

Package ‘BayesSUR’

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Type Package

Title Bayesian Seemingly Unrelated Regression

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Description Bayesian seemingly unrelated regression with general variable selection and dense/sparse covariance matrix. The sparse seemingly unrelated regression is described in Banterle et al. (2018) <doi:10.1101/467019>.

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BayesSUR	<i>main function of the package</i>
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Description

Main function of the package. Fits a range of models introduced in the package vignette BayesSUR.pdf. Returns an object of S3 class BayesSUR. There are three options for the prior on the residual covariance matrix (i.e., independent inverse-Gamma, inverse-Wishart and hyper-inverse Wishart) and three options for the prior on the latent indicator variable (i.e., independent Bernoulli, hotspot and Markov random field). So there are nine models in total. See details for their combinations.

Usage

```
BayesSUR(
  Y,
  X,
  X_0 = NULL,
  data = NULL,
```

```

outFilePath = "",
nIter = 10000,
burnin = 5000,
nChains = 2,
covariancePrior = "HIW",
gammaPrior = "",
betaPrior = "independent",
gammaSampler = "bandit",
gammaInit = "R",
mrfG = NULL,
standardize = TRUE,
standardize.response = TRUE,
maxThreads = 1,
output_gamma = TRUE,
output_beta = TRUE,
output_G = TRUE,
output_sigmaRho = TRUE,
output_pi = TRUE,
output_tail = TRUE,
output_model_size = TRUE,
output_model_visit = FALSE,
output_CPO = FALSE,
output_Y = TRUE,
output_X = TRUE,
hyperpar = list(),
tmpFolder = "tmp/"
)

```

Arguments

Y, X, X_0	vectors of indexes (with respect to the data matrix) for the outcomes, the covariates to select and the fixed covariates respectively if data is either a path to a file or a matrix; if the 'data' argument is not provided, these needs to be matrices containing the data instead.
data	a data frame if using formula. If not using formula, it is either a matrix/dataframe or the path to (a plain text) data file with variables on the columns and observations on the rows
outFilePath	path to where the output files are to be written. The default path is the current working directory.
nIter	number of iterations for the MCMC procedure.
burnin	number of iterations (or fraction of iterations) to discard at the start of the chain. Default is 0.
nChains	number of parallel chains to run.
covariancePrior	string indicating the prior for the covariance Σ ; it has to be either "HIW" for the hyper-inverse-Wishart (which will result in a sparse covariance matrix), "IW" for the inverse-Wishart prior (dense covariance) or "IG" for independent

	inverse-Gamma on all the diagonal elements and 0 otherwise. See the details for the model specification
gammaPrior	string indicating the gamma prior to use, either "hotspot" for the Hotspot prior of Bottolo (2011), "MRF" for the Markov Random Field prior or "hierarchical" for a simpler hierarchical prior. See the details for the model specification
betaPrior	string indicating the beta prior to use, either "independent" for the independent spike-and-slab prior or "reGroup" for the random effects for χ_0 and independent spike-and-slab priors for other predictors
gammaSampler	string indicating the type of sampler for gamma, either "bandit" for the Thompson sampling inspired sampler or "MC3" for the usual MC^3 sampler
gammaInit	gamma initialisation to either all-zeros ("0"), all ones ("1"), MLE-informed ("MLE") or (default) randomly ("R").
mrfg	either a matrix or a path to the file containing the G matrix for the MRF prior on gamma (if necessary)
standardize	logical flag for X variable standardization. Default is standardize=TRUE. The coefficients are returned on the standardized scale.
standardize.response	Standardization for the response variables. Default is standardize.response=TRUE.
maxThreads	maximum threads used for parallelization. Default is 1.
output_gamma	allow (TRUE) or suppress (FALSE) the output for gamma. See the return value below for more information.
output_beta	allow (TRUE) or suppress (FALSE) the output for beta. See the return value below for more information.
output_G	allow (TRUE) or suppress (FALSE) the output for G. See the return value below for more information.
output_sigmaRho	allow (TRUE) or suppress (FALSE) the output for sigmaRho. See the return value below for more information.
output_pi	allow (TRUE) or suppress (FALSE) the output for pi. See the return value below for more information.
output_tail	allow (TRUE) or suppress (FALSE) the output for tail (hotspot tail probability). See the return value below for more information.
output_model_size	allow (TRUE) or suppress (FALSE) the output for model_size. See the return value below for more information.
output_model_visit	allow (TRUE) or suppress (FALSE) the output for all visited models over the MCMC iterations. Default is FALSE. See the return value below for more information.
output_CPO	allow (TRUE) or suppress (FALSE) the output for *; possible outputs are gamma, G, beta, sigmaRho, pi, tail (hotspot tail probability), model_size, CPO. See the return value below for more information.
output_Y	allow (TRUE) or suppress (FALSE) the output for responses dataset Y.
output_X	allow (TRUE) or suppress (FALSE) the output for predictors dataset X.

