

A new R package 

# statTarget

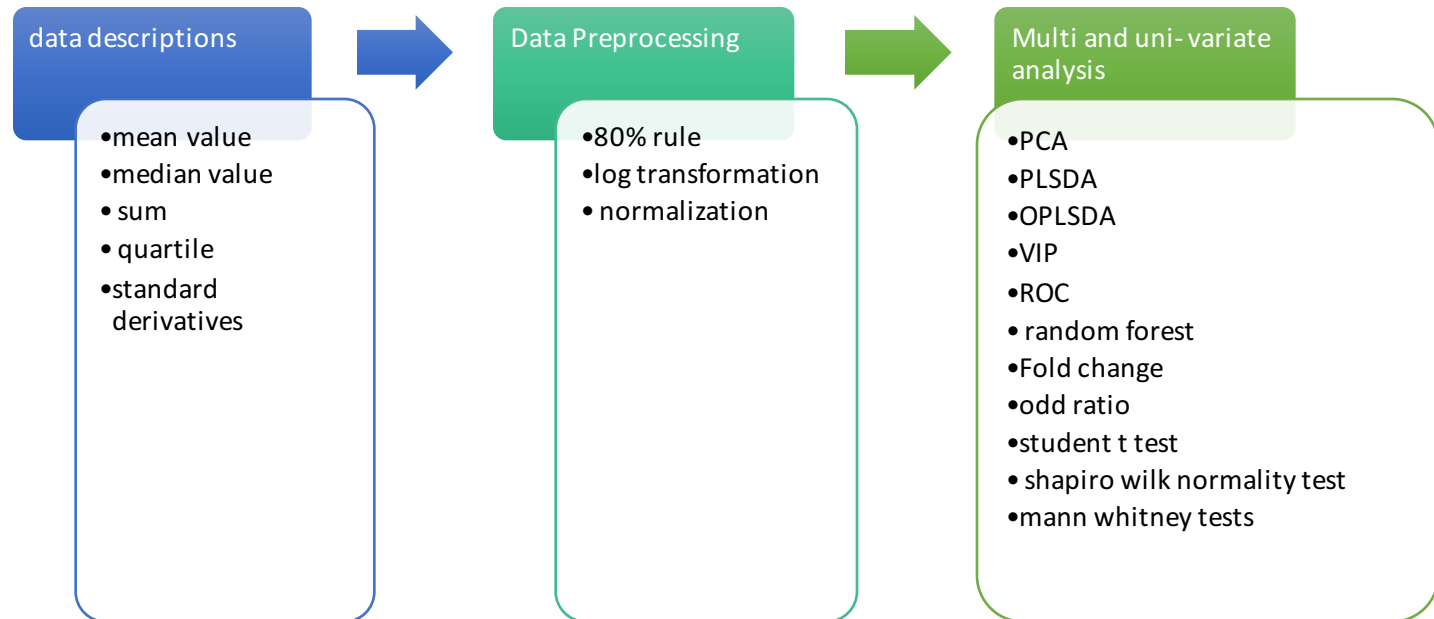
# StatTarget

A tool provide the basic data analysis for metabolomics data.

## ① Simple operation, only 3 steps



## ② Comprehensively statistical results



Data input

Sample name Group Factor

Saved as .csv

Metabolites ID

Order	Group	1	2	3	4	5
21	1	0.0269394	0.212481308	0.421938647	0.072731082	0.476999498
71	1	0.004056653	0.104999071	0.014279731	0.024105957	0.167094773
50	1	0.004056653	0.570556469	0.171406702	0.02019163	0.061832702
14	2	0.014602305	4.650099858	0.022114445	0.007105695	0.156819962
74	1	0.045739012	0.36876884	0.019088228	0.006108264	0.278668387
9	2	0.008098186	0.235025541	0.182280343	0.025622084	0.046807751
32	1	0.019498917	0.683527006	0.035527196	0.014959372	0.430006029
20	2	0.004056653	0.060402839	0.015232417	0.007500019	0.149098523
168	1	0.015402529	1.036678761	0.155572884	0.022977097	0.152309431
28	2	0.036884932	6.041892945	0.103977726	0.017530557	0.299275534
62	2	0.031621389	6.028034401	0.352036582	0.086246923	0.935893131

Concentration

Execute R

- 1 Copy this code into R
- 2 Replace the file name
- 3 Execute

```
> library(statTarget)
> data <- read.csv("data.csv",header=TRUE)
> statTarget("data.csv", glog = TRUE,
test.multi=TRUE, nvarRF = 30, scaling = "Pareto")
```

## You can use the <?statTarget> to get the information of parameters

Wed May 18 13:31:20 2016\Statistic Summary Finished

Wed May 18 13:31:20 2016\Preglog Finished!

