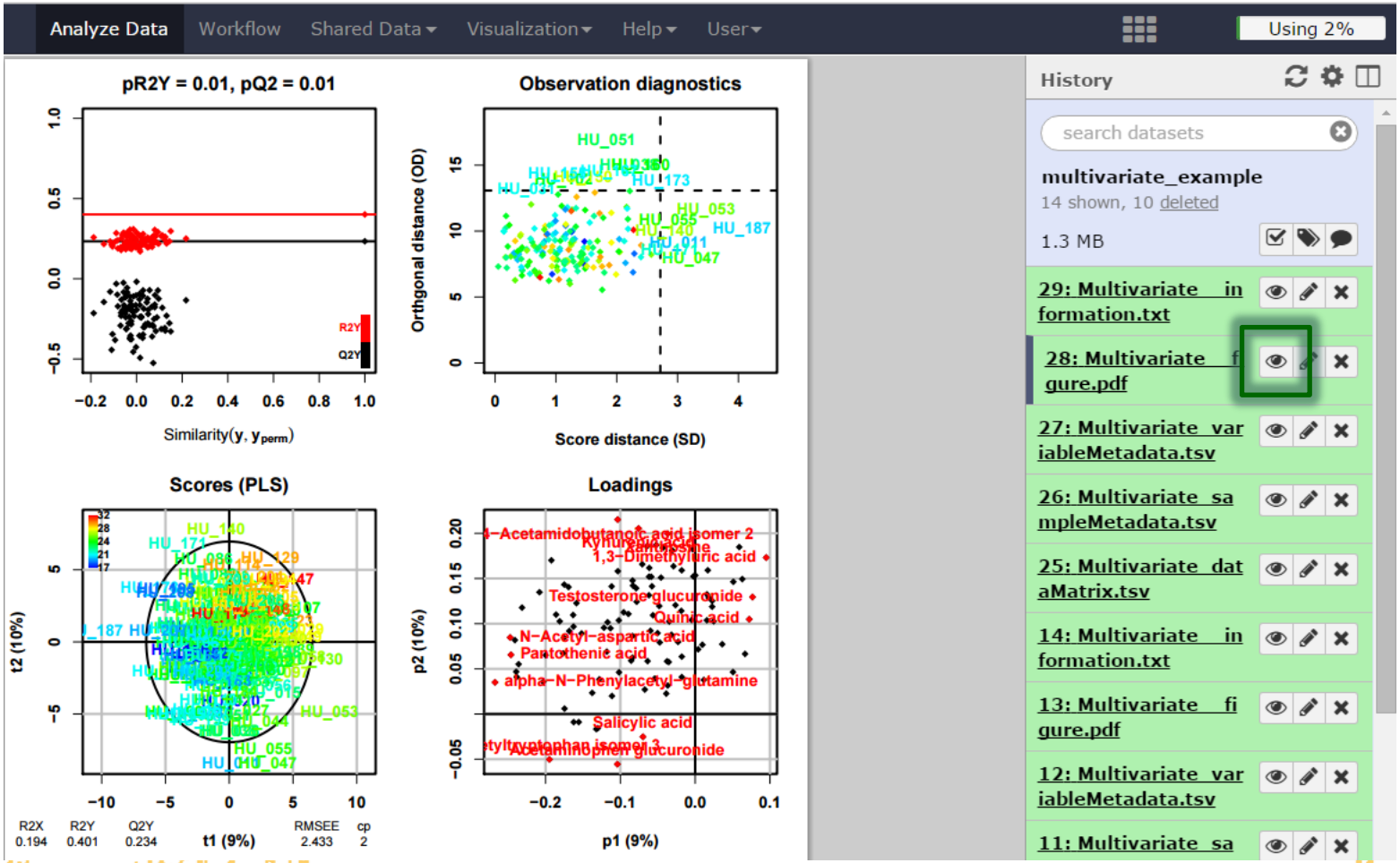
Note: $Q2Y_h = 1 - \frac{PRESS_h}{RSS_{h-1}}$ where $PRESS_h$ is estimated by cross-validation



Graphical results

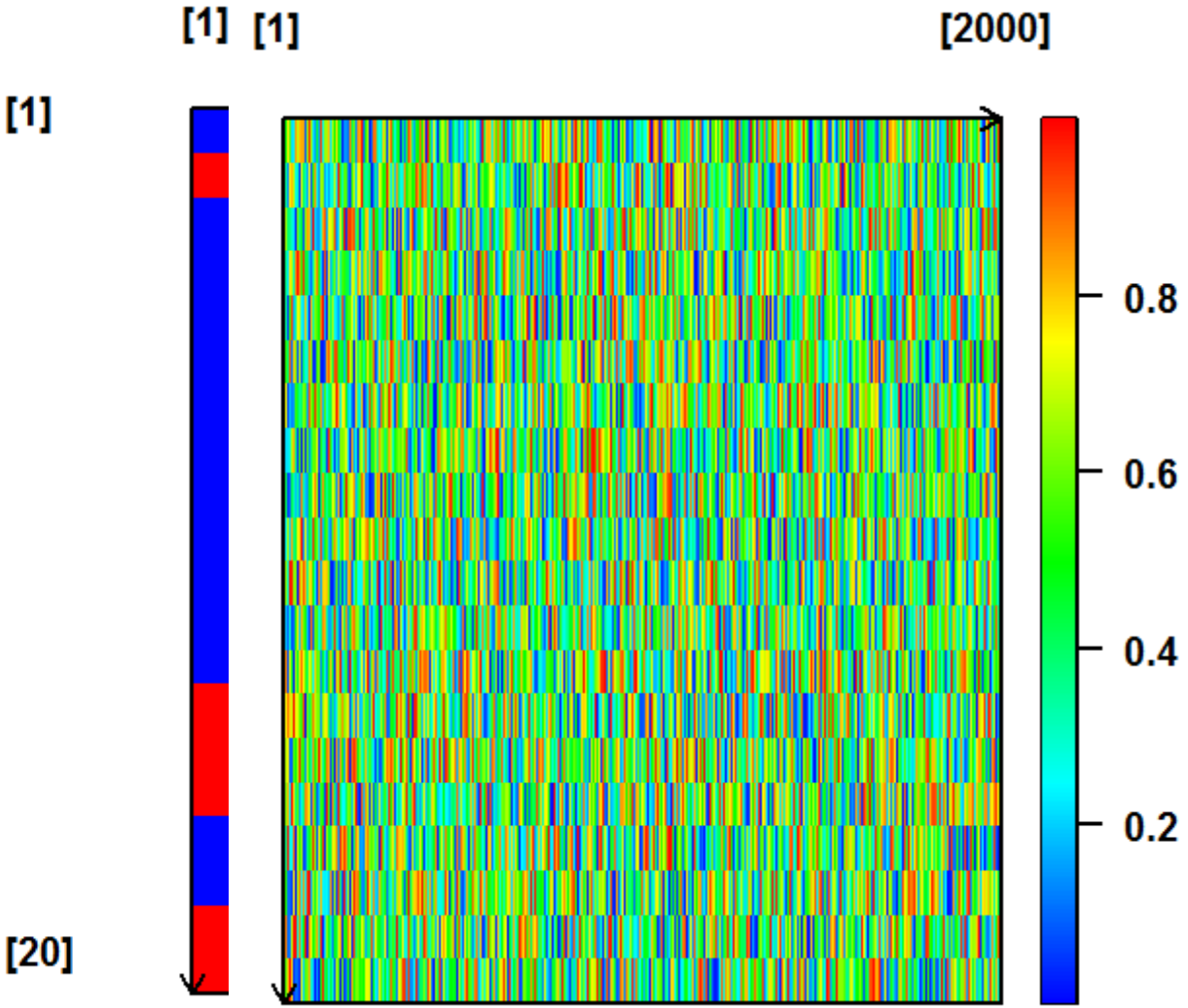
- permutation, overview, outlier, and score plots displayed as the default ('summary')

