Package 'gramm4R'

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Type Package

Title Generalized correlation analysis and model construction strategy
for metabolome and microbiome

Version 1.2.0

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Description Generalized Correlation Analysis for Metabolome and Microbiome (GRaMM), for inter-
correlation pairs discovery among metabolome and microbiome.

License GPL-2

Encoding UTF-8

biocViews GraphAndNetwork,Microbiome

Depends R (>= 3.6.0)

LazyData true

Imports basicTrendline,investr,minerva,psych,grDevices, graphics,
stats,DelayedArray,SummarizedExperiment,DMwR,phyloseq

VignetteBuilder knitr

Suggests knitr, rmarkdown

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R topics documented:

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covariates   *Test data of covariates*

Description

The test data for examples at functionnaiveGramm, Gramm,nlfitGramm

Usage

```
data("covariates")
```

Format

The format is: Formal class 'SummarizedExperiment' [package "SummarizedExperiment"] with 5 slots ..@ colData :Formal class 'DataFrame' [package "S4Vectors"] with 6 slots .. .. ..@ rownames : chr [1:42] "B1" "B2" "B3" "B4" ... .@ nrows : int 42 .. .. ..@ listData : Named list() .. .. ..@ elementType : chr "ANY" .. .. ..@ elementMetadata: NULL .. .. ..@ metadata : list() ..@ assays :Formal class 'SimpleAssays' [package "SummarizedExperiment"] with 1 slot .. .. ..@ data:Formal class 'SimpleList' [package "S4Vectors"] with 4 slots .. ..@ listData :List of 1 .. ..$ counts: int [1:3, 1:42] 25 1 90 26 1 70 27 1 68 28 ... .- attr(*, "dimnames")=List of 2 .. ..$: NULL .. ..$: chr [1:42] "B1" "B2" "B3" "B4" ... .@ elementType : chr "ANY" .. ..@ elementMetadata: NULL .. ..@ metadata : list() ..@ NAMES : NULL ..@ elementMetadata:Formal class 'DataFrame' [package "S4Vectors"] with 6 slots .. .. ..@ rownames : NULL .. .. ..@ nrows : int 3 .. .. ..@ listData :List of 1 .. ..$ X: Factor w/ 3 levels "age","gender",..: 1 2 3 .. .. ..@ elementType : chr "ANY" .. .. ..@ elementMetadata: NULL .. .. ..@ metadata : list() ..@ metadata : list()

Examples

```
data(covariates)
## maybe str(covariates) ; plot(covariates) ...
```

Gramm   *Get the association between metabolites and microbes*

Description

The entire strategy to get the association between metabolites and microbes, using linear and non-linear methods, and plot the regression figures.

Usage

```
Gramm(A,B,C,metaNor,rarefaction,r,alpha)
```

Arguments

A	A SummarizedExperiment object contains data of metabolome, where rows represent features of metabolites and columns represent samples.
B	A SummarizedExperiment object contains data of microbiome, where rows represent features of microbes and columns represent samples.
C	A SummarizedExperiment object contains data of covariates, where rows represent features of covariates and columns represent samples.
metaNor	Should metabolome data normalized? Using normalization when your metabolites are qualitative; and no normalization when the metabolites are quantitative. Default:TRUE.
rarefaction	Resample an OTU table such that all samples have the same library size. Here refers to a repeated sampling procedure to assess species richness, first proposed in 1968 by Howard Sanders.(see wikipedia for more detail.) Default:FALSE.
r	The linear regression coefficients threshold for using nonlinear method. Default: 0.5.
alpha	The linear regression p-value threshold for using nonlinear method.Default: 0.05.

Value

pretreatment	The result of pretreatment
correlation	The result of correlation, see naiveGramm for detail

A file named "R value top 10 pairs.pdf" will be created automatically (corrlation coefficient top 10 pairs) .

Author(s)

Mengci Li, Dandan Liang, Tianlu Chen and Wei Jia

References

Gloor, G. B., Macklaim, J. M., Pawlowsky-Glahn, V., Egozcue, J. J., Microbiome Datasets Are Compositional: And This Is Not Optional. Front. Microbiol. 2017, 8 (2224). Chambers, J. M. (1992) Linear models. Chapter 4 of Statistical Models in S eds J. M. Chambers and T. J. Hastie, Wadsworth & Brooks/Cole. D. Reshef, Y. Reshef, H. Finucane, S. Grossman, G. McVean, P. Turnbaugh, E. Lander, M. Mitzenmacher, P. Sabeti. (2011) Detecting novel associations in large datasets. Science 334, 6062. D. Albanese, M. Filosi, R. Visintainer, S. Riccadonna, G. Jurman, C. Furlanello. minerva and minepy: a C engine for the MINE suite and its R, Python and MATLAB wrappers. Bioinformatics (2013) 29(3): 407-408.