Wed May 18 13:31:20 2016\PCA-PLSDA start...

Loading required package: robustbase

Scalable Robust Estimators with High Breakdown Point (version 1.3-11)

[1] "Pairs of Principal Components giving highest statistical cluster separation are:"

	Pair_of_PCs	Sum_p_values(F_statistics)	Variance(%)
1	PC1vsPC13	7.911175e-10	21.9
2	PC1vsPC6	1.279460e-09	24.3
3	PC1vsPC3	6.595059e-09	28.1
4	PC1vsPC11	1.786467e-08	22.2
5	PC1vsPC21	3.030638e-08	20.4

[1] "No outliers are detected"

Wed May 18 13:31:42 2016\Variable List

[1]	"X1"	"X2"	"X3"	"X4"	"X5"	"X6"	"X7"	"X8"	"X9"	"X10"	"X11"	"X12"
[14]	"X14"	"X15"	"X16"	"X17"	"X18"	"X19"	"X20"	"X21"	"X22"	"X23"	"X24"	"X25"
[27]	"X27"	"X28"	"X29"	"X30"	"X31"	"X32"	"X33"	"X34"	"X35"	"X36"	"X37"	"X38"
[40]	"X40"	"X41"	"X42"	"X43"	"X44"	"X45"	"X46"	"X47"	"X48"	"X49"	"X50"	"X51"

Wed May 18 13:31:42 2016\PLS-DA Start...!

Attaching package: 'pls'

The following object is masked from 'package:stats':

loadings

Data: X dimension: 193 325

Y dimension: 193 2

Fit method: oscorespls

Number of components considered: 172

VALIDATION: RMSEP

Cross-validated using 10 random segments.

Response: Y1

	(Intercept)	1 comps	2 comps	3 comps	4 comps	5 comps	6 comps	7 comps	8 comps
CV	0.4977	0.4444	0.4265	0.4217	0.4242	0.4349	0.4419	0.4477	0.4552
adjCV	0.4977	0.4439	0.4245	0.4192	0.4212	0.4300	0.4349	0.4405	0.4468

Wed May 18 13:31:46 2016\PLS-DA Finished!

Wed May 18 13:31:46 2016\permutation 500 time START...!

\.....Tea Time! Take A Rest!.....

Wed May 18 13:55:38 2016\R2!

	R2Y(cum)	Q2(cum)
Y1.1 comps	0.2535865	0.1941836
Y2.1 comps	0.2535865	0.1941836
Y1.2 comps	0.3898557	0.2579649
Y2.2 comps	0.3898557	0.2579649
Y1.3 comps	0.4447295	0.2744668
Y2.3 comps	0.4447295	0.2744668

Wed May 18 13:55:38 2016\permutation 500 time Finished!

Wed May 18 13:55:41 2016\p-value Start...

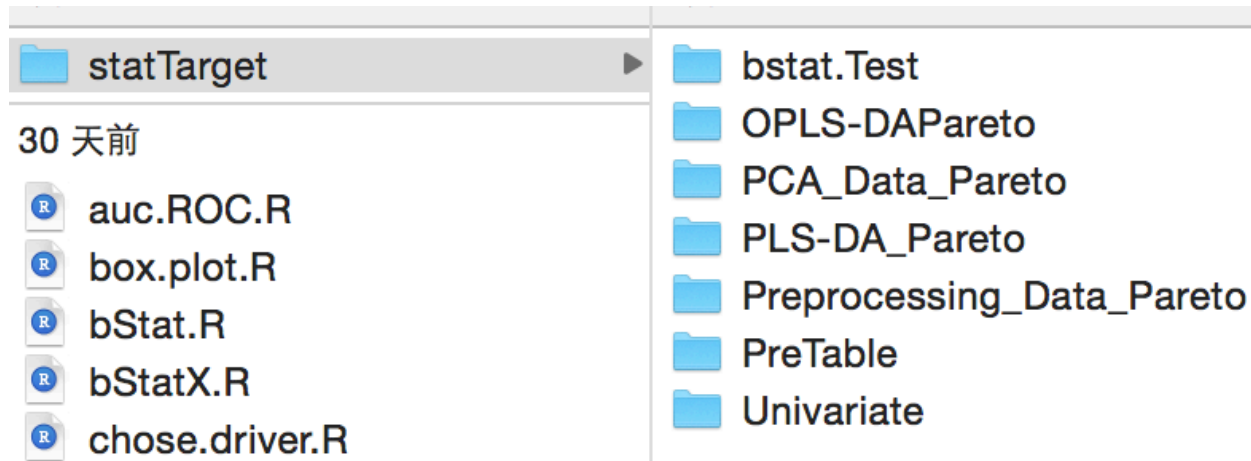
Wed May 18 13:55:45 2016\ROC Start...