'summary'



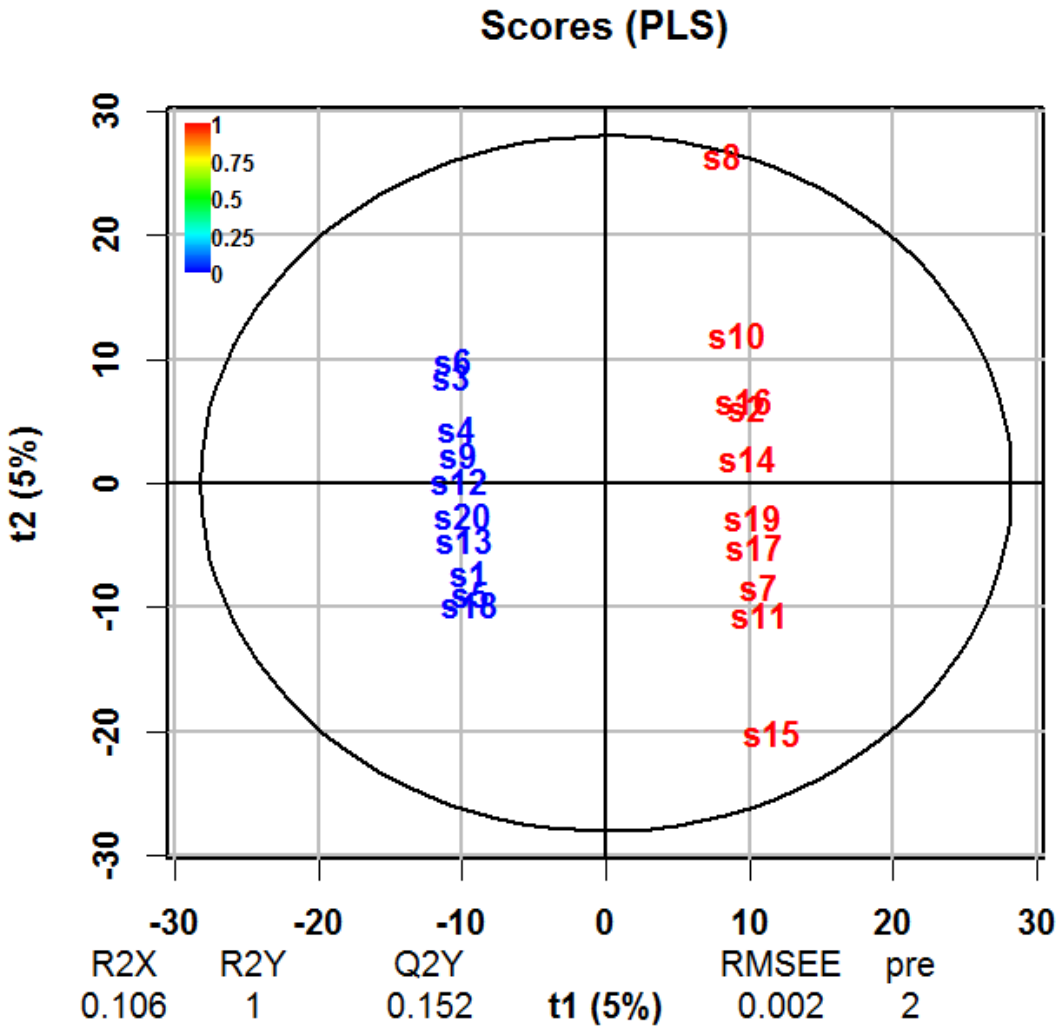
Overfitting

- X: 20 × 2,000 matrix of **random** numbers
  - Uniform distribution between 0 and 1
- Y: 20 x 1 matrix of **random** labels
  - 0 or 1 values



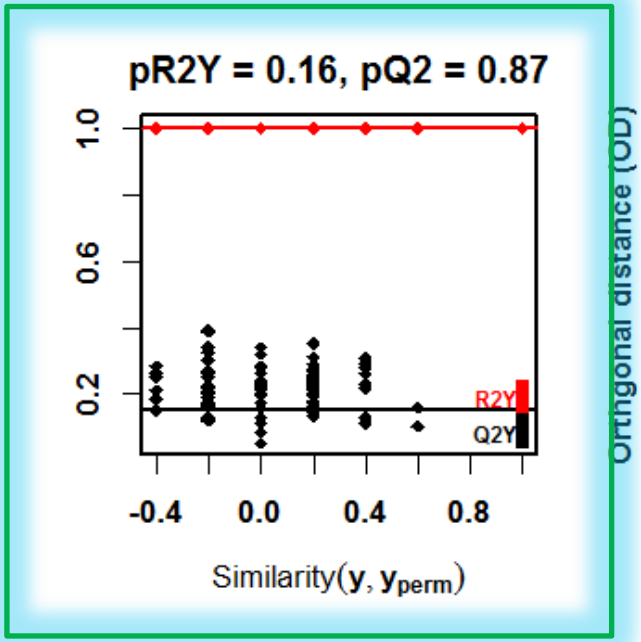
adpated from Wehrens (2011). Chemometrics with R. Springer.

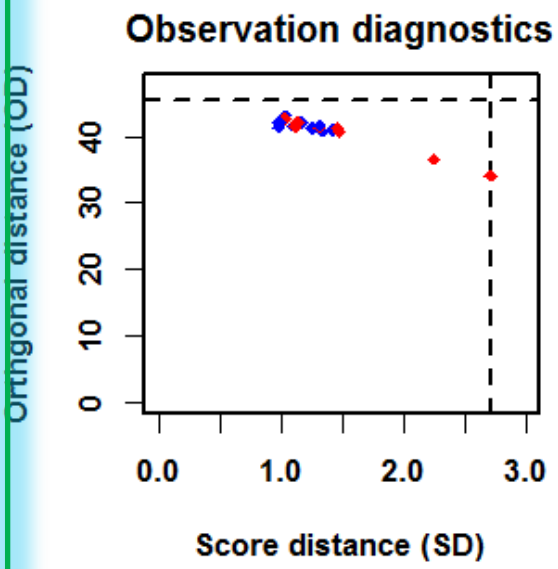
Score plot!

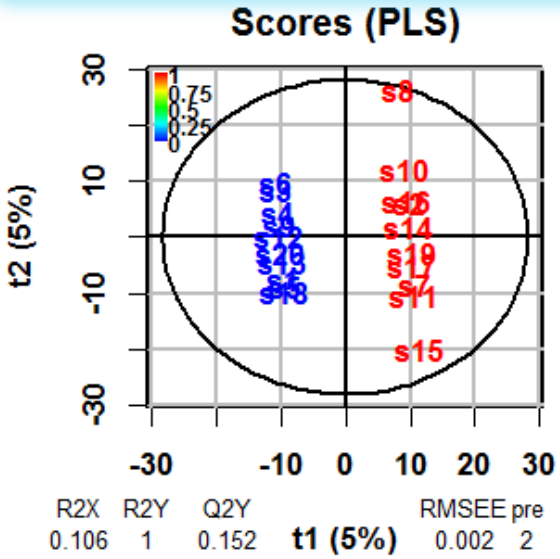

Scores (PLS)
1
0.75
0.5
0.25
0
s8
s10
s6
s3
s16
s2
s4
s9
s14
s12
s20
s19
s13
s17
s1
s7
s18
s11
s15
t2 (5%)
30
20
10
0
-10
-20
-30
-30
-20
-10
0
10
20
30
R2X
0.106
R2Y
1
Q2Y
0.152
t1 (5%)
RMSEE
0.002
pre
2