hyperpar	a list of named hyperparameters to use instead of the default values. Valid names are mrf_d, mrf_e, a_sigma, b_sigma, a_tau, b_tau, nu, a_eta, b_eta, a_o, b_o, a_pi, b_pi, a_w and b_w. Their default values are a_w=2, b_w=5, a_omega=2, b_omega=1, a_o=2, b_o=p-2, a_pi=2, b_pi=1, nu=s+2, a_tau=0.1, b_tau=10, a_eta=0.1, b_eta=1, a_sigma=1, b_sigma=1, mrf_d=-3 and mrf_e=0.03. See the vignette for more information.
tmpFolder	the path to a temporary folder where intermediate data files are stored (will be erased at the end of the chain) default to local tmpFolder

Details

The arguments covariancePrior and gammaPrior specify the model HRR, dSUR or SSUR with different gamma prior. Let γ_{jk} be latent indicator variable of each coefficient and C be covariance matrix of response variables. The nine models specified through the arguments covariancePrior and gammaPrior are as follows.

	$\gamma_{jk} \sim \text{Bernoulli}$	$\gamma_{jk} \sim \text{hotspot}$	$\gamma_{jk} \sim \text{MRF}$
$C \sim \text{indep}$	HRR-B	HRR-H	HRR-M
$C \sim \text{IW}$	dSUR-B	dSUR-H	dSUR-M
$C \sim \text{HIW}$	SSUR-B	SSUR-H	SSUR-M

Value

An object of class "BayesSUR":

- status - the running status
- input - a list of all input parameters by the user
- output - a list of the all output filenames:
 - `"*_logP_out.txt"` - contains each row for the 1000t-th iteration's log-likelihoods of parameters, i.e., Tau, Eta, JunctionTree, SigmaRho, O, Pi, Gamma, W, Beta and data conditional log-likelihood depending on the models.
 - `"*_gamma_out.txt"` - posterior mean of the latent indicator matrix.
 - `"*_pi_out.txt"` - posterior mean of the predictor effects (propensity) by decomposing the probability of the latent indicator.
 - `"*_hotspot_tail_p_out.txt"` - posterior mean of the hotspot tail probability. Only available for the hotspot prior on the gamma.
 - `"*_beta_out.txt"` - posterior mean of the coefficients matrix.
 - `"*_G_out.txt"` - posterior mean of the response graph. Only available for the HIW prior on the covariance.
 - `"*_sigmaRho_out.txt"` - posterior mean of the transformed parameters. Not available for the IG prior on the covariance.
 - `"*_model_size_out.txt"` - contains each row for the 1000t-th iteration's model sizes of the multiple response variables.
 - `"*_model_visit_g_out.txt"` - contains each row for the nonzero indices of the vectorized estimated graph matrix for each iteration.
 - `"*_model_visit_gamma_out.txt"` - contains each row for the nonzero indices of the vectorized estimated gamma matrix for each iteration.

- "*_CPO_out.txt" - the (scaled) conditional predictive ordinates (CPO).
 - "*_CPOsumy_out.txt" - the (scaled) conditional predictive ordinates (CPO) with joint posterior predictive of the response variables.
 - "*_WAIC_out.txt" - the widely applicable information criterion (WAIC).
 - "*_Y.txt" - responses dataset.
 - "*_X.txt" - predictors dataset.
 - "*_X0.txt" - fixed predictors dataset.
- call - the matched call.

References

Banterle M, Bottolo L, Richardson S, Ala-Korpela M, Jarvelin MR, Lewin A (2018). *Sparse variable and covariance selection for high-dimensional seemingly unrelated Bayesian regression*. bioRxiv: 467019.

