

Package ‘equSA’

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Type Package

Title Estimate Graphical Models from Multiple Types of Datasets and Construct Networks

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Description Provides an equivalent measure of partial correlation coefficients for high-dimensional Gaussian Graphical Models to learn and visualize the underlying relationships between variables from single or multiple datasets. You can refer to <doi:10.1080/01621459.2015.1012391> for more detail. Based on this method, the package also provides the method for constructing networks for Next Generation Sequencing Data.

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R topics documented:

equSA-package	2
combineR	3
Cont2Gaus	4
ContSim	5
ContTran	8
count	9
diffR	9
equSAR	10

pcorSelR	11
plotGraph	13
psical	14
solcov	15
SR0	16
SR0_mat	16
TR0	17
TR0_mat	17
Index	18

equSA-package	<i>Estimate Graphical Models from Multiple Types of Datasets and Construct Networks</i>
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Description

Provides an equivalent measure of partial correlation coefficients for high-dimensional Gaussian Graphical Models to learn and visualize the underlying relationships between variables from single or multiple datasets. The package also provides the method for constructing networks for Next Generation Sequencing Data.

Details

Package: equSA
Type: Package
Version: 1.1.2
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License: GPL-2

We propose an equivalent measure of partial correlation coefficient estimator called ψ estimators which enable us to estimate these networks via sparse, high-dimensional undirected graphical models. (Liang, F et al, 2015)

Here, we provide the community a convenient and useful tool to learn a Gaussian Graphical Models. To estimate the network structures from Gaussian distributed data with this package, users simply need to specify the "method" in the main function, for example `equSAR(data, ...)` to fit GGM to get the estimated adjacency matrix.

In this package, we also provide the code for combining Networks from two different dataset `combineR(data1,data2,...)` and the code for detecting difference between two Networks, for example `diffR(data1,data2,...)`. `data1` and `data2` should share the same dimension of variables (p) but allow have different samples (n).

This package also implement the Algorithm 17.1 of Friedman et al(2001), i.e estimate the covariance and precision matrix of the data given its structure. `solcov(data,struct,...)`

If the data are not Normalized, for example, the count data, we propose a random effect model-based transformation to continuized data `ContTran(data, ...)`, and then we transform the continuized data to Gaussian via a semiparametric transformation and then apply ψ -learning algorithm to reconstruct networks. The proposed method is consistent, and the resulting network satisfies the faithfulness and global Markov properties. The most common application is to estimate Gene Regulatory Networks from Next Generation Sequencing Data (Jia, B et al, 2017)

Author(s)

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References

- Friedman, J., Hastie, T., & Tibshirani, R. (2001). The elements of statistical learning (Vol. 1). Springer, Berlin: Springer series in statistics.
- Liang, F., Song, Q. and Qiu, P. (2015). An Equivalent Measure of Partial Correlation Coefficients for High Dimensional Gaussian Graphical Models. J. Amer. Statist. Assoc., 110, 1248-1265.<doi:10.1080/01621459.2015.1012391>
- Liang, F. and Zhang, J. (2008) Estimating FDR under general dependence using stochastic approximation. Biometrika, 95(4), 961-977.<doi:10.1093/biomet/asn036>
- Liu, H., Lafferty, J. and Wasserman, L. (2009). The Nonparanormal: Semiparametric Estimation of High Dimensional Undirected Graphs. Journal of Machine Learning Research , 10, 2295-2328.
- Jia, B., Xu, S., Xiao, G., Lamba, V., Liang, F. (2017) Inference of Genetic Networks from Next Generation Sequencing Data. Biometrics.

Examples

```
#library(equSA)
#data(SR0)
#equSAR(SR0)
```

combineR

Combine two networks.

Description

Combine two networks to a single one from datasets of two groups by our calculated ψ scores.

Usage

```
combineR(Data1,Data2,ALPHA1=0.05,ALPHA2=0.05)
```

Arguments

Data1	a $n_1 \times p$ data matrix.
Data2	a $n_2 \times p$ data matrix.
ALPHA1	The significance level of correlation screening for each dataset. In general, a high significance level of correlation screening will lead to a slightly large separator set S_{ij} , which reduces the risk of missing some important variables in the conditioning set. Including a few false variables in the conditioning set will not hurt much the accuracy of the ψ -partial correlation coefficient.
ALPHA2	The significance level of ψ screening for integrative estimation of ψ scores.