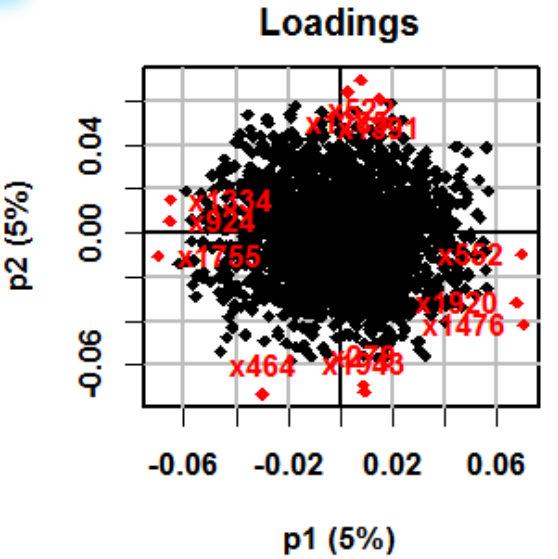
Importance of diagnostics

- **Permutation testing:** comparing the R2Y and Q2Y values of the model built with the true Y labels with n_{perm} **models built with random permutation of Y labels**







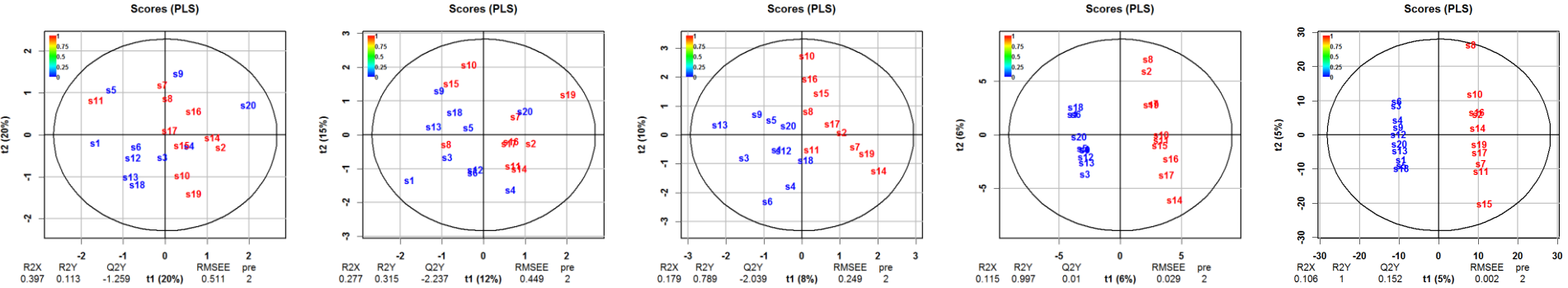


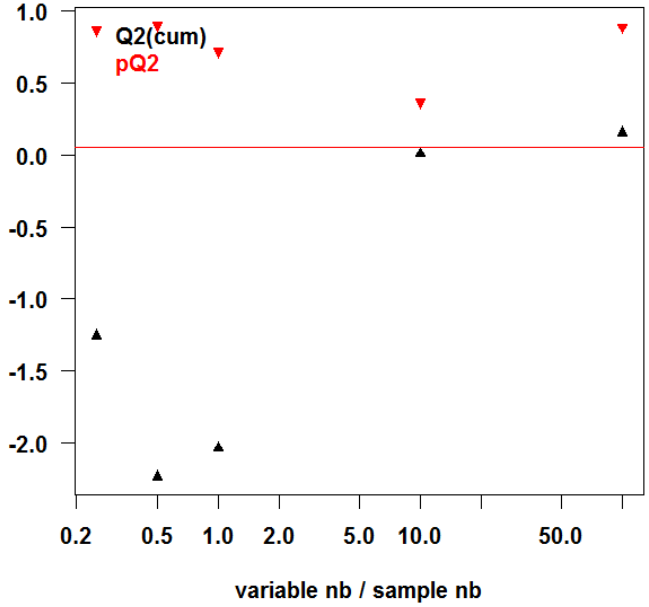
Szymanska E., Saccenti E., Smilde A. and Westerhuis J. (2012). Double-check: validation of diagnostic statistics for PLS-DA models in metabolomics studies. *Metabolomics*, **8:**3-16. DOI: 10.1007/s11306-011-0330-3

Risk of overfitting when *n* < *p*

$$\frac{\text{variables}}{\text{samples}} =$$

0.2 | 0.5 | 1 | 10 | 100





Significance of the model

- The algorithm randomly permutates the **y** labels, builds the models and computes the $R2X$, $R2Y$, $Q2Y$

1 response

p = 30 (quantitative) variables

***n* = 20 samples**

	bmi
H011	19.8
H023	29.6
H033	18.4
H042	19.8
H052	20.1
H062	22.2
H073	25.4
H083	29.8
H092	21.8
H103	26.8
H114	29.4
H124	22.2
H134	22.9
H145	29.1
H157	22.0
H168	20.8
H180	23.7
H189	19.4
H199	21.0
H209	21.5

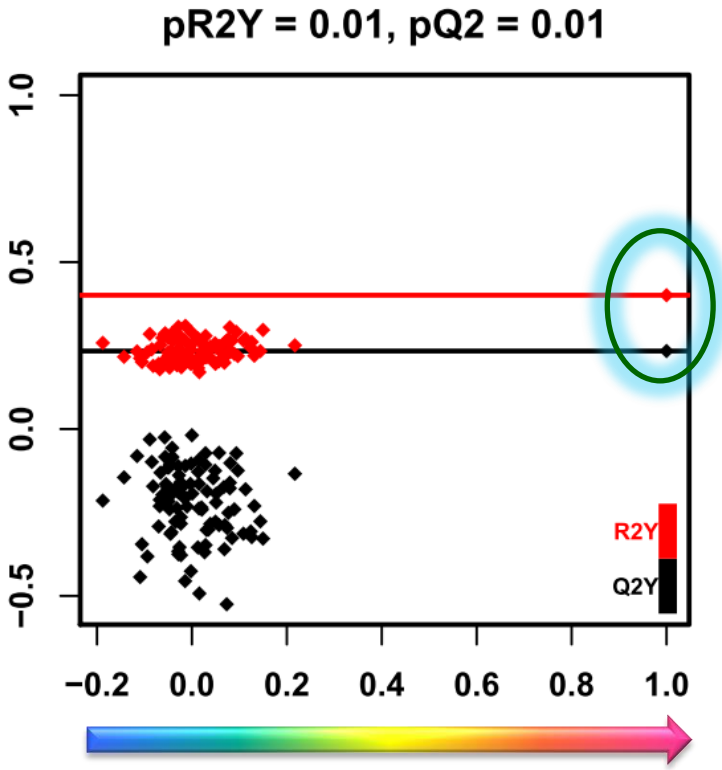
	1,7-Dimethyluric acid	Dehydroepiandrosterone sulfate	...
H011	3.33	4.46	
H023	4.64	2.81	
H033	4.35	2.51	
H042	3.91	4.14	
H052	4.35	2.55	
H062	3.80	2.47	
H073	4.00	4.36	
H083	4.48	2.02	
H092	3.82	4.55	
H103	4.08	0.21	
H114	4.52	5.17	
H124	4.05	4.93	
H134	4.27	4.53	
H145	4.16	5.33	
H157	4.50	4.29	
H168	4.01	1.89	
H180	4.36	2.67	
H189	4.16	3.02	
H199	3.46	4.09	
H209	4.10	5.00	

y_{random}

X

Significance of the model

- Counting the number of $R2Y$ (and $Q2Y$) metrics from random models which are superior to the values of the true model gives an indication of the significance of the PLS modelling