Banterle M#, Zhao Z#, Bottolo L, Richardson S, Lewin A, Zucknick M (2019). *BayesSUR: An R package for high-dimensional multivariate Bayesian variable and covariance selection in linear regression*. URL: <https://cran.r-project.org/web/packages/BayesSUR/vignettes/BayesSUR.pdf>

Examples

```
data("example_eQTL", package = "BayesSUR")
hyperpar <- list( a_w = 2 , b_w = 5 )
set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/", output_CPO=TRUE)

## check output
# show the summary information
summary(fit)

# show the estimated beta, gamma and graph of responses Gy
## Not run:
estimators <- get.estimated(fit, estimator=c("beta", "gamma", "Gy"))
plot(estimators)

#Set up temporary work directory for saving a pdf figure
td <- tempdir()
oldwd <- getwd()
setwd(td)

# Produce authentic math formulas in the graph
plot(estimators, fig.tex = TRUE)
system(paste(getOption("pdfviewer"), "ParamEstimator.pdf"))
setwd(oldwd)

## End(Not run)
```

BayesSUR_internal	<i>BayesSUR_internal</i>
-------------------	--------------------------

Description

Run a SUR Bayesian sampler – internal function

Arguments

dataFile	path to data file
outFilePath	path to where the output is to be written
nIter	number of iterations
nChains	number of parallel chains to run

NOTE THAT THIS IS BASICALLY JUST A WRAPPER

coef.BayesSUR	<i>extract the posterior mean of the coefficients of a "BayesSUR" class object</i>
---------------	--

Description

Extract the posterior mean of the coefficients of a "BayesSUR" class object

Usage

```
## S3 method for class 'BayesSUR'
coef(object, Pmax = 0, ...)
```

Arguments

object	an object of class "BayesSUR"
Pmax	threshold that truncates the estimated coefficients based on thresholding the estimated latent indicator variable. Default is 0.
...	other arguments

Value

Estimated coefficients are from an object of class "BayesSUR". If the BayesSUR specified data standardization, the fitted values are base based on standardized data.

Examples

```
data("example_eQTL", package = "BayesSUR")
hyperpar <- list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/" )

## check prediction
beta.hat <- coef(fit)
```

elpd	<i>measure the prediction accuracy by the expected log pointwise predictive density</i>
------	---

Description

Measure the prediction accuracy by the elpd (expected log pointwise predictive density). The out-of-sample predictive fit can either be estimated by Bayesian leave-one-out cross-validation (LOO) or by widely applicable information criterion (WAIC) (Vehtari et al. 2017).

Usage

```
elpd(object, method = "LOO")
```

Arguments

object	an object of class "BayesSUR"
method	the name of the prediction accuracy index. Default is the "LOO" (Bayesian LOO estimate of out-of-sample predictive fit). The other index is the "WAIC" (widely applicable information criterion). For the HRR models, both "LOO" and "WAIC" are computed based on the multivariate t-distribution of the posterior predictive rather than approximation of importance sampling.

Value

Return the prediction accuracy measure from an object of class "BayesSUR". It is `elpd.loo` if the argument `method="LOO"` and `elpd.WAIC` if `method="WAIC"`.

References

Vehtari, A., Gelman, A., Gabry, J. (2017). *Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC*. *Statistics and Computing*, 27(5): 1413–1432.

Examples

```

data("example_eQTL", package = "BayesSUR")
hyperpar = list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/", output_CPO=TRUE)

## check output
# print the prediction accuracy elpd (expected log pointwise predictive density)
# by the Bayesian LOO estimate of out-of-sample predictive fit
elpd(fit, method="LOO")

```

example_eQTL	<i>Simulated data set to mimic a small expression quantitative trait loci (eQTL) example</i>
--------------	--

Description

Simulated data set to mimic a small expression quantitative trait loci (eQTL) example, with p=150 single nucleotide polymorphisms (SNPs) as explanatory variables, s=10 gene expression features as response variables and data for n=100 observations. Loading the data will load the associated blockList object needed to fit the model with BayesSUR(). The R code for generating the simulated data is given in the Examples paragraph.

```
#importFrom BDgraph rgwish #importFrom gRbase mcsMAT #importFrom scime simulateSNPs
```

Usage

```
example_eQTL
```

Format

An object of class list of length 4.

