

Package ‘MetSizeR’

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Type Package

Title GUI Tool for Estimating Sample Sizes for Metabolomic Experiments

Version 1.1

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Description An easy to use Graphical User Interface for estimating sample sizes required for metabolomic experiments even when experimental pilot data is not available.

Depends mvtnorm, MetabolAnalyze, cairoDevice, gWidgets, gWidgetsRGtk2

License GPL (>= 2)

LazyLoad yes

NeedsCompilation no

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MetSizeR-package *MetSizeR Graphical User Interface*

Description

Start the Graphical User Interface for MetSizeR.
MetSizeR can be used to determine sample sizes for both targeted and NMR metabolomic experiments even when experimental pilot data is not available.

Details

```

Package:  MetSizeR
Type:    Package
Version:  1.1
Date:    2013-09-08
License:  GPL (>= 2)
LazyLoad: yes

```

The manual and example can be found with `vignette("MetSizeR")`.

Author(s)

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MetSizeR

MetSizeR GUI

Description

Start the Graphical User Interface for MetSizeR. The MetSizeR GUI provides a user friendly method for sample size estimation for both targeted and NMR metabolomic experiments even when experimental pilot data is not available.

Usage

`MetSizeR()`

Details

MetSizeR GUI options:

File

Open

covariates

demo_nmr_pilot_data

Quit

Read in data and covariates, quit

upload the txt file containing the spectrum

upload the txt file containing the covariates

upload the demonstration NMR data already in MetSizeR

dispose the GUI

Sample size

pilot data

no pilot data

NMR data

Targeted

Spectral bins

Metabolites

Proportion of significant bins

sample size estimation

sample size estimation with experimental pilot data

sample size estimation with no experimental pilot data

sample size estimation for a NMR experiment

sample size estimation for a targeted experiment

number of spectral bins from the NMR experiment

number of metabolites for targeted analysis

proportion of spectral bins expected to be significant

Proportion of significant metabolites	proportion of metabolites expected to be significant
Models	different types of models available
ncovars	number of covariates for the PPCCA model
Target FDR	level of control over type I errors
Sample size per group	smallest sample size to be considered in each group
Save results in R directory	save results in the R working directory
calculate	estimate the sample size
Plot proportion of significant bins	assess the effect of varying the expected proportion of significant bins
Plot proportion of significant metabolites	assess the effect of varying the expected proportion of proportion of significant metabolites
MetSizeR status	displays if MetSize has finished estimating the sample size
<hr/>	
Help	manual for MetSizeR
manual	manual for MetSizeR

Note

MetSizeR is built upon gWidgets package. Make sure gWidgets package is properly installed.

Author(s)

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Examples

```
MetSizeR()
```

```
nmr_spectra
```

NMR Metabolomic Spectra from Urine Samples of Eighteen Mice

Description

NMR metabolomic spectra from urine samples of 18 mice. Each spectrum has 189 spectral bins, measured in parts per million (ppm). Covariate associated with the mice was also recorded: the weight.

Usage

```
data(nmr_spectra)
```

Format

A data frame with 18 observations on the following 190 variables.

weight a numeric vector

spectra a numeric vector

Details

The *nmr_spectra* data is included in *nmr_spectra.txt* which can be uploaded into MetSizeR.

Source

Nyamundanda, G., Gormley, I.C. and Brennan, L. (2010) Probabilistic principal components analysis for metabolomic data, *Bioinformatics*, 11.

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