Wed May 18 13:59:09 2016\RandomForest Start...

Wed May 18 14:01:04 2016\Multiglog Finished!

Wed May 18 14:01:04 2016\ttest.multi done!

## Statistical results



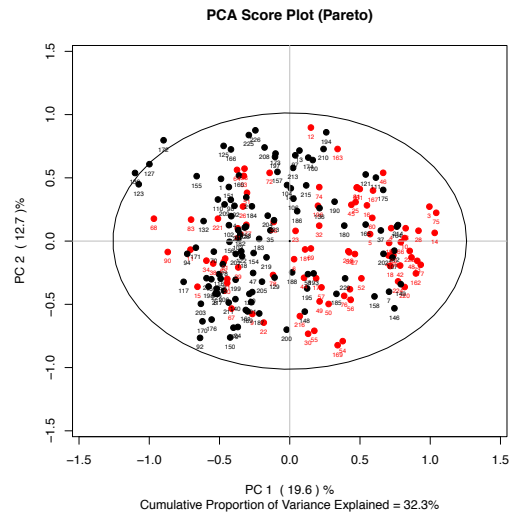
**Bstat.test** includes the basic data descriptions, mean value, median value, sum, quartile, standard derivatives, etc.

**OPLS-DAPareto, PCA-Data\_Pareto and PLS-DA\_Pareto** include the multivariate analysis, PCA, PLSDA, OPLSDA, VIP, Scoreplot, Loadingplot, S-plot, Permutation.

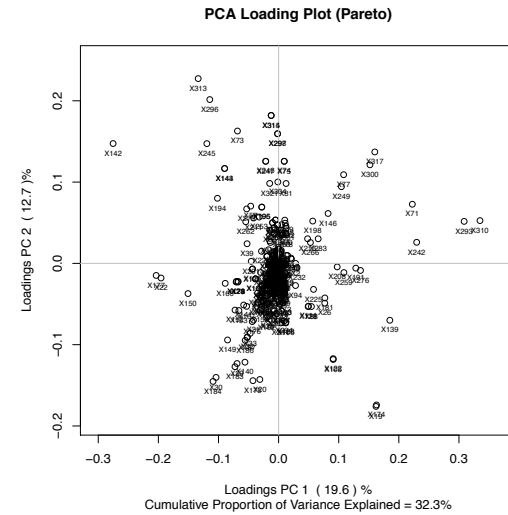
**Preprocessing\_Data\_Pareto and Pretable** include the Normalize data.

**Univariate** includes univariate analysis, ROC, random forest, odd ratio, student t test, shapiro wilk normality test and mann whitney tests, fold changes, P values, volcano plot, box plot.