Examples

```

# Load the eQTL sample dataset
data("example_eQTL", package = "BayesSUR")
str(example_eQTL)

## Not run:
#=====
# The code below is to show how to generate the dataset "example_eQTL.rda" above
#=====

```

```

requireNamespace("BDgraph", quietly = TRUE)
requireNamespace("gRbase", quietly = TRUE)
requireNamespace("scrim", quietly = TRUE)

##### Problem Dimensions
n = 100
p = 150
s = 10

##### Select a set of n x p (SNPs) covariates

## The synthetic data in the paper use a subset of the real SNPs as covariates,
# but as the NFBC66 dataset is confidential we'll use scrim to sample similar data

x = scrim::simulateSNPs(c(n,10), p, c(3, 2),prop.explain = c(0.9, 0.95))$data[1:n,]
x = cbind(rep(1,n),x)

#####

graph_pattern = 2 # in 2,3,4

snr = 25 # in 5,15,25

corr_param = 0.9 # in 0.3 , 0.6 , 0.9

### Create the underlying graph
if(graph_pattern==1){
  ### 1) Random but full
  G = matrix(1,s,s)
  Prime = list(c(1:s))
  Res = Prime
  Sep = list()
}else if(graph_pattern==2){

  ### 2) Block Diagonal structure
  Prime = list(c(1:floor(s*2/3)),
              c((floor(s*2/3)+1):(ceiling(s*4/5)-1)),
              c(ceiling(s*4/5):s))

  Res = Prime
  Sep = lapply(Res,function(x) which(x==99))

  G = matrix(0,s,s)
  for(i in Prime){
    G[i,i] = 1
  }
}else if(graph_pattern==3){

  ### 3) Decomposable model
  Prime = list(c(1:floor(s*5/12),ceiling(s*9/10):s),

```

```

        c(floor(s*2/9):(ceiling(s*2/3)-1)),
        c(ceiling(s*2/3):(ceiling(s*4/5)-1)),
        c(ceiling(s*4/5):s))

Sep = list(); H=list()
for( i in 2:length(Prime)){
  H = union(H,Prime[[i-1]])
  Sep[[i-1]] = intersect( H,Prime[[i]])
}

Res = list()
Res[[1]] = Prime[[1]]
for( i in 2:length(Prime)){
  Res[[i]] = setdiff( Prime[[i]],Sep[[i-1]])
}

G = matrix(0,s,s)
for(i in Prime)
  G[i,i] = 1

## decomp check
dimnames(G) = list(1:s,1:s)
length( gRbase::mcsMAT(G - diag(s)) ) > 0
}else if(graph_pattern==4){

### 4) Non-decomposable model
nblocks = 5
nElemPerBlock =c(floor(s/4),floor(s/2)-1-floor(s/4),
                  ceiling(s*2/3)-1-floor(s/2),7)
nElemPerBlock = c(nElemPerBlock , s-sum(nElemPerBlock))
res = 1:s; blockIdx = list()
for(i in 1:nblocks){
  # blockIdx[[i]] = sample(res,nElemPerBlock[i])
  blockIdx[[i]] = res[1:nElemPerBlock[i]]
  res = setdiff(res,blockIdx[[i]])
}

G = matrix(0,s,s)
## add diagonal
for(i in 1:nblocks)
  G[blockIdx[[i]],blockIdx[[i]]] = 1
## add cycle
G[blockIdx[[1]],blockIdx[[2]]] = 1 ; G[blockIdx[[2]],blockIdx[[1]]] = 1
G[blockIdx[[1]],blockIdx[[5]]] = 1 ; G[blockIdx[[5]],blockIdx[[1]]] = 1
G[blockIdx[[2]],blockIdx[[3]]] = 1 ; G[blockIdx[[3]],blockIdx[[2]]] = 1
G[blockIdx[[3]],blockIdx[[5]]] = 1 ; G[blockIdx[[5]],blockIdx[[3]]] = 1

## decomp check
dimnames(G) = list(1:s,1:s)
length( gRbase::mcsMAT(G -diag(s)) ) > 0

# Prime = blockIdx