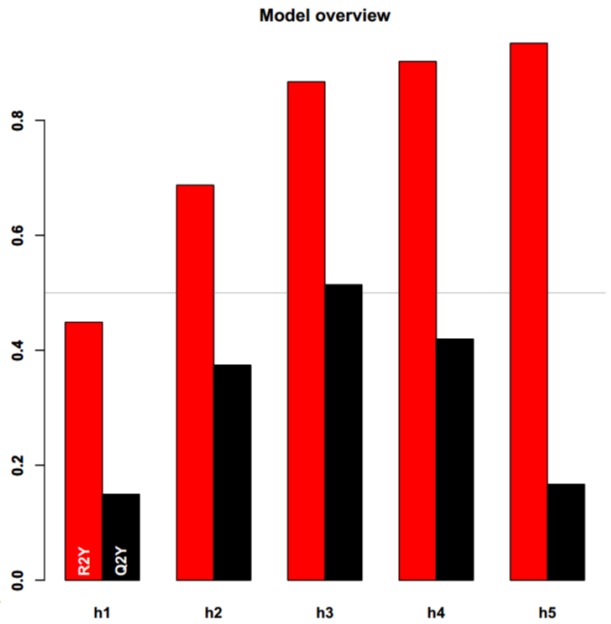
$R2Y$ and $Q2Y$ of the model with the true $\mathbf{y}$ values

'permutation'

Diagnostic metrics

- $0 \leq R2X \leq 1$: percentage of X inertia explained by the model
- $0 \leq R2Y \leq 1$: percentage of Y inertia explained by the model
- $0 \leq Q2Y \leq 1$: estimation of the predictive performance of the model by cross-validation

- $R2X$ and $R2Y$ increase with the number of components while $Q2Y$ reaches a maximum (due to overfitting):



'overview'

Numerical results

- The details of the $R2X$, $R2Y$, and $Q2Y$ values are stored in the "information.txt" file

olomics Analyze Data | Workflow | Shared Data | Visualization | Help | User | Using 2%

```
Y: mean-centering and unit-variance scaling

PLS ('nipals' algorithm)
Number of predictive components: 3

Number of reference observations: 183 (100%)

Correlations between variables and components:
                                    h1     h2 cor_h1 cor_h2
alpha-N-Phenylacetyl-glutamine    -0.220     NA  -0.64     NA
Phe-Tyr-Asp (and isomers)         -0.220     NA  -0.63     NA
Glucuronic acid and/or isomers    -0.220     NA  -0.62     NA
Asp-Leu/Ile isomer 1               0.080     NA   0.22     NA
6-(carboxymethoxy)-hexanoic acid   0.097     NA   0.27     NA
Testosterone glucuronide           0.180     NA   0.50     NA
Acetaminophen glucuronide             NA -0.093     NA -0.240
p-Anisic acid                         NA -0.066     NA -0.180
Malic acid                            NA -0.030     NA -0.078
p-Hydroxymandelic acid                NA  0.200     NA  0.520
1-Methyluric acid                     NA  0.200     NA  0.530
Porphobilinogen                       NA  0.200     NA  0.530

Model overview:
      R2X R2X(cum)    R2Y R2Y(cum)    Q2 Q2(cum) Signif. Iter.
h1 0.0984   0.0984 0.4791    0.479 0.401   0.401      R1     1
h2 0.0861   0.1846 0.1892    0.668 0.256   0.555      R1     1
h3 0.0907   0.2752 0.0615    0.730 0.065   0.584      R1     1

Model summary:
   R2X(cum) R2Y(cum) Q2(cum) RMSEE ncp nco
h3    0.275     0.73   0.584 0.262   3   0
```

History

search datasets

multivariate_example
14 shown, 10 deleted

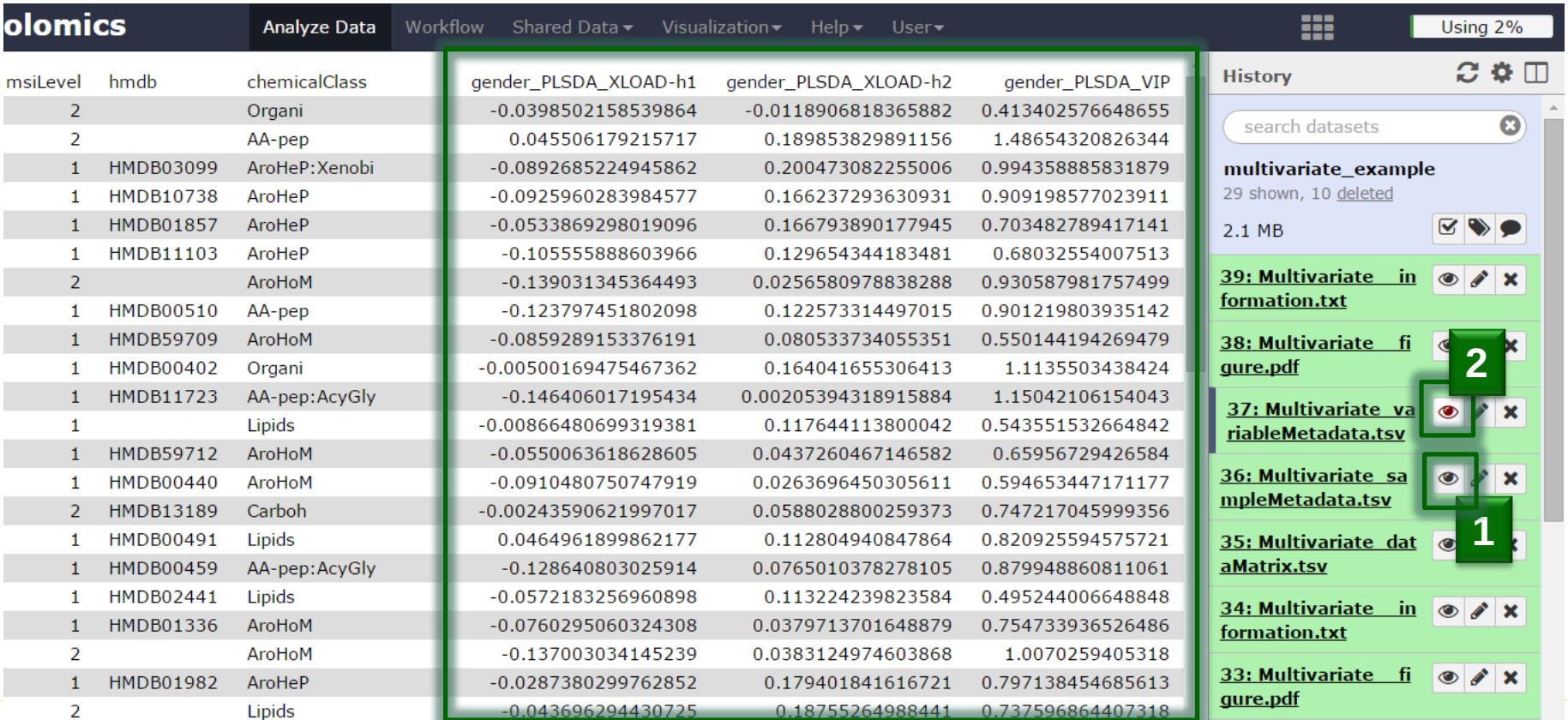
2.1 MB

1

39: Multivariate__information.txt
38: Multivariate__figure.pdf
37: Multivariate_variableMetadata.tsv
36: Multivariate_sampleMetadata.tsv
35: Multivariate_dataMatrix.tsv
34: Multivariate__information.txt
33: Multivariate__figure.pdf
32: Multivariate_variableMetadata.tsv

