

# Package ‘simulatorZ’

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**Type** Package

**Title** Simulator for Collections of Independent Genomic Data Sets

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**Description** simulatorZ is a package intended primarily to simulate collections of independent genomic data sets, as well as performing training and validation with predicting algorithms. It supports ExpressionSet and RangedSummarizedExperiment objects.

**License** Artistic-2.0

**Depends** R (>= 3.5), Biobase, SummarizedExperiment, survival, CoxBoost, BiocGenerics

**Imports** graphics, stats, gbm, Hmisc, GenomicRanges, methods

**Suggests** RUnit, BiocStyle, curatedOvarianData, parathyroidSE, superpc

**URL** <https://github.com/zhangyuqing/simulatorZ>

**BugReports** <https://github.com/zhangyuqing/simulatorZ>

**biocViews** Survival

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cvSubsets	<i>cvSubsets</i>
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### Description

To generate a list of subsets(indices of observations) from one set

### Usage

```
cvSubsets(obj, fold)
```

### Arguments

obj	a ExpressionSet, matrix or RangedSummarizedExperiment object. If it is a matrix, columns represent samples
fold	the number of folds in cross validation. Number of observations in the set does not need to be a multiple of fold

### Value

returns the list of indices of subsets

### Author(s)

Yuqing Zhang, Christoph Bernau, Levi Waldron

### Examples

```
library(curatedOvarianData)

data(E.MTAB.386_eset)

id <- cvSubsets(E.MTAB.386_eset, 3)

subsets <- lapply(1:3, function(i){E.MTAB.386_eset[1:10, id[[i]]]})

sapply(subsets, dim)
```

```

rm(subsets)

## Number of observations in the set does not need to be a multiple of

## the fold parameter

id2 <- cvSubsets(E.MTAB.386_eset, 5)

subsets <- lapply(1:5, function(j){E.MTAB.386_eset[1:10, id2[[j]]]})

sapply(subsets, dim)

rm(subsets)

```

---

funCV

*funCV*


---

### Description

Cross validation function

### Usage

```

funCV(obj, fold, y.var, trainFun = masomenos, funCvSubset = cvSubsets,

      covar = NULL)

```

### Arguments

obj	a ExpressionSet, matrix or RangedSummarizedExperiment object. If it is a matrix, columns represent samples
fold	the number of folds in cross validation
y.var	response variable, matrix, data.frame(with 2 columns) or Surv object
trainFun	training function, which takes gene expression matrix X and response variable y as input, the coefficients as output
funCvSubset	function to divide one Expression Set into subsets for cross validation
covar	other covariates to be added in as predictors

**Value**

returns the c statistics of cross validation(CV)

**Author(s)**

Yuqing Zhang, Christoph Bernau, Levi Waldron

**Examples**

```
library(curatedOvarianData)
```

```
library(GenomicRanges)
```

```
set.seed(8)
```

```
data( E.MTAB.386_eset )
```

```
eset <- E.MTAB.386_eset[1:100, 1:30]
```

```
rm(E.MTAB.386_eset)
```

```
time <- eset$days_to_death
```

```
cens.chr <- eset$vital_status
```

```
cens <- rep(0, length(cens.chr))
```

```
cens[cens.chr=="living"] <- 1
```

```
y <- Surv(time, cens)
```

```
y1 <- cbind(time, cens)
```

```
nrows <- 200; ncols <- 6
```

```
counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)

rowRanges <- GRanges(rep(c("chr1", "chr2"), c(50, 150)),

                     IRanges(floor(runif(200, 1e5, 1e6)), width=100),

                     strand=sample(c("+", "-"), 200, TRUE))

colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),

                    row.names=LETTERS[1:6])

sset <- SummarizedExperiment(assays=SimpleList(counts=counts),

                             rowRanges=rowRanges, colData=colData)

time <- c(1588,1929,1813,1542,1830,1775)

cens <- c(1,0,1,1,1,1)

y.vars <- Surv(time, cens)

funCV(eset, 3, y)

funCV(exprs(eset), 3, y1)

funCV(sset, 3, y.vars)

## any training function will do as long as it takes the gene expression matrix X

## and response variable y(matrix, data.frame or Surv object) as parameters, and

## return the coefficients as its value
```