```

```

Res = blockIdx ## this is not correct but not used in the non-decomp case
}

### Gamma Pattern
gamma = matrix(0,p+1,s)
gamma[1,] = 1

### 2) Extra Patterns

## outcomes (correlated in the decomp model) have some predictors in common
gamma[6:10,6:9] = 1

## outcomes (correlated in the decomp model) have some predictors in common
#gamma[16:20,14:15] = 1

## outcomes (sort-of correlated [pair-wise] in the decomp model)
# have predictors in common 6:15
gamma[26:30,4:8] = 1

## outcomes (NOT correlated in the decomp model) have predictors in common 16:17
gamma[36:40,c(3:5,9:10)] = 1

## these predictors are associated with ALL the outcomes
gamma[46:50,] = 1

combn11 = combn(rep((6:9-1)*p,each=length(6:10-1)) + rep(6:10-1,times=length(6:9)), 2)
combn31 = combn(rep((4:8-1)*p,each=length(26:30-1)) + rep(26:30-1,times=length(4:8)), 2)
combn32 = combn(rep((4:8-1)*p,each=length(46:50-1)) + rep(46:50-1,times=length(4:8)), 2)
combn41 = combn(rep((3:5-1)*p,each=length(36:40-1)) + rep(36:40-1,times=length(3:5)), 2)
combn42 = combn(rep((3:5-1)*p,each=length(46:50-1)) + rep(46:50-1,times=length(3:5)), 2)
combn51 = combn(rep((9:10-1)*p,each=length(36:40-1)) + rep(36:40-1,times=length(9:10)), 2)
combn52 = combn(rep((9:10-1)*p,each=length(46:50-1)) + rep(46:50-1,times=length(9:10)), 2)

Gmrf = rbind(t(combn11), t(combn31), t(combn32), t(combn41), t(combn42), t(combn51), t(combn52))

## get for every correlated bunch in the decomposable model,

if(graph_pattern<4){
  # a different set of predictors
  for(i in 1:length(Prime))
    gamma[6:10 + (i+6) * 10, Prime[[i]]] = 1 ## for each Prime component

  ## for every Residual instead
  for(i in 1:length(Res))
    gamma[6:10 + (i+10) * 10, Res[[i]]] = 1
}else{

  for(i in 1:length(Prime))
    gamma[6:10 + (i+4) * 10, Prime[[i]]] = 1 ## for each Prime component

```

```

## for every Residual instead
for(i in 1:length(Res))
  gamma[6:10 + (i+9) * 10, Res[[i]]] = 1
}

#### Sample the betas
sd_b = 1
b = matrix(rnorm((p+1)*s,0,sd_b),p+1,s)

xb = matrix(NA,n,s)

for(i in 1:s){
  if(sum(gamma[,i])>1){
    xb[,i] = x[,gamma[,i]==1] %*% b[gamma[,i]==1,i]
  }else{
    xb[,i] = rep(1,n) * b[1,i]
  }
}

##Sample the variance
v_r = mean(diag(var(xb))) / snr

nu = s+1

M = matrix(corr_param,s,s)
diag(M) = rep(1,s)

P = BDgraph::rgwish(n=1,adj=G,b=3,D=v_r*M)

var = solve(P)

factor = 10 ; factor_min = 0.01; factor_max = 1000
count = 0 ; maxit = 10000

factor_prev = 1

repeat{

  var = var / factor * factor_prev

  ### Sample the errors and the Ys
  cVar = chol(as.matrix(var))
  #err = matrix(rnorm(n*s),n,s) %*% cVar
  err = matrix(rnorm(n*s,sd=0.5),n,s) %*% cVar
  y = xb+err

## Reparametrisation ( assuming PEO is 1:s )
  cVar = t(cVar) # make it lower-tri
  S = diag(diag(cVar))
  sigma = S*S
  L = cVar %*% solve(S)
  rho = diag(s) - solve(L)
}

```

```

### S/N Ratio
emp_snr = mean( diag( var(xb) %** solve(sigma) ))
emp_g_snr = mean( diag( var( (err)%**t(rho) ) %** solve(sigma) ))

#####

if( abs(emp_snr - snr) < (snr/10) | count > maxit ){
  break
}else{
  if( emp_snr < snr ){ # increase factor
    factor_min = factor
  }else{ # decrease factor
    factor_max = factor
  }
  factor_prev = factor
  factor = (factor_min + factor_max)/2
}
count = count+1
}

#####
colnames(y) <- paste("GEX",1:ncol(y),sep="")
colnames(G) <- colnames(y); Gy <- G
gamma <- gamma[-1,]
mrfG <- Gmrf[!duplicated(Gmrf),]
data = cbind(y,x[,-1]) # leave out the intercept because is coded inside already

example_eQTL = list(data=data, blockList=list(1:s,s+1:p))

## Write data file to the user's directory by save()

## End(Not run)