Scores, loadings and VIPs

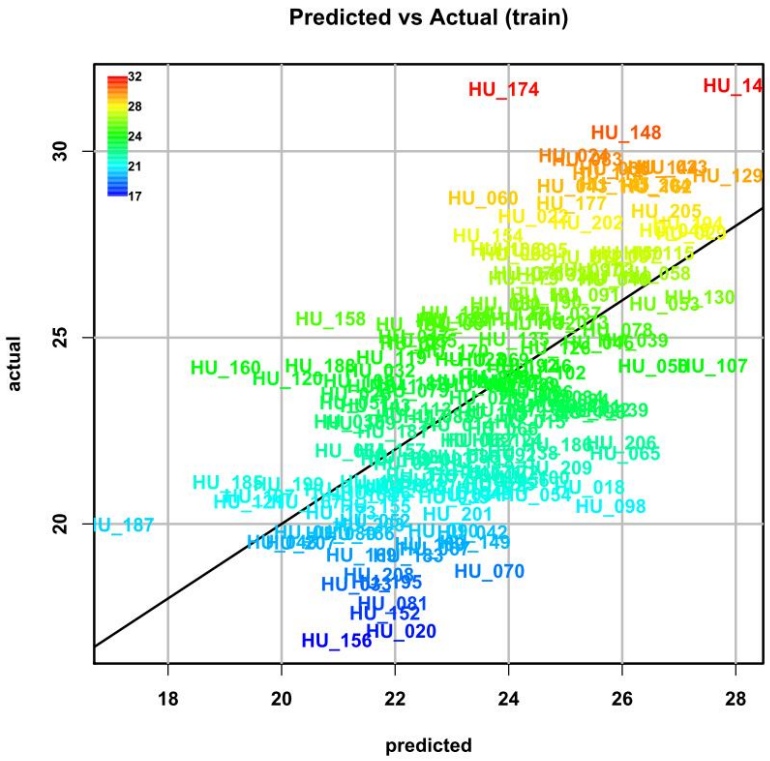
- The score (resp. loading and VIPs) of the selected components have been added as columns in the sampleMetadata (resp. variableMetadata) files



msiLevel	hmdb	chemicalClass	gender_PLSDA_XLOAD-h1	gender_PLSDA_XLOAD-h2	gender_PLSDA_VIP
2		Organi	-0.0398502158539864	-0.0118906818365882	0.413402576648655
2		AA-pep	0.045506179215717	0.189853829891156	1.48654320826344
1	HMDB03099	AroHeP:Xenobi	-0.0892685224945862	0.200473082255006	0.994358885831879
1	HMDB10738	AroHeP	-0.0925960283984577	0.166237293630931	0.909198577023911
1	HMDB01857	AroHeP	-0.0533869298019096	0.166793890177945	0.703482789417141
1	HMDB11103	AroHeP	-0.105555888603966	0.129654344183481	0.68032554007513
2		AroHoM	-0.139031345364493	0.0256580978838288	0.930587981757499
1	HMDB00510	AA-pep	-0.123797451802098	0.122573314497015	0.901219803935142
1	HMDB59709	AroHoM	-0.0859289153376191	0.080533734055351	0.550144194269479
1	HMDB00402	Organi	-0.00500169475467362	0.164041655306413	1.1135503438424
1	HMDB11723	AA-pep:AcyGly	-0.146406017195434	0.00205394318915884	1.15042106154043
1		Lipids	-0.00866480699319381	0.117644113800042	0.543551532664842
1	HMDB59712	AroHoM	-0.0550063618628605	0.0437260467146582	0.65956729426584
1	HMDB00440	AroHoM	-0.0910480750747919	0.0263696450305611	0.594653447171177
2	HMDB13189	Carboh	-0.00243590621997017	0.0588028800259373	0.747217045999356
1	HMDB00491	Lipids	0.0464961899862177	0.112804940847864	0.820925594575721
1	HMDB00459	AA-pep:AcyGly	-0.128640803025914	0.0765010378278105	0.879948860811061
1	HMDB02441	Lipids	-0.0572183256960898	0.113224239823584	0.495244006648848
1	HMDB01336	AroHoM	-0.0760295060324308	0.0379713701648879	0.754733936526486
2		AroHoM	-0.137003034145239	0.0383124974603868	1.0070259405318
1	HMDB01982	AroHeP	-0.0287380299762852	0.179401841616721	0.797138454685613
2		Lipids	-0.043696294430725	0.18755264988441	0.737596864407318

Advanced parameters: Graphics

- Several types of graphics are available:
  - e.g., predict-train and predict-test (the latter being available only if the train/test partition has been selected)



'predict-train'

PLS-DA

- The two response levels are encoded as numbers

Qualitative

	gender
H011	M
H023	M
H033	F
H042	M
H052	F
H062	M
H073	M
H083	M
H092	M
H103	M
H114	M
H124	M
H134	M
H145	M
H157	F
H168	F
H180	F
H189	F
H199	M
H209	F

y

n = 20 samples

Quantitative

	gender
HU_017	0.5
HU_028	0.5
HU_034	-0.5
HU_051	0.5
HU_060	-0.5
HU_078	0.5
HU_091	0.5
HU_093	0.5
HU_099	0.5
HU_110	0.5
HU_130	0.5
HU_134	0.5
HU_138	0.5
HU_149	0.5
HU_152	-0.5
HU_175	-0.5
HU_178	-0.5
HU_185	-0.5
HU_204	0.5
HU_208	-0.5

y

PLS

Quantitative

	gender
H011	0.40
H023	0.10
H033	-0.61
H042	0.39
H052	-0.47
H062	0.46
H073	0.36
H083	0.11
H092	0.47
H103	0.23
H114	0.25
H124	0.56
H134	0.12
H145	0.93
H157	-0.19
H168	-0.49
H180	-0.20
H189	0.00
H199	0.54
H209	0.05