See Also

preGramm for pretreatment;nlfitGramm for nonlinear fitting;naiveGramm for naive correlation method.

Examples

```
data("metabolites");data("microbes");data("covariates")
Gramm(metabolites,microbes,covariates)
```

---

metabolites   *Test data of metabolome*

Description

The test data for examples at function naiveGramm, Gramm,nlfitGramm

Usage

```
data("metabolites")
```

Format

The format is: Formal class 'SummarizedExperiment' [package "SummarizedExperiment"] with 5 slots ..@ colData :Formal class 'DataFrame' [package "S4Vectors"] with 6 slots .. .. ..@ rownames : chr [1:42] "B1" "B2" "B3" "B4" ... .@ nrows : int 42 .. .. ..@ listData : Named list() .. .. ..@ elementType : chr "ANY" .. .. ..@ elementMetadata: NULL .. .. ..@ metadata : list() ..@ assays :Formal class 'SimpleAssays' [package "SummarizedExperiment"] with 1 slot .. .. ..@ data:Formal class 'SimpleList' [package "S4Vectors"] with 4 slots .. ..@ listData :List of 1 .. ..$ counts: num [1:40, 1:42] 8.75 3.31 5.09 1.49 6.2 8.81 2.37 1.76 4.47 2.18 ... .- attr(*, "dimnames")=List of 2 .. ..$: NULL .. ..$: chr [1:42] "B1" "B2" "B3" "B4" ... .@ elementType : chr "ANY" .. ..@ elementMetadata: NULL .. ..@ metadata : list() ..@ NAMES : NULL ..@ elementMetadata:Formal class 'DataFrame' [package "S4Vectors"] with 6 slots .. .. ..@ rownames : NULL .. .. ..@ nrows : int 40 .. .. ..@ listData :List of 1 .. ..$ X: Factor w/ 40 levels "Decadienylcarnitine",..: 16 35 31 25 3 4 1 8 9 6 ... .@ elementType : chr "ANY" .. .. ..@ elementMetadata: NULL .. .. ..@ metadata : list() ..@ metadata : list()

Examples

```
data(metabolites)
## maybe str(metabolites) ; plot(metabolites) ...
```

---

microbes   *Test data of microbiome*

Description

The test data for examples at functionnaiveGramm, Gramm,nlfitGramm

Usage

```
data("microbes")
```

Format

The format is: Formal class 'SummarizedExperiment' [package "SummarizedExperiment"] with 5 slots ..@ colData :Formal class 'DataFrame' [package "S4Vectors"] with 6 slots .. .. ..@ rownames : chr [1:42] "B1" "B2" "B3" "B4" ... .@ nrows : int 42 .. .. ..@ listData : Named list() .. .. ..@ elementType : chr "ANY" .. .. ..@ elementMetadata: NULL .. .. ..@ metadata : list() ..@ assays :Formal class 'SimpleAssays' [package "SummarizedExperiment"] with 1 slot .. .. ..@ data:Formal class 'SimpleList' [package "S4Vectors"] with 4 slots .. ..@ listData :List of 1 .. ..$ counts: num [1:85, 1:42] 1 1 13 2 4 8 11 24 6 1 ... .- attr(*, "dimnames")=List of 2 .. ..$: NULL .. ..$: chr [1:42] "B1" "B2" "B3" "B4" ... .@ elementType : chr "ANY" .. ..@ elementMetadata: NULL .. ..@ metadata : list() ..@ NAMES : NULL ..@ elementMetadata:Formal class 'DataFrame' [package "S4Vectors"] with 6 slots .. .. ..@ rownames : NULL .. .. ..@ nrows : int 85 .. .. ..@ listData :List of 1 .. ..$ X: Factor w/ 84 levels "[Ruminococcus] spp",..: 74 24 1 12 20 21 29 70 65 20 ... .@ elementType : chr "ANY" .. .. ..@ elementMetadata: NULL .. .. ..@ metadata : list() ..@ metadata : list()

Examples

```
data(microbes)
## maybe str(microbes) ; plot(microbes) ...
```

---

naiveGramm *Corrlation methods of Gramm*

Description

A function to test the association among metabolites and microbes. Using linear (linear regression) or nonlinear (Maximal Information Coefficient) methods.