```

example_GDSC

Preprocessed data set to mimic a small pharmacogenetic example

Description

Preprocessed data set to mimic a small pharmacogenetic example from the Genomics of Drug Sensitivity in Cancer (GDSC) database, with $p=850$ gene features as explanatory variables, $s=7$ drugs sensitivity data as response variables and data for $n=498$ cell lines. Gene features include $p_1=343$ gene expression features (GEX), $p_2=426$ by copy number variations (CNV) and $p_3=68$ mutated genes (MUT). Loading the data will load the associated `blockList` (and `mrfG`) objects needed to fit the model with `BayesSUR()`. The R code for generating the simulated data is given in the Examples paragraph.

```
#importFrom plyr mapvalues #importFrom data.table like
```

Usage

```
example_GDSC
```

Format

An object of class list of length 3.

Examples

```
# Load the GDSC sample dataset
data("example_GDSC", package = "BayesSUR")
str(example_GDSC)

## Not run:
#=====
# This code below is to do preprocessing of GDSC data and obtain the complete dataset
# "example_GDSC.rda" above. The user needs load the datasets from
# ftp://ftp.sanger.ac.uk/pub4/cancerrxgene/releases/release-5.0/.
# But downloading and transforming the three used datasets below to *.csv files first.
#=====

requireNamespace("plyr", quietly = TRUE)
requireNamespace("data.table", quietly = TRUE)

features <- data.frame(read.csv("/gdsc_en_input_w5.csv", head=T))
names.fea <- strsplit(rownames(features), "")
features <- t(features)
p <- c(13321, 13747-13321, 13818-13747)
Cell.Line <- rownames(features)
features <- data.frame(Cell.Line, features)

ic50_00 <- data.frame(read.csv("gdsc_drug_sensitivity_fitted_data_w5.csv", head=T))
ic50_0 <- ic50_00[,c(1,4,7)]
drug.id <- data.frame(read.csv("gdsc_tissue_output_w5.csv", head=T))[,c(1,3)]
drug.id2 <- drug.id[!duplicated(drug.id$drug.id),]
# delete drug.id=1066 since ID1066 and ID156 both correspond drug AZD6482,
# and no ID1066 in the "suppl.Data1" by Garnett et al. (2012)
drug.id2 <- drug.id2[drug.id2$drug.id!=1066,]
drug.id2$drug.name <- as.character(drug.id2$drug.name)
drug.id2$drug.name <- substr(drug.id2$drug.name, 1, nchar(drug.id2$drug.name)-6)
drug.id2$drug.name <- gsub(" ", "-", drug.id2$drug.name)

ic50 <- ic50_0
# mapping the drug_id to drug names in drug sensitivity data set
ic50$drug_id <- plyr::mapvalues(ic50$drug_id, from = drug.id2[,2], to = drug.id2[,1])
colnames(ic50) <- c("Cell.Line", "compound", "IC50")

# transform drug sensitivity overall cell lines to a data matrix
y0 <- reshape(ic50, v.names="IC50", timevar="compound", idvar="Cell.Line", direction="wide")
y0$Cell.Line <- gsub("-", ".", y0$Cell.Line)
```

```

#####
# select nonmissing pharmacological data
#####
y00 <- y0
m0 <- dim(y0)[2]-1
eps <- 0.05
# r1.na is better to be not smaller than r2.na
r1.na <- 0.3
r2.na <- 0.2
k <- 1
while(sum(is.na(y0[,2:(1+m0)]))>0){
  r1.na <- r1.na - eps/k
  r2.na <- r1.na - eps/k
  k <- k + 1
  ## select drugs with <30% (decreasing with k) missing data overall cell lines
  na.y <- apply(y0[,2:(1+m0)], 2, function(xx) sum(is.na(xx))/length(xx))
  while(sum(na.y<r1.na)<m0){
    y0 <- y0[,-c(1+which(na.y>=r1.na))]
    m0 <- sum(na.y<r1.na)
    na.y <- apply(y0[,2:(1+m0)], 2, function(xx) sum(is.na(xx))/length(xx))
  }

  ## select cell lines with treatment of at least 80% (increasing with k) drugs
  na.y0 <- apply(y0[,2:(1+m0)], 1, function(xx) sum(is.na(xx))/length(xx))
  while(sum(na.y0<r2.na)<(dim(y0)[1])){
    y0 <- y0[na.y0<r2.na,]
    na.y0 <- apply(y0[,2:(1+m0)], 1, function(xx) sum(is.na(xx))/length(xx))
  }
  num.na <- sum(is.na(y0[,2:(1+m0)]))
  message("#{NA}=", num.na, "\n", "r1.na =", r1.na, ", r2.na =", r2.na, "\n")
}

#####
# combine drug sensitivity, tissues and molecular features
#####
yx <- merge(y0, features, by="Cell.Line")
names.cell.line <- yx$Cell.Line
names.drug <- colnames(yx)[2:(dim(y0)[2])]
names.drug <- substr(names.drug, 6, nchar(names.drug))
# numbers of gene expression features, copy number features and mutation features
p <- c(13321, 13747-13321, 13818-13747)
num.nonpen <- 13
yx <- data.matrix(yx[,-1])
y <- yx[,1:(dim(y0)[2]-1)]
x <- cbind(yx[,dim(y0)[2]-1+sum(p)+1:num.nonpen], yx[,dim(y0)[2]-1+1:sum(p)])

# delete genes with only one mutated cell line
x <- x[,-c(num.nonpen+p[1]+p[2]+which(colSums(x[,num.nonpen+p[1]+p[2]+1:p[3]])<=1))]
p[3] <- ncol(x) - num.nonpen - p[1] - p[2]

GDSC <- list(y=y, x=x, p=p, num.nonpen=num.nonpen, names.cell.line=names.cell.line,
            names.drug=names.drug)