Value

A	$p \times p$ Adjacency matrix of the combined graph.
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Author(s)

Bochao Jia<jbc409@ufl.edu> and Faming Liang

References

- Liang, F., Song, Q. and Qiu, P. (2015). An Equivalent Measure of Partial Correlation Coefficients for High Dimensional Gaussian Graphical Models. J. Amer. Statist. Assoc., 110, 1248-1265.
- Liang, F. and Zhang, J. (2008) Estimating FDR under general dependence using stochastic approximation. Biometrika, 95(4), 961-977.

Examples

```
#library(equSA)
#data(SR0)
#data(TR0)
#combineR(SR0, TR0)
```

Cont2Gaus

A transformation from count data into Gaussian data

Description

To transform count data into Gaussian distributed and also keep the consistency for constructing networks.

Usage

```
Cont2Gaus(iData, total_iteration=5000, stepsize=0.05)
```

Arguments

`iData` a $n \times p$ count data matrix.

`total_iteration` Total iteration number for Bayesian random effect model-based transformation, default of 5000.

`stepsize` The stepsize of updating parameters in transformation, default of 0.05.

Details

This is the function that transform the count data into Gaussian data which include two steps. First, we do data continuized transformation `ContTran(data, ...)` and then we apply the semiparametric transformation (Liu, H et al, 2009) provided in "*huge*" packages to tranform continuized data into Gaussian distributed.

Value

`Gaus` $n \times p$ matrix of Normalized data with Gaussian distribution.

Author(s)

Bochao Jia<jbc409@ufl.edu> and Faming Liang

References

Jia, B., Xu, S., Xiao, G., Lamba, V., Liang, F. (2017) Inference of Genetic Networks from Next Generation Sequencing Data. Biometrics, in press.

Liu, H., Lafferty, J. and Wasserman, L. (2009). The Nonparanormal: Semiparametric Estimation of High Dimensional Undirected Graphs. Journal of Machine Learning Research , 10, 2295-2328.

Examples

```
#library(equSA)
#data(count)
#Cont2Gaus(count,total_iteration=1000)
```

ContSim	<i>A simulation method for generating count data from multivariate Zero-Inflated Negative Binomial distributions</i>
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Description

Implements the data generation from multivariate Zero-Inflated Negative Binomial (ZINB) distributions with different graph structures, including "random", "hub", "cluster", "AR(2)" and "scale-free".

Usage

```
ContSim(n, p, v = NULL, u = NULL, g = NULL,
prob = NULL, vis = FALSE, verbose = TRUE,
graph.type="AR(2)", k=3.30, lambda=515, omega=0.003,
lower.tail = TRUE, log.p = FALSE)
```

Arguments

n	The number of observations (sample size).
p	The number of variables (dimension).
graph.type	The graph structure with 4 options: "random", "hub", "cluster", "AR(2)" and "scale-free".
v	The off-diagonal elements of the precision matrix, controlling the magnitude of partial correlations with u. The default value is 0.3.
u	A positive number being added to the diagonal elements of the precision matrix, to control the magnitude of partial correlations. The default value is 0.1.
g	For "cluster" or "hub" graph, g is the number of hubs or clusters in the graph. The default value is about $d/20$ if $d \geq 40$ and 2 if $d < 40$. NOT applicable to "random" and "AR(2)" graph.
prob	For "random" graph, it is the probability that a pair of nodes has an edge. The default value is $3/d$. For "cluster" graph, it is the probability that a pair of nodes has an edge in each cluster. The default value is $6*g/d$ if $d/g \leq 30$ and 0.3 if $d/g > 30$. NOT applicable to "hub" or "AR(2)" graphs.
vis	Visualize the adjacency matrix of the true graph structure, the graph pattern, the covariance matrix and the empirical covariance matrix. The default value is FALSE
verbose	If verbose = FALSE, tracing information printing is disabled. The default value is TRUE.
k	dispersion parameter of ZINB distribution, default of 3.30.
lambda	vector of (non-negative) means of ZINB distribution, default of 515.
omega	zero-inflation parameter of ZINB distribution, default of 0.003.
lower.tail	logical; if TRUE (default), probabilities are $P[X \leq x]$, otherwise, $P[X > x]$.
log.p	logical; if TRUE, probabilities p are given as $\log(p)$.