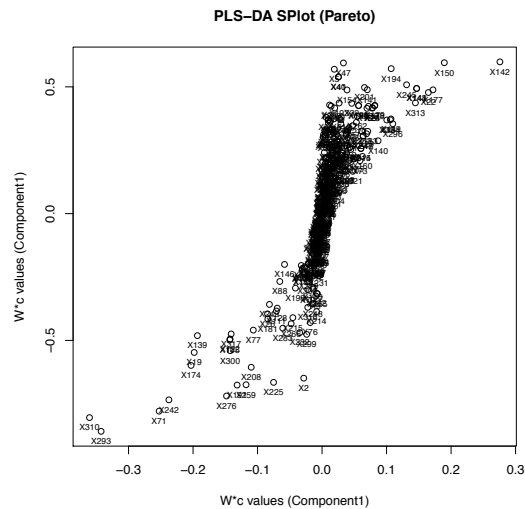
# PCA Score Plot



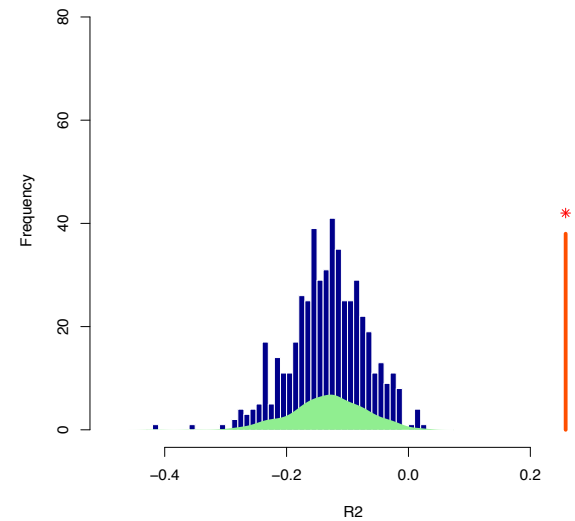
# PCA Loading Plot



# PLS-DA S-Plot

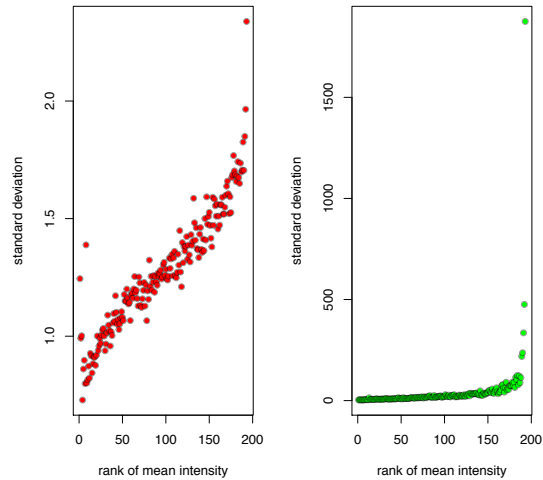


# PLS-DA Permutation Plot

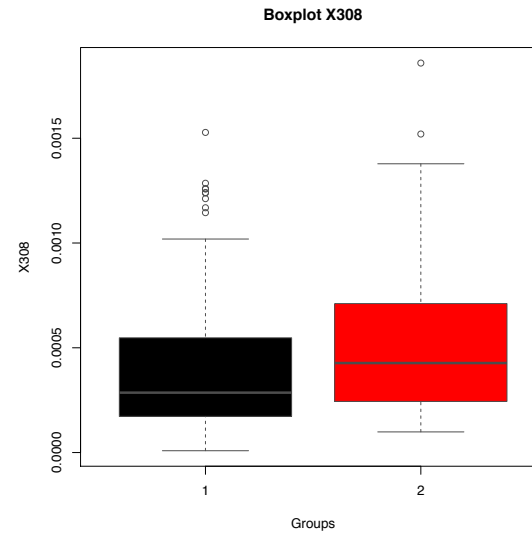




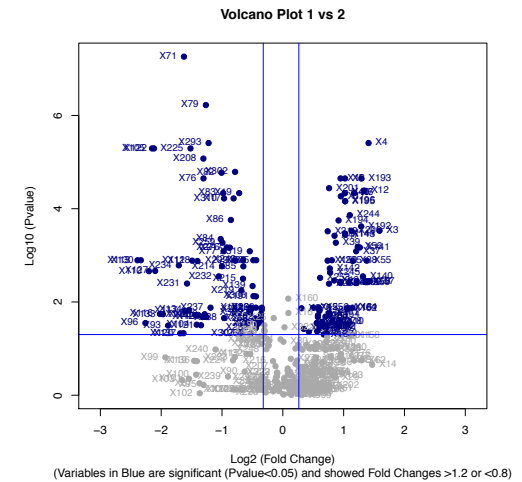
# gLog transformation Plot



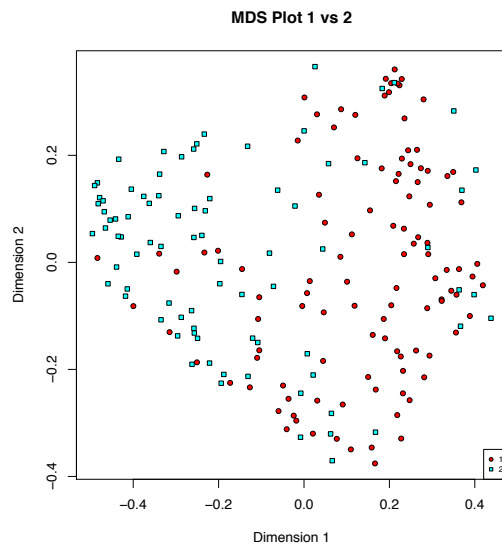
# Box Plot



# Volcano Plot



# MDS Plot



# Gini Plot