geneFilter

*geneFilter*

---

**Description**

the function to filter genes by Intergrative Correlation

**Usage**

```
geneFilter(obj, cor.cutoff = 0.5)
```

**Arguments**

obj	a list of ExpressionSet, matrix or RangedSummarizedExperiment objects. If its elements are matrices, columns represent samples, rows represent genes
cor.cutoff	the cutoff threshold for filtering genes. Only when the integrative correlation between every pair of sets is larger than the cutoff value, will the gene be selected.

**Value**

returns a list of ExpressionSets matrix or RangedSummarizedExperiment objects with genes filtered

**Author(s)**

Yuqing Zhang, Christoph Bernau, Levi Waldron

**References**

Garrett-Mayer, E., Parmigiani, G., Zhong, X., Cope, L., Gabrielson, E., Cross-study validation and combined analysis of gene expression microarray data. *Biostatistics*. 2008 Apr;9(2):333-354.

**Examples**

```
set.seed(8)
```

```
library(curatedOvarianData)
```

```
library(GenomicRanges)
```

```
data(GSE17260_eset)
```

```
data(E.MTAB.386_eset)
```

```
data(GSE14764_eset)

## to save time, we take a small subset from each dataset

esets.list <- list(GSE17260=GSE17260_eset[1:50, 1:10],

                  E.MTAB.386=E.MTAB.386_eset[1:50, 1:10],

                  GSE14764=GSE14764_eset[1:50, 1:10])

rm(E.MTAB.386_eset, GSE14764_eset, GSE17260_eset)

result.set <- geneFilter(esets.list, 0.1)

dim(result.set[[1]])

## as we cannot calculate correlation with one set, this function just

## delivers the same set if esets has length 1

result.oneset <- geneFilter(esets.list[1])

dim(result.oneset[[1]])

## Support matrices

X.list <- lapply(esets.list, function(eset){

  return(exprs(eset)) ## Columns represent samples!
```

```
})

result.set <- geneFilter(X.list, 0.1)

dim(result.set[[1]])

## Support RangedSummarizedExperiment

nrows <- 200; ncols <- 6

counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)

rowRanges <- GRanges(rep(c("chr1", "chr2"), c(50, 150)),

                      IRanges(floor(runif(200, 1e5, 1e6)), width=100),

                      strand=sample(c("+", "-"), 200, TRUE))

colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),

                    row.names=LETTERS[1:6])

sset <- SummarizedExperiment(assays=SimpleList(counts=counts),

                             rowRanges=rowRanges, colData=colData)

s.list <- list(sset, sset)

result.set <- geneFilter(s.list, 0.9)

## the same set should resemble each other, no genes filtered

dim(assay(result.set[[1]]))
```



---

getTrueModel	<i>getTrueModel</i>
--------------	---------------------

---

### Description

The parametric bootstrap simulation depends on the true model of original sets.  
This function is to generate useful values from the true models for further analysis.  
We fit CoxBoost to the original sets and use the coefficients to simulate the survival and censoring time. grid, survH, censH, which are useful for this purpose.  
grid=grid corresponding to hazard estimations censH and survH  
survH=cumulative hazard for survival times distribution  
censH=cumulative hazard for censoring times distribution

### Usage

```
getTrueModel(esets, y.vars, parstep, balance.variables = NULL)
```

### Arguments

esets	a list of ExpressionSets, matrix or SummarizedExperiment
y.vars	a list of response variables
parstep	CoxBoost parameter
balance.variables	variable names to be balanced.