Details

This is the function that can generate dataset from multivariate Zero-Inflated Negative Binomial distributions with different graph structures, including "random", "hub", "cluster", "AR(2)" and "scale-free".

Given the adjacency matrix θ , the graph patterns are generated as below:

(I) "random": Each pair of off-diagonal elements are randomly set $\theta[i, j] = \theta[j, i] = 1$ for $i \neq j$ with probability prob, and 0 other wise. It results in about $d*(d-1)*prob/2$ edges in the graph.

(II) "hub": The row/columns are evenly partitioned into g disjoint groups. Each group is associated with a "center" row i in that group. Each pair of off-diagonal elements are set $\theta_{i,j} = \theta_{j,i} = 1$ for $i \neq j$ if j also belongs to the same group as i and 0 otherwise. It results in $d - g$ edges in the graph.

(III) "cluster": The row/columns are evenly partitioned into g disjoint groups. Each pair of off-diagonal elements are set $\theta_{i,j} = \theta_{j,i} = 1$ for $i \neq j$ with the probability prob if both i and j belong to the same group, and 0 otherwise. It results in about $g \cdot (d/g) \cdot (d/g - 1) \cdot \text{prob} / 2$ edges in the graph.

(IV) "AR(2)": The off-diagonal elements are set to be $\theta_{i,j} = 1$ if $1 \leq |i - j| \leq g$ and 0 otherwise. It results in $(2d - 1 - g) \cdot g / 2$ edges in the graph.

(V) "scale-free": The graph is generated using B-A algorithm. The initial graph has two connected nodes and each new node is connected to only one node in the existing graph with the probability proportional to the degree of the each node in the existing graph. It results in d edges in the graph.

The adjacency matrix θ has all diagonal elements equal to 0 . To obtain a positive definite precision matrix, the smallest eigenvalue of $\theta + v$ (denoted by e) is computed. Then we set the precision matrix equal to $\theta + v + (|e| + 0.1 + u)I$. The covariance matrix is then computed for generating multivariate ZINB dataset.

The default values for parameters k , λ and ω of ZINB distribution are estimated from a real TCGA dataset. See Jia.B et al(2017) for more detail.

Value

A list of two elements:

data	The simulated count dataset in a $n \times p$ matrix.
Adj	$p \times p$ The adjacency matrix of true graph structure (in sparse matrix representation) for the generated data

Author(s)

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References

- Jia, B., Xu, S., Xiao, G., Lamba, V., Liang, F. (2017) Inference of Genetic Networks from Next Generation Sequencing Data. Biometrics, in press.
- T. Zhao and H. Liu.(2012) The huge Package for High-dimensional Undirected Graph Estimation in R. Journal of Machine Learning Research.
- Yahav, I., and Shmueli, G. (2012). On generating multivariate Poisson data in management science applications. Applied Stochastic Models in Business and Industry, 28(1), 91-102.

Examples

```
#library(equSA)
#ContSim(100,200)
```

ContTran

A data continuized transformation

Description

To transform count data into continuous data.

Usage

```
ContTran(iData, total_iteration=5000, stepsize=0.05)
```

Arguments

`iData` a *nxp* count data matrix.

`total_iteration` total iteration number for Bayesian random effect model-based transformation, default of 5000.

`stepsize` The stepsize of updating parameters in transformation, default of 0.05.

Details

This is the function that transform the count data into continuized data.

Value

`continuz` *nxp* matrix of continuized data.

Author(s)

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References

Jia, B., Xu, S., Xiao, G., Lamba, V., Liang, F. (2017) Inference of Genetic Networks from Next Generation Sequencing Data. Biometrics, in press.