Usage

```
naiveGramm(x,y,z,r,alpha)
```

Arguments

x	A SummarizedExperiment object contains data of preproccessed data, where rows represent features of metabolites and columns represent samples.
y	A SummarizedExperiment object contains data of microbiome preproccessed data , where rows represent features of microbes and columns represent samples.
z	An optional SummarizedExperiment object containing the confounders.
r	The linear regression coefficients threshold for using nonlinear method. Default: 0.5.
alpha	The linear regression p-value threshold for using nonlinear method.Default: 0.05.

Value

r	Correlation coefficients.
p	Correlation p values.
type	Correlation methods for computing (linear or nonlinear).

Author(s)

Mengci Li, Dandan Liang, Tianlu Chen and Wei Jia

References

Chambers, J. M. (1992) Linear models. Chapter 4 of Statistical Models in S eds J. M. Chambers and T. J. Hastie, Wadsworth & Brooks/Cole. D. Reshef, Y. Reshef, H. Finucane, S. Grossman, G. McVean, P. Turnbaugh, E. Lander, M. Mitzenmacher, P. Sabeti. (2011) Detecting novel associations in large datasets. Science 334, 6062. D. Albanese, M. Filosi, R. Visintainer, S. Riccadonna, G. Jurman, C. Furlanello. minerva and minepy: a C engine for the MINE suite and its R, Python and MATLAB wrappers. Bioinformatics (2013) 29(3): 407-408.

See Also

preGramm for pretreatment;nlfitGramm for nonlinear fitting;Gramm: the whole strategy of this method.

Examples

```
data("metabolites")
data("microbes")
data("covariates")
naiveGramm(metabolites,microbes,covariates)
```

---

nlfitGramm   *Plot the nonlinear fitting of input data*

Description

Plot, draw regression line and confidence interval, and show regression equation, R-square and P-value. The function includes the following models in the latest version: "line2P" (formula as: y=a*x+b), "line3P" (y=a*x^2+b*x+c), "log2P" (y=a*ln(x)+b), "exp2P" (y=a*exp(b*x)),"exp3P" (y=a*exp(b*x)+c), "power2P" (y=a*x^b), "power3P" (y=a*x^b+c), and "S" (y=a/(1+exp((x-b)/c))). Of each correlation pairs the figure who has the highest R-square among these models will be saved in a "pdf" file at working dirctory.

Usage

```
nlfitGramm(X,Y)
```

Arguments

X	Metabolome preproccessed data (SummarizedExperiment object).
Y	Microbiome preproccessed data (SummarizedExperiment object).

Details

nothing

Value

A file named "curve fit.pdf" will be created automatically.

Author(s)

Mengci Li, Dandan Liang, Tianlu Chen and Wei Jia

References

Bates, D. M., and Watts, D. G. (2007) Nonlinear Regression Analysis and its Applications. Wiley.

Greenwell B. M., and Schubert-Kabban, C. M. (2014) investr: An R Package for Inverse Estimation. The R Journal, 6(1), 90-100.

See Also

naiveGramm for naive correlation method; preGramm for pretreatment; Gramm: the whole strategy of this method.

Examples

```
data("metabolites")
data("microbes")
nlfitGramm(metabolites,microbes)
```

---

preGramm	*Preproccess the metabolome data and microbiome data*

Description

Preproccess the input data of metabolome and microbiome. Missing values may be imputed and filled (KNN method). Metabolome data and microbiomedata may be normalized and transformed by logarithm transformation and centered log-ratio (CLR) algorithm.

Usage

```
preGramm(A,B,metaNor = TRUE,rarefaction = FALSE)
```

Arguments

A	The metabolome data under pretreatment (SummarizedExperiment object).
B	The microbiome data under pretreatment (SummarizedExperiment object).
metaNor	Should metabolome data normalized? Using normalization when your metabolites are qualitative; and no normalization when the metabolites are quantitative. Default:TRUE.
rarefaction	Resample an OTU table such that all samples have the same library size. Here refers to a repeated sampling procedure to assess species richness, first proposed in 1968 by Howard Sanders.(see wikipedia for more detail.) Default:FALSE.

Value

x	Metabolome preprocessed data
y	Microbiome preprocessed data

Author(s)

Mengci Li, Dandan Liang, Tianlu Chen and Wei Jia

References

Gloor, G. B., Macklaim, J. M., Pawlowsky-Glahn, V., Egozcue, J. J., Microbiome Datasets Are Compositional: And This Is Not Optional. Front. Microbiol. 2017, 8 (2224).

See Also

naiveGramm for naive correlation method; nlfitGramm for nonlinear fitting; Gramm: the whole strategy of this method.

Examples

```
data("metabolites")
data("microbes")
preGramm(metabolites,microbes)
```

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