### Value

returns a list of values:  
beta: True coefficients obtained by fitting CoxBoost to the original ExpressionSets  
grid: timeline grid corresponding to hazard estimations censH and survH  
survH: cumulative hazard for survival times distribution  
censH: cumulative hazard for censoring times distribution  
lp: true linear predictors

### Author(s)

Yuqing Zhang, Christoph Bernau, Levi Waldron

### Examples

```
library(curatedOvarianData)

data(GSE14764_eset)
```

```
data(E.MTAB.386_eset)

esets.list <- list(GSE14764=GSE14764_eset[1:500, 1:20],
                  E.MTAB.386=E.MTAB.386_eset[1:500, 1:20])

rm(E.MTAB.386_eset, GSE14764_eset)

## simulate on multiple ExpressionSets

set.seed(8)

y.list <- lapply(esets.list, function(eset){

  time <- eset$days_to_death

  cens.chr <- eset$vital_status

  cens <- rep(0, length(cens.chr))

  cens[cens.chr=="living"] <- 1

  return(Surv(time, cens))

})

res1 <- getTrueModel(esets.list, y.list, 100)

## Get true model from one set

res2 <- getTrueModel(esets.list[1], y.list[1], 100)
```

```
names(res2)

res2$lp

## note that y.list[1] cannot be replaced by y.list[[1]]
```

---

masomenos

*masomenos*

---

## Description

function for Mas-o-menos algorithm

## Usage

```
masomenos(X, y, option = "fast", ...)
```

## Arguments

X	matrix with rows corresponding to subjects and columns to features resp
y	response variable, a data.frame, matrix, or Surv object: c(time, event)
option	whether to use C or R code to fit the marginal Cox models
...	

## Value

return the coefficients

## Author(s)

Yuqing Zhang, Christoph Bernau, Levi Waldron

## References

Zhao, S., Huttenhower, G. P. C., and Waldron, L. (2013). Mas-o-menos: a simple sign averaging method for discrimination in genomic data analysis. <http://biostats.bepress.com/harvardbiostat/paper158/>. Accessed: 2013-10-24.

## Examples

```
set.seed(8)

library(curatedOvarianData)
```

```
data( E.MTAB.386_eset )

eset <- E.MTAB.386_eset[1:100, 1:30]

rm(E.MTAB.386_eset)

X <- t(exprs(eset))

time <- eset$days_to_death

cens <- sample(0:1, 30, replace=TRUE)

y <- Surv(time, cens)

beta <- masomenos(X=X, y=y)

beta
```

---

plusMinus

*plusMinus*

---

### **Description**

function for plusMinus algorithm

### **Usage**

```
plusMinus(X, y, lambda = NULL, tuningpar = "nfeatures", standardize = FALSE,
```

```
directionality = "posneg", ties.method = "average", votingthresholdquantile = 0.5,
```

```
modeltype = "plusminus")
```

**Arguments**

<code>X</code>	gene expression matrix
<code>y</code>	response variables
<code>lambda</code>	lambda
<code>tuningpar</code>	tuning parameter
<code>standardize</code>	standardize or not
<code>directionality</code>	directionality
<code>ties.method</code>	ties.method
<code>votingthresholdquantile</code>	votingthresholdquantile
<code>modeltype</code>	modeltype

**Value**

returns regression coefficients

**Author(s)**

Yuqing Zhang, Christoph Bernau, Levi Waldron

**Examples**

```
set.seed(8)

library(curatedOvarianData)

data( E.MTAB.386_eset )

eset <- E.MTAB.386_eset[1:100, 1:30]

rm(E.MTAB.386_eset)

X <- t(exprs(eset))

time <- eset$days_to_death

cens <- sample(0:1, 30, replace=TRUE)
```

```
y <- Surv(time, cens)
```

```
beta <- plusMinus(X, y)
```

```
beta
```

---

rowCoxTests

*rowCoxTests*


---

### Description

method for performing Cox regression

### Usage

```
rowCoxTests(X, y, option = c("fast", "slow"), ...)
```

### Arguments

X	Gene expression data. The following formats are available: matrix Rows correspond to observations, columns to variables. data.frame Rows correspond to observations, columns to variables. ExpressionSet rowCoxTests will extract the expressions using exprs().
y	Survival Response, an object of class: Surv if X is of type data.frame or matrix character if X is of type ExpressionSet. In this case y is the name of the survival response in the phenoData of X. If survival time and indicator are stored separately in the phenoData one can specify a two-element character vector the first element representing the survival time variable.
option	"fast" loops over rows in C, "slow" calls coxph directly in R. The latter method may be used if something goes wrong with the "fast" method.
...	currently unused

### Value

dataframe with two columns: coef = Cox regression coefficients, p.value = Wald Test p-values. Rows correspond to the rows of X.