Examples

```
#library(equSA)
#data(count)
#ContTran(count, total_iteration=1000)
```

count	<i>An example of count dataset for constructing networks</i>
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Description

count is a simulated dataset for illustrating our proposed method for inferencing networks from next generation sequencing data.

Usage

```
data(count)
```

Format

count dataset is a 100x200 matrix. Each row represents a observation and each column represents a variable. It is generated from an overdispersion and zero-inflated Poission distribution.

References

Jia, B., Xu, S., Xiao, G., Lamba, V., Liang, F. (2017) Inference of Genetic Networks from Next Generation Sequencing Data. Biometrics, in press.

diffR	<i>Detect difference between two networks.</i>
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Description

Detecting significant different edges between two networks using our calculated ψ scores.

Usage

```
diffR(Data1,Data2,ALPHA1=0.05,ALPHA2=0.05)
```

Arguments

Data1	a $n_1 \times p$ data matrix.
Data2	a $n_2 \times p$ data matrix.
ALPHA1	The significance level of correlation screening for each dataset. In general, a high significance level of correlation screening will lead to a slightly large separator set S_{ij} , which reduces the risk of missing some important variables in the conditioning set. Including a few false variables in the conditioning set will not hurt much the accuracy of the ψ -partial correlation coefficient.
ALPHA2	The significance level of ψ screening for integrative estimation of ψ scores.

Value

A $p \times p$ adjacency matrix of the combined graph.

Author(s)

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References

Liang, F., Song, Q. and Qiu, P. (2015). An Equivalent Measure of Partial Correlation Coefficients for High Dimensional Gaussian Graphical Models. J. Amer. Statist. Assoc., 110, 1248-1265.

Liang, F. and Zhang, J. (2008) Estimating FDR under general dependence using stochastic approximation. Biometrika, 95(4), 961-977.

Examples

```
#library(equSA)
#data(SR0)
#data(TR0)
#diffR(SR0,TR0,ALPHA2=0.2)
```

equSAR

An equivalent measure of partial correlation coefficients

Description

Infer networks from Gaussian data using our proposed ψ -learning algorithm.

Usage

```
equSAR(iData,iMaxNei=as.integer(iDataNum/log(iDataNum)),
ALPHA1=0.05,ALPHA2=0.05)
```

Arguments

iData	a $n \times p$ data matrix.
iMaxNei	Neighborhood size in correlation screening step, default to $n/\log(n)$.
ALPHA1	The significance level of correlation screening. In general, a high significance level of correlation screening will lead to a slightly large separator set S_{ij} , which reduces the risk of missing some important variables in the conditioning set. Including a few false variables in the conditioning set will not hurt much the accuracy of the ψ -partial correlation coefficient.
ALPHA2	The significance level of ψ screening.

Details

This is the main function of the package that fit the Gaussian Graphical Models and obtain the ψ scores and adjacency matrix.

Value

A list of two elements:

Adj	$p \times p$ adjacency matrix of the generated graph.
score	Estimated ψ score matrix which has 3 columns. The first two columns denote the pair indices of variables i and j and the last column denote the calculated ψ scores for this pair.

Author(s)

Bochao Jia and Faming Liang<faliang@ufl.edu>

References

Liang, F., Song, Q. and Qiu, P. (2015). An Equivalent Measure of Partial Correlation Coefficients for High Dimensional Gaussian Graphical Models. J. Amer. Statist. Assoc., 110, 1248-1265.

Liang, F. and Zhang, J. (2008) Estimating FDR under general dependence using stochastic approximation. Biometrika, 95(4), 961-977.

Examples

```
#library(equSA)
#data(SR0)
#equSAR(SR0)
```

pcorSelR	<i>Multiple hypothesis test</i>
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Description

Infer networks from ψ scores using multiple hypothesis test in ψ screening procedure.

Usage

```
pcorSelR(score, ALPHA2=0.05)
```

Arguments

score	ψ score matrix which has 3 columns. The first two columns denote the pair of variables i and j and the last column denote the calculated ψ scores for this pair.
ALPHA2	The significance level of ψ screening, default of 0.05.

Details

This is the function that conduct multiple hypothesis test for ψ scores, thus we called it ψ screening procedure.