y_{fitted}

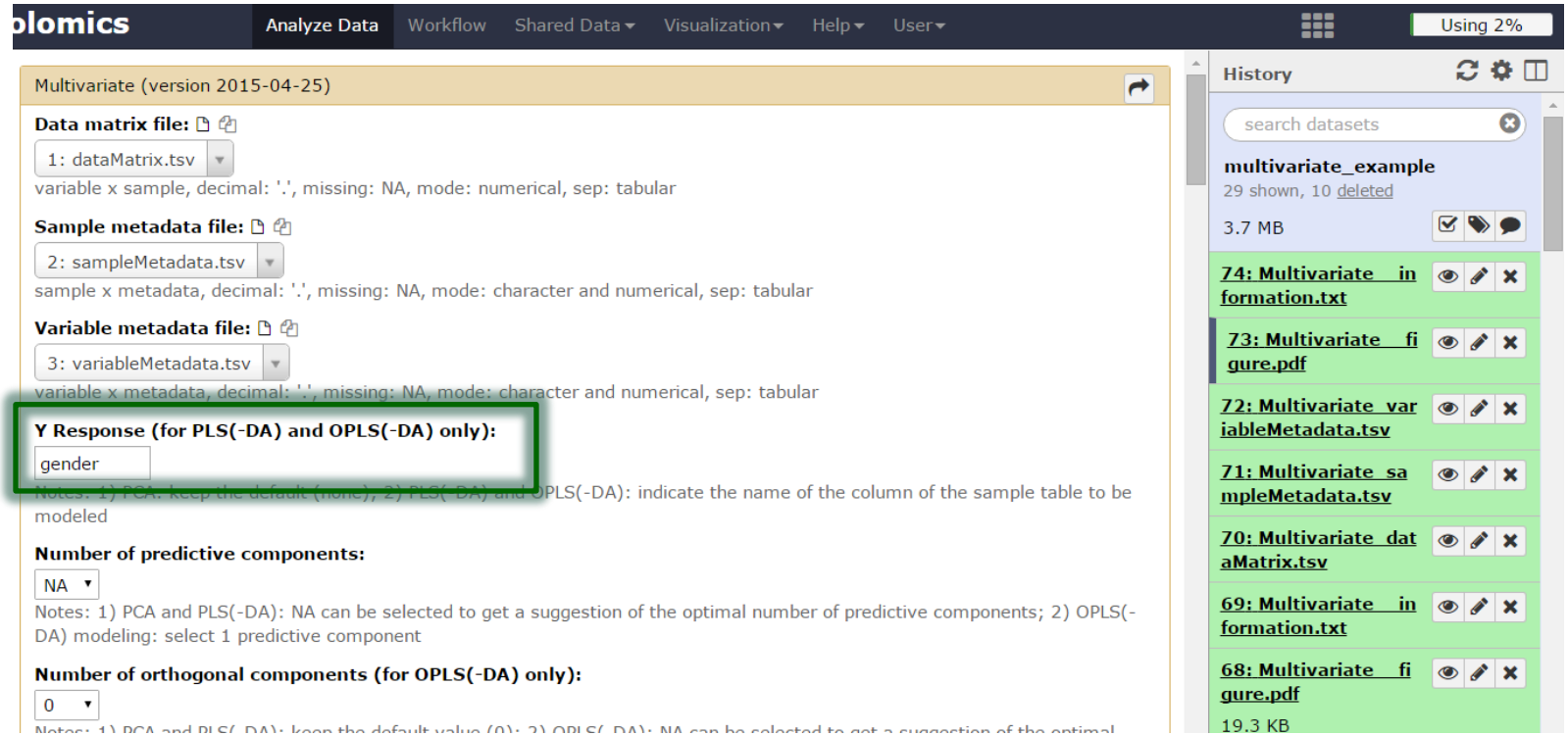
Qualitative

	pred
H011	M
H023	M
H033	F
H042	M
H052	F
H062	M
H073	M
H083	M
H092	M
H103	M
H114	M
H124	M
H134	M
H145	M
H157	F
H168	F
H180	F
H189	M
H199	M
H209	M

y_{fitted}

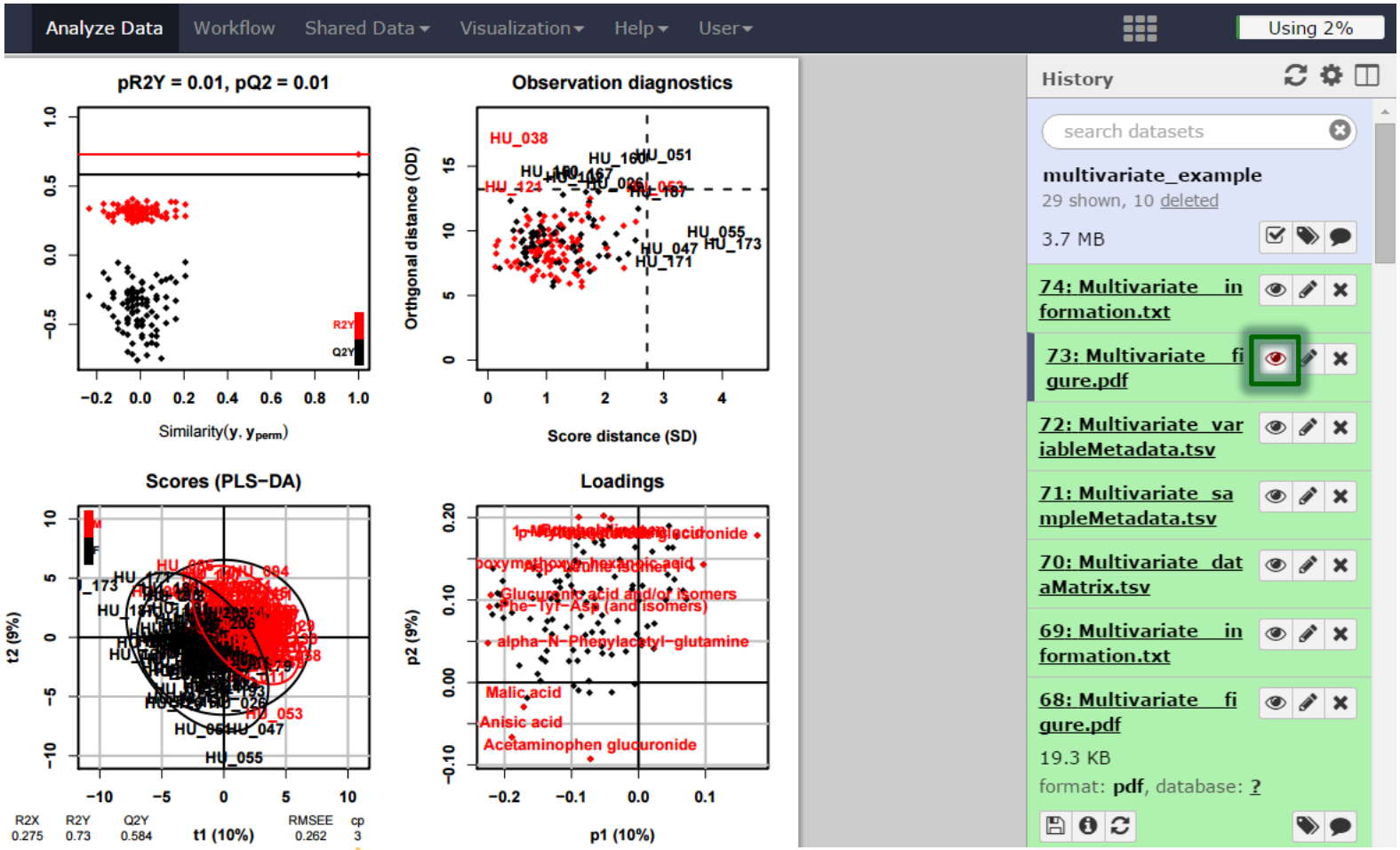
PLS-DA

- Automatically selected when the response is qualitative (i.e. the column of sampleMetadata only contains characters)



Warning: Use balanced datasets (similar proportions of samples in each of the two classes)

PLS-DA


Analyze Data
Workflow
Shared Data
Visualization
Help
User
Using 2%
pR2Y = 0.01, pQ2 = 0.01
R2Y
Q2Y
Similarity(y, y perm)
Observation diagnostics
Orthgonal distance (OD)
Score distance (SD)
HU_038
HU_051
HU_053
HU_055
HU_173
HU_047
HU_171
Scores (PLS-DA)
t2 (9%)
t1 (10%)
R2X 0.275
R2Y 0.73
Q2Y 0.584
RMSEE 0.262
cp 3
Loadings
p2 (9%)
p1 (10%)
Glucuronic acid and/or isomers
alpha-N-Phenylacetyl-glutamine
Malic acid
Anisic acid
Acetaminophen glucuronide
History
search datasets
multivariate_example
29 shown, 10 deleted
3.7 MB
74: Multivariate information.txt
73: Multivariate figure.pdf
72: Multivariate variableMetadata.tsv
71: Multivariate sampleMetadata.tsv
70: Multivariate dataMatrix.tsv
69: Multivariate information.txt
68: Multivariate figure.pdf
19.3 KB
format: pdf, database: ?

ORTHOGONAL PARTIAL LEAST SQUARES REGRESSION (OPLS) AND DISCRIMINANT ANALYSIS (OPLS-DA)