**Author(s)**

Yuqing Zhang, Christoph Bernau, Levi Waldron

**Examples**

```
#test

##regressor-matrix (gene expressions)

X<-matrix(rnorm(1e6),nrow=10000)

#seed

set.seed(123)

#times

time<-rnorm(n=ncol(X),mean=100)

#censoring(1->death)

status<-rbinom(n=ncol(X),size=1, prob=0.8)

##survival object

y<-Surv(time,status)

## Do 10,000 Cox regressions:

system.time(output <- rowCoxTests(X=X,y=y, option="fast"))
```

---

 simBootstrap

*simBootstrap*


---

### Description

the driver function to perform three-step bootstrap resampling  
to get independent genomic data sets

### Usage

```
simBootstrap(obj, y.vars, n.samples, parstep, type = "two-steps",
            balance.variables = NULL, funSimData = simData, funTrueModel = getTrueModel,
            funSurvTime = simTime)
```

### Arguments

obj	a list of ExpressionSet, matrix or RangedSummarizedExperiment
y.vars	a list of reponse variables, elements can be class Surv, matrix or data.frame
n.samples	number of samples to resample in each set
parstep	step number to fit CoxBoost
type	whether to include resampling set labels
balance.variables	covariate names to balance in the simulated sets
funSimData	function to perform non-parametric bootstrap
funTrueModel	function to construct true models in original sets
funSurvTime	function to perform parametric bootstrap

### Value

a list of values including:

obj.list = a list of simulated objects the same type as input

indices.list = a list of indices indicating which sample the simulated sample is in the original set

setsID = a vector to indicate the original ID of simulated sets, if type=="original", setsID should be 1,2,3,...

lp.list = a list of true linear predictor of each original data sets

beta.list = a list of true coefficients used for simulating observations

survH.list = list of cumulative survival hazard

censH.list = list of cumulative censoring hazard

grid.list = list of timeline grid corresponding to survH and censH respectively



**Author(s)**

Yuqing Zhang, Christoph Bernau, Levi Waldron

**Examples**

```
library(curatedOvarianData)

library(GenomicRanges)

data(E.MTAB.386_eset)

data(GSE14764_eset)

esets.list <- list(E.MTAB.386=E.MTAB.386_eset[1:200, 1:20], GSE14764=GSE14764_eset[1:200, 1:20])

rm(E.MTAB.386_eset, GSE14764_eset)

## simulate on multiple ExpressionSets

set.seed(8)

y.list <- lapply(esets.list, function(eset){

  time <- eset$days_to_death

  cens.chr <- eset$vital_status

  cens <- rep(0, length(cens.chr))

  cens[cens.chr=="living"] <- 1

  return(Surv(time, cens))

})
```



```

s.list <- list(sset[,1:5], sset[,6:10])

time <- c(540, 527, 668, 587, 620, 540, 527, 668, 587, 620)

cens <- c(1, 0, 0, 1, 0, 1, 0, 0, 1, 0)

y.vars <- Surv(time, cens)

y.vars <- list(y.vars[1:5,],y.vars[1:5,])

simmodels <- simBootstrap(obj=s.list, y.vars=y.vars, 20, 100)

```

---

simData

*simData*


---

### Description

simData is a function to perform non-parametric bootstrap resampling on a list of (original) data sets, both on set level and patient level, in order to simulate independent genomic sets.

