

statTarget: Statistical Analysis of Metabolite Profile

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1 statTarget installation guide

statTarget package needs GTK2 libraries to run. Below, it is described how to install GTK2 libraries on Mac OS and Windows.

1.1 For Mac OS users

1 - Install Xcode developer tools (at least version 5.0.1) from Apple Store (it is free).

2 - Install XQuartz-2.7.5.dmg from <http://xquartz.macosforge.org/landing/>

3 - Install GTK_2.24.17_X11.pkg from <http://r.research.att.com> .

4 - `install.packages("statTarget")` .

5 - `library(statTarget)`

1.2 For Windows users

1 - download `gtk+-bundle_2.22.1-20101229_win64.zip` from <http://ftp.gnome.org/pub/gnome/binaries/win64/gtk+/2.22/> .

2 - This is a bundle containing the GTK+ stack and its dependencies for Windows. To use it, create some empty folder like `C : \opt\gtk` .

3 - Unzip this bundle.

4 - Now, you have to add the bin folder to your PATH variable. Make sure you have no other versions of GTK+ in PATH variable. To do this, execute the following instructions: Open Control Panel, click on System and Security, click on System, click on Advanced System Settings, click on Environment Variables. In the Environment Variables window you will notice two columns User variables for a user name and System variables. Change the PATH variable in the System variables to be `C : \opt\gtk\bin` .

This is all you need to install the GTK2 libraries.

5 - `install.packages("statTarget")` .

6 - `library(statTarget)`.

2 Overview of statTarget

A graphical user interface, easy to use tool provide quality control based signal correction, integration of metabolomic data from multiple batches, and the comprehensive statistic analysis for non-targeted and targeted approaches. The user controls statTarget through a Graphical User Interface (GUI).

3 statTarget in detail

The main GUI of statTarget has two basic components. The first is shift correction. It includes quality control-based robust LOESS signal correction (QC-RLSC) that is a widely accepted method for quality control based signal correction and integration of metabolomic data from multiple analytical batches (Dunn WB., et al. 2011; Luan H., et al. 2015).

3.1 statTarget Shift Correction

statTarget - Shift Correction provide QC-RLSC algorithm that fit the QC data, and each metabolites in the true sample will be normalized to the QC sample.

Additionally, LOESS based generalised cross-validation (GCV) would be automatically applied to avoid overfitting of the observed data, when the QCspan was set at 0.

3.2 statTarget Statistical Analysis

statTarget - Statistical Analysis provide features including Data preprocessing, Data descriptions, Multivariate statistics analysis and Univariate analysis.

Data preprocessing : 80-percent rule, log transformation, KNN imputation, Median imputation and Minimum values imputation.

Data descriptions : Mean value, Median value, Sum, Quartile, Standard derivatives, etc.

Multivariate statistics analysis : PCA, PLSDA, OPLSDA, VIP, Random forest.

Univariate analysis : Student T-test, Shapiro-Wilk normality test and Mann-Whitney tests.

Biomarkers analysis for Clinical research : ROC, Odd ratio.

4 Session Info

- R version 3.3.0 (2016-05-03), x86_64-apple-darwin13.4.0
- Locale:
en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
- Base packages: base, datasets, graphics, grDevices, methods, stats, utils
- Other packages: devtools 1.11.1, digest 0.6.9, gWidgets2 1.0-7, gWidgets2RGtk2 1.0-5, memoise 1.0.0, RGtk2 2.20.31, statTarget 1.2.0, testthat 1.0.2
- Loaded via a namespace (and not attached): BiocInstaller 1.22.3, cluster 2.0.4, crayon 1.3.1, DEoptimR 1.0-4, grid 3.3.0, impute 1.46.0, lattice 0.20-33, LMGene 2.28.0, magrittr 1.5, mvtnorm 1.0-5, pcaPP 1.9-60, pls 2.5-0, plyr 1.8.3, pracma 1.8.8, pROC 1.8, R6 2.1.2, randomForest 4.6-12, Rcpp 0.12.4, robustbase 0.92-5, roxygen2 5.0.1, rrcov 1.3-11, stats4 3.3.0, stringi 1.0-1, stringr 1.0.0, tools 3.3.0, withr 1.0.1