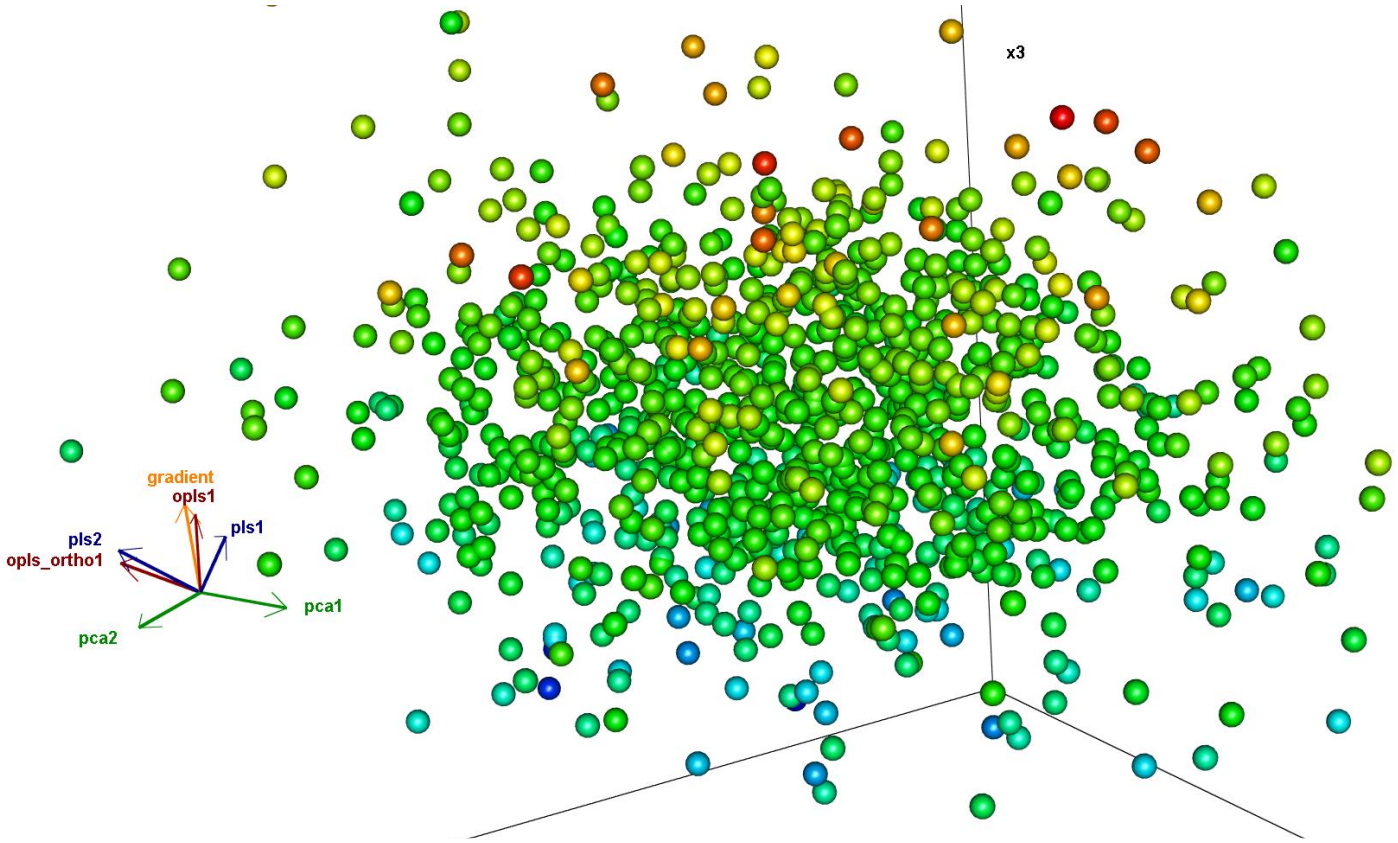
Principles

- Separately models the variations of the predictors correlated and orthogonal to the response
- Improves the interpretation of the components but not the overall predictive performance of the model
- Only one predictive component required for single response models
- Note: As with PLS, care should be taken to avoid too many (orthogonal) components (which would result in overfitting)

OPLS vs PLS

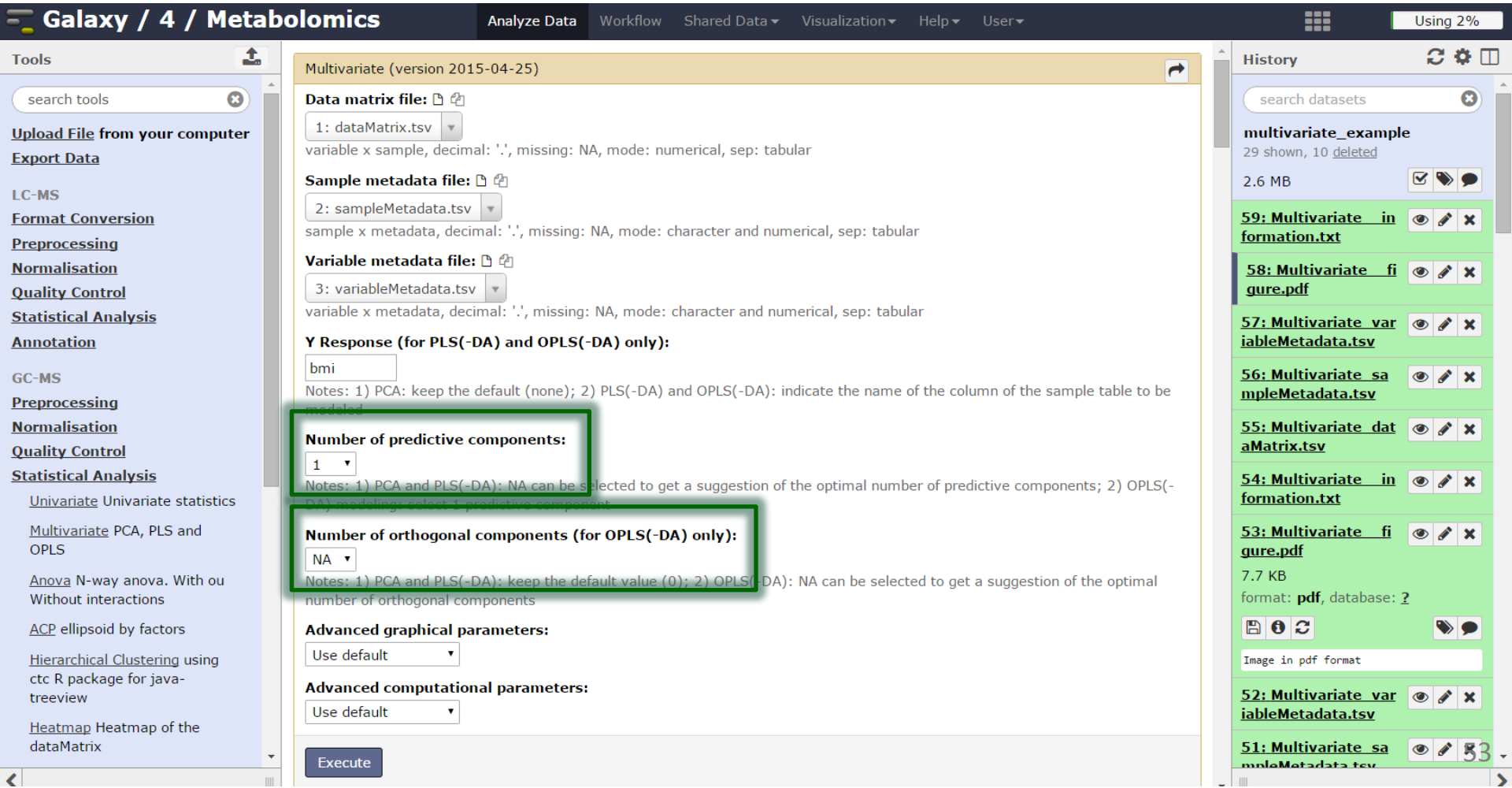
- Variation not correlated to the response (e.g., technical bias) is modelled separately by the orthogonal component(s)