### Usage

```

simData(obj, n.samples, y.vars = list(), type = "two-steps",

        balance.variables = NULL)

```

### Arguments

obj	a list of ExpressionSets, matrices or RangedSummarizedExperiments. If elements are matrices, columns represent samples
n.samples	an integer indicating how many samples should be resampled from each set
y.vars	a list of response variables, can be Surv object, or matrix or data.frame with two columns
type	string "one-step" or "two-steps". If type="one-step", the function will skip resampling the datasets, and directly resample from the original list of obj

**balance.variables**

balance.variables will be a vector of covariate names that should be balanced in the simulation. After balancing, the prevalence of covariate in each result set should be the same as the overall distribution across all original data sets. Default is set as NULL, when it will not balance over any covariate. if isn't NULL, esets parameter should only be of class ExpressionSet

**Value**

returns a list of simulated ExpressionSets, with names indicating its original set, and indices of the original patients.

prob.desired and prob.real are only useful when balance.variables is set.

prob.desired shows overall distribution of the specified covariate. prob.list

shows the sampling probability in each set after balancing

**Author(s)**

Yuqing Zhang, Christoph Bernau, Levi Waldron

**Examples**

```
library(curatedOvarianData)
```

```
library(GenomicRanges)
```

```
data(E.MTAB.386_eset)
```

```
data(GSE14764_eset)
```

```
esets.list <- list(E.MTAB.386=E.MTAB.386_eset[1:100, 1:10], GSE14764=GSE14764_eset[1:100, 1:10])
```

```
rm(E.MTAB.386_eset, GSE14764_eset)
```

```
## simulate on multiple ExpressionSets
```

```
set.seed(8)
```

```
# one-step bootstrap: skip resampling set labels

simmodels <- simData(esets.list, 20, type="one-step")

# two-step-non-parametric bootstrap

simmodels <- simData(esets.list, 10, type="two-steps")

## simulate one set

simmodels <- simData(list(esets.list[[1]]), 10, type="two-steps")

## balancing covariates

# single covariate

simmodels <- simData(list(esets.list[[1]]), 5, balance.variables="tumorstage")

# multiple covariates

simmodels <- simData(list(esets.list[[1]]), 5,

                    balance.variables=c("tumorstage", "age_at_initial_pathologic_diagnosis"))

## Support matrices

X.list <- lapply(esets.list, function(eset){

  return(exprs(eset))
```

```

})

simmodels <- simData(X.list, 20, type="two-steps")

## Support RangedSummarizedExperiment

nrows <- 200; ncols <- 6

counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)

rowRanges <- GRanges(rep(c("chr1", "chr2"), c(50, 150)),

                      IRanges(floor(runif(200, 1e5, 1e6)), width=100),

                      strand=sample(c("+", "-"), 200, TRUE))

colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),

                    row.names=LETTERS[1:6])

sset <- SummarizedExperiment(assays=SimpleList(counts=counts),

                             rowRanges=rowRanges, colData=colData)

s.list <- list(sset[,1:3], sset[,4:6])

simmodels <- simData(s.list, 20, type="two-steps")

```

---

simTime

*simTime*

---

### Description

simTime is a function to perform the parametric-bootstrap step, where we use the true coefficients and cumulative hazard to simulate survival and censoring.

**Usage**

```
simTime(simmodels, original.yvars, result)
```

**Arguments**

**simmodels** a list in the form of the return value of `simData()` which consists of three lists:  
**obj**: a list of `ExpressionSets`, matrices or `RangedSummarizedExperiments`  
**setsID**: a list of set labels indicating which original set the simulated one is from  
**indices**: a list of patient labels to tell which patient in the original set is drawn

**original.yvars** response variable in the order of original sets(without sampling)

**result** a list in the form of return of `getTrueModel()` which consists of five lists:  
**Beta**: a list of coefficients obtained by  
**grid**: timeline grid corresponding to hazard estimations `censH` and `survH`  
**survH**: cumulative hazard for survival times distribution  
**censH**: cumulative hazard for censoring times distribution  
**lp**: true linear predictors

**Value**

survival time is saved in `phenodata`, here the function still returns the `ExpressionSets`