Value

qqqscore The threshold value of ψ scores which indicates that if one pair of variables has larger ψ scores than this threshold value in the ψ score matrix, this pair is considered as connected, i.e there is an edge between this pair of variables.

Author(s)

Bochao Jia, Faming liang<faliang@ufl.edu>

References

Liang, F., Song, Q. and Qiu, P. (2015). An Equivalent Measure of Partial Correlation Coefficients for High Dimensional Gaussian Graphical Models. J. Amer. Statist. Assoc., 110, 1248-1265.

Liang, F. and Zhang, J. (2008) Estimating FDR under general dependence using stochastic approximation. Biometrika, 95(4), 961-977.

Examples

```
# library(equSA)
# data(SR0)
# U <- psical(SR0, ALPHA1=0.05)
# ## probit transformation for psi scores ###
# z<-U[,3]
# q<-pnorm(-abs(z), log.p=TRUE)
# q<-q+log(2.0)
# s<-qnorm(q,log.p=TRUE)
# s<-(-1)*s
# U<-cbind(U[,1:2],s)
# ## subsampling for psi scores ###
# N <- length(U[,1])
# ratio<-ceiling(N/100000)
# U<-U[order(U[,3]), 1:3]
# m<-floor(N/ratio)
# m0<-N-m*ratio
# s<-sample.int(ratio,m,replace=TRUE)
# for(i in 1:length(s)) s[i]<-s[i]+(i-1)*ratio
# if(m0>0){
#   s0<-sample.int(m0,1)+length(s)*ratio
#   s<-c(s,s0)
# }
# Us<-U[s,]
# y <- round(Us,6)
# ## multiple hypothesis tests ###
# pcorseIR(y,ALPHA2=0.05)
```

`plotGraph`*Plot Single Network*

Description

Plot a network with specific layout.

Usage

```
plotGraph(net, fn = "", th = 1e-06, mylayout = NULL)
```

Arguments

<code>net</code>	a square adjacency matrix of the network to be plotted.
<code>fn</code>	file name to save the network plot. Default to be an empty string, so the network is plotted to the standard output (screen). NOTE: if a file name is specified, it should be file name for PDF file.
<code>th</code>	numeric value, default to 1e-06. To specify the threshold if the estimated coefficient between two variables is to be considered connected.
<code>mylayout</code>	graph layout to draw the network, default to NULL.

Details

This function serves as the alternative plotting function to allow users to plot a specific network with specific layout, such as plotting the simulated network.

Value

Returns the layout object from igraph package - numeric matrix of two columns and the rows with the same number as the number of vertices.

Examples

```
#library(equSA)
#data(SR0_mat)
#plotGraph(as.matrix(SR0_mat))
```

psical

An calculation of ψ scores.

Description

To compute an equivalent measure of partial correlation coefficients called ψ scores.

Usage

```
psical(iData, iMaxNei=as.integer(iDataNum/log(iDataNum)), ALPHA1=0.05)
```

Arguments

iData	a $n \times p$ data matrix.
iMaxNei	Neighborhood size in correlation screening step, default to $n/\log(n)$.
ALPHA1	The significance level of correlation screening. In general, a high significance level of correlation screening will lead to a slightly large separator set S_{ij} , which reduces the risk of missing some important variables in the conditioning set. Including a few false variables in the conditioning set will not hurt much the accuracy of the ψ -partial correlation coefficient.

Details

This is the function to calculate ψ scores and can be used in combining or detecting difference of two networks.

Value

score	Estimated ψ score matrix which has 3 columns. The first two columns denote the pair indices of variables i and j and the last column denote the calculated ψ scores for this pair.
-------	--

Author(s)

Bochao Jia, Faming liang<faliang@ufl.edu>

References

Liang, F., Song, Q. and Qiu, P. (2015). An Equivalent Measure of Partial Correlation Coefficients for High Dimensional Gaussian Graphical Models. J. Amer. Statist. Assoc., 110, 1248-1265.

Liang, F. and Zhang, J. (2008) Estimating FDR under general dependence using stochastic approximation. Biometrika, 95(4), 961-977.