=> The first predictive component is strongly correlated to the response



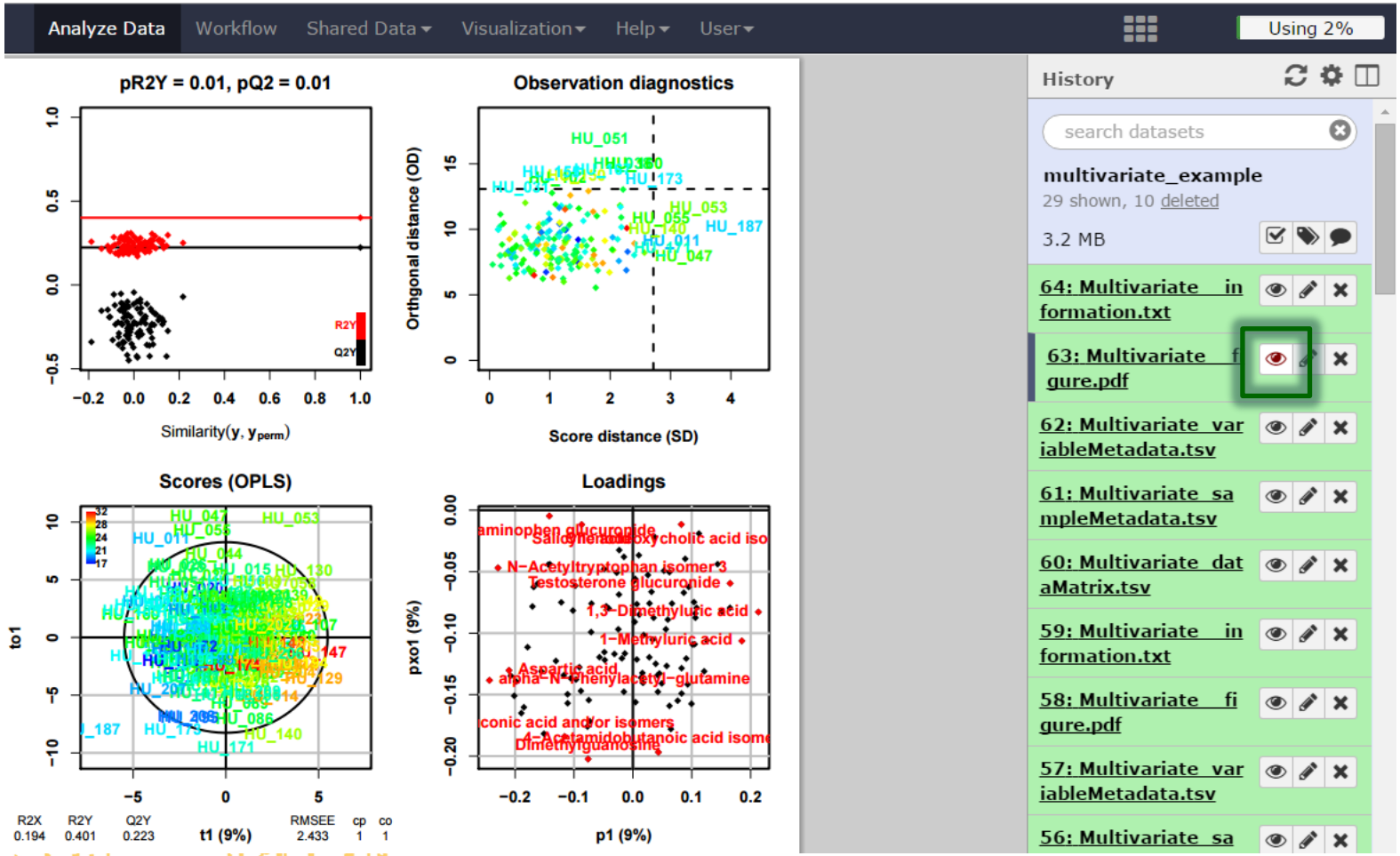
Selection of OPLS(-DA) as the type of analysis

- Set the number of predictive component to 1
- Select the number of orthogonal components (e.g., NA)



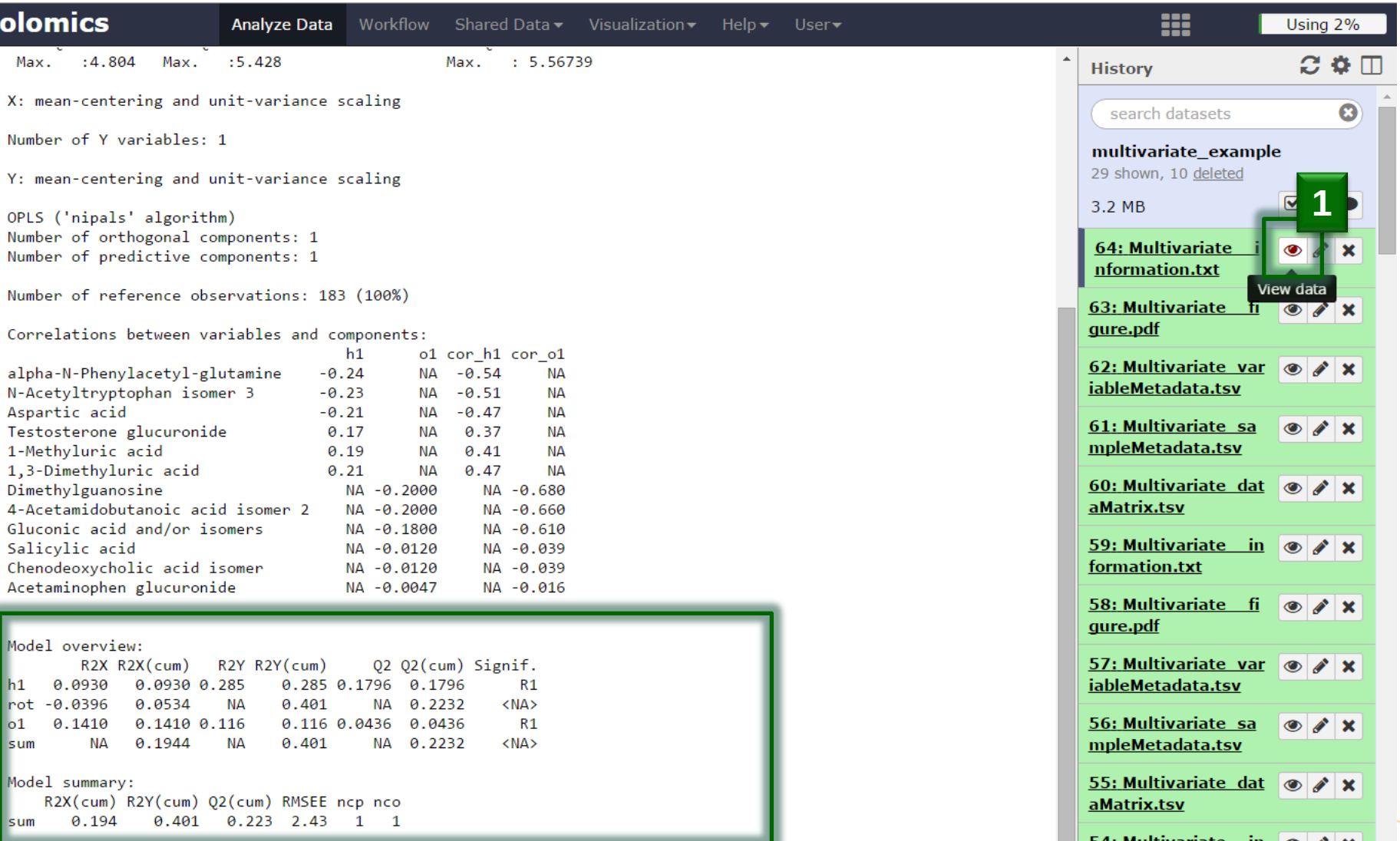
Graphical results

- permutation, overview, outlier, and score plots displayed as the default ('summary')



Numerical results

- The details of the $R2X$, $R2Y$, and $Q2Y$ values are stored in the "information.txt" file



References

- Wold S., Sjöström M. and Eriksson L. (2001). PLS-regression: a basic tool of chemometrics. *Chemometrics and Intelligent Laboratory Systems,* **58:**109-130. http://dx.doi.org/10.1016/S0169-7439(01)00155-1

- Trygg J., Holmes E. and Lundstedt T. (2007). Chemometrics in Metabonomics. *Journal of Proteome Research*, **6**:469-479. http://dx.doi.org/10.1021/pr060594q

- Brereton R.G. and Lloyd G.R. (2014). Partial least squares discriminant analysis: taking the magic away. *Journal of Chemometrics,* **28:**213-225. http://dx.doi.org/10.1002/cem.2609