**Author(s)**

Yuqing Zhang, Christoph Bernau, Levi Waldron

**Examples**

```
library(curatedOvarianData)

data(E.MTAB.386_eset)

data(GSE14764_eset)

esets.list <- list(E.MTAB.386=E.MTAB.386_eset[1:100, 1:20], GSE14764=GSE14764_eset[1:100, 1:20])

rm(E.MTAB.386_eset, GSE14764_eset)

## simulate on multiple ExpressionSets

set.seed(8)
```

```
y.list <- lapply(esets.list, function(eset){

  time <- eset$days_to_death

  cens.chr <- eset$vital_status

  cens <- rep(0, length(cens.chr))

  cens[cens.chr=="living"] <- 1

  return(Surv(time, cens))

})

# To perform both parametric and non-parametric bootstrap, you can call simBootstrap()

# or, you can divide the steps into:

res <- getTrueModel(esets.list, y.list, 100)

simmodels <- simData(obj=esets.list, y.vars=y.list, n.samples=10)

# Then, use this function

simmodels <- simTime(simmodels=simmodels, original.yvars=y.list, result=res)

# it also supports performing only the parametric bootstrap step on a list of expressionsets

# but you need to construct the parameter by scratch
```



```

res <- getTrueModel(esets.list, y.list, 100)

setsID <- seq_along(esets.list)

indices <- list()

for(i in setsID){

  indices[[i]] <- seq_along(sampleNames(esets.list[[i]]))

}

simmodels <- list(obj=esets.list, y.vars=y.list, indices=indices, setsID=setsID)

new.simmodels <- simTime(simmodels=simmodels, original.yvars=y.list, result=res)

```

---

zmatrix

*zmatrix*


---

### Description

generate a matrix of c statistics

### Usage

```

zmatrix(obj, y.vars, fold, trainingFun = masomenos, cvFun = funCV,

        cvSubsetFun = cvSubsets, covar = NULL)

```

### Arguments

obj	a list of ExpressionSet, matrix or RangedSummarizedExperiment objects. If its elements are matrices, columns represent samples
y.vars	a list of response variables, all the response variables should be matrix, data.frame(with 2 columns) or Surv object
fold	cvFun parameter, in this case passes to funCV()
trainingFun	training function

cvFun	function to perform cross study within one set
cvSubsetFun	function to divide the expression sets into subsets for cross validation
covar	other covariates to be added as predictors

**Value**

outputs one matrix of validation statistics

**Author(s)**

Yuqing Zhang, Christoph Bernau, Levi Waldron

**Examples**

```
library(curatedOvarianData)

library(GenomicRanges)

data(E.MTAB.386_eset)

data(GSE14764_eset)

esets.list <- list(E.MTAB.386=E.MTAB.386_eset[1:100, 1:30], GSE14764=GSE14764_eset[1:100, 1:30])

rm(E.MTAB.386_eset, GSE14764_eset)

## simulate on multiple ExpressionSets

set.seed(8)

y.list <- lapply(esets.list, function(eset){

  time <- eset$days_to_death

  cens.chr <- eset$vital_status

  cens <- rep(0, length(cens.chr))
```

```
cens[cens.chr=="living"] <- 1

return(Surv(time, cens))

})

# generate on original ExpressionSets

z <- zmatrix(esets.list, y.list, 3)

# generate on simulated ExpressionSets

simmodels <- simBootstrap(esets.list, y.list, 100, 100)

z <- zmatrix(simmodels$obj.list, simmodels$y.vars.list, 3)

# support matrix

X.list <- lapply(esets.list, function(eset){

  return(exprs(eset)) ### columns represent samples !!

})

z <- zmatrix(X.list, y.list, 3)

# support RangedSummarizedExperiment

nrows <- 200; ncols <- 6
```

```
counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)

rowRanges <- GRanges(rep(c("chr1", "chr2"), c(50, 150)),

                     IRanges(floor(runif(200, 1e5, 1e6)), width=100),

                     strand=sample(c("+", "-"), 200, TRUE))

colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),

                    row.names=LETTERS[1:6])

sset <- SummarizedExperiment(assays=SimpleList(counts=counts),

                             rowRanges=rowRanges, colData=colData)

time <- sample(4500:4700, 6, replace=TRUE)

cens <- sample(0:1, 6, replace=TRUE)

y.vars <- Surv(time, cens)

z <- zmatrix(list(sset[,1:3], sset[,4:6]), list(y.vars[1:3,],y.vars[4:6,]), 3)
```

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