Examples

```
#library(equSA)
#data(SR0)
#psical(SR0)
```

solcov	<i>Calculate covariance matrix and precision matrix</i>
--------	---

Description

Calculate the adjusted covariance matrix and precision matrix given the network structure from high dimensional dataset.

Usage

```
solcov(data, struct, tol=10^-5)
```

Arguments

data	A <i>n</i> × <i>p</i> data matrix.
struct	A preacquired adjacency matrix
tol	Tolerant value, default is 10 ⁻⁵

Value

A list of two elements:

COV	Adjusted covariance matrix
PRE	Precision matrix

Author(s)

Bochao Jia & Runmin Shi <jbc409@ufl.edu>

References

Friedman, J., Hastie, T., & Tibshirani, R. (2001). The elements of statistical learning (Vol. 1). Springer, Berlin: Springer series in statistics.

Examples

```
#data(SR0)
#data(SR0_mat)
#solcov(SR0, SR0_mat)
```

SR0

One example dataset for equSA

Description

SR0 is a simulated dataset for illustration our equSA alogorithm.

Usage

```
data(SR0)
```

Format

SR0 dataset is a 100x200 matrix. Each row represents a observation and each column represents a variable.

References

Liang, F., Song, Q. and Qiu, P. (2015). An Equivalent Measure of Partial Correlation Coefficients for High Dimensional Gaussian Graphical Models. J. Amer. Statist. Assoc., 110, 1248-1265.

SR0_mat

The adjacency matrix for SR0 dataset.

Description

SR0_mat is an estimated adjacency matrix by ψ - learning alogorithm.

Usage

```
data(SR0_mat)
```

Format

SR0_mat a 200x200 matrix with binary values. When its element (i,j) equals to 1, there exists an edge between variable i and j. Otherwise, it equals to 0.

References

Liang, F., Song, Q. and Qiu, P. (2015). An Equivalent Measure of Partial Correlation Coefficients for High Dimensional Gaussian Graphical Models. J. Amer. Statist. Assoc., 110, 1248-1265.

TR0

One example dataset for equSA

Description

TR0 is a simulated dataset for illustration our equSA alogorithm.

Usage

`data(TR0)`

Format

TR0 dataset is a 100x200 matrix. Each row represents a observation and each column represents a variable.

References

Liang, F., Song, Q. and Qiu, P. (2015). An Equivalent Measure of Partial Correlation Coefficients for High Dimensional Gaussian Graphical Models. J. Amer. Statist. Assoc., 110, 1248-1265.

TR0_mat

The adjacency matrix for TR0 dataset.

Description

TR0_mat is an estimated adjacency matrix by ψ - learning alogorithm.

Usage

`data(TR0_mat)`

Format

TR0_mat a 200x200 matrix with binary values. When its element (i,j) equals to 1, there exists an edge between variable i and j. Otherwise, it equals to 0.

References

Liang, F., Song, Q. and Qiu, P. (2015). An Equivalent Measure of Partial Correlation Coefficients for High Dimensional Gaussian Graphical Models. J. Amer. Statist. Assoc., 110, 1248-1265.

Index

*Topic **Cont2Gaus**

Cont2Gaus, [4](#)

*Topic **ContSim**

ContSim, [5](#)

*Topic **ContTran**

ContTran, [8](#)

*Topic **combineR**

combineR, [3](#)

*Topic **datasets**

count, [9](#)

SR0, [16](#)

SR0_mat, [16](#)

TR0, [17](#)

TR0_mat, [17](#)

*Topic **diffR**

diffR, [9](#)

*Topic **equSAR**

equSAR, [10](#)

*Topic **package**

equSA-package, [2](#)

*Topic **pcorselR**

pcorselR, [11](#)

*Topic **psical**

psical, [14](#)

*Topic **solcov**

solcov, [15](#)

combineR, [3](#)

Cont2Gaus, [4](#)

ContSim, [5](#)

ContTran, [8](#)

count, [9](#)

diffR, [9](#)

equSA-package, [2](#)

equSAR, [10](#)

pcorselR, [11](#)

plotGraph, [13](#)

psical, [14](#)

solcov, [15](#)

SR0, [16](#)

SR0_mat, [16](#)

TR0, [17](#)

TR0_mat, [17](#)