```



```

#####
#####
## select a small set of drugs
#####
#####

name_drugs <- c("Methotrexate","RDEA119","PD-0325901","CI-1040","AZD6244","Nilotinib",
               "Axitinib")

# extract the drugs' pharmacological profiling and tissue dummy
YX0 <- cbind(GDSC$y[,colnames(GDSC$y) %in% paste("IC50.",name_drugs,sep="")]
            [,c(1,3,6,4,7,2,5)], GDSC$x[,1:GDSC$num.nonpen])
colnames(YX0) <- c(name_drugs, colnames(GDSC$x)[1:GDSC$num.nonpen])
# extract the genetic information of CNV & MUT
X23 <- GDSC$x[, GDSC$num.nonpen+GDSC$p[1]+1:(p[2]+p[3])]
colnames(X23)[1:p[2]] <- paste(substr(colnames(X23)[1:p[2]], 1,
                                   nchar(colnames(X23)[1:p[2]] )-3), ".CNV", sep="")

# locate all genes with CNV or MUT information
name_genes_duplicate <- c( substr(colnames(X23)[1:p[2]], 1, nchar(colnames(X23)[1:p[2]]-4),
                             substr(colnames(X23)[p[2]+1:p[3]], 1, nchar(colnames(X23)[p[2]+1:p[3]]-4) )
name_genes <- name_genes_duplicate[!duplicated(name_genes_duplicate)]

# select the GEX which have the common genes with CNV or MUT
X1 <- GDSC$x[,GDSC$num.nonpen+which(colnames(GDSC$x)[GDSC$num.nonpen+1:p[1]] %in% name_genes)]

p[1] <- ncol(X1)
X1 <- log(X1)

# summary the data information
example_GDSC <- list( data=cbind( YX0, X1, X23 ) )
example_GDSC$blockList <- list(1:length(name_drugs), length(name_drugs)+1:GDSC$num.nonpen,
                               ncol(YX0)+1:sum(p))

#####
# construct the G matrix: edge potentials in the MRF prior
#####

# edges between drugs: Group1 ("RDEA119","17-AAG","PD-0325901","CI-1040" and "AZD6244")
# indexed as (2:5)
# http://software.broadinstitute.org/gsea/msigdb/cards/KEGG_MAPK_SIGNALING_PATHWAY
pathway_genes <- read.table("MAPK_pathway.txt")[[1]]
Idx_Pathway1 <- which(c(colnames(X1),name_genes_duplicate) %in% pathway_genes)
Gmrf_Group1Pathway1 <- t(combn(rep(Idx_Pathway1,each=length(2:5)) +
                              rep((2:5-1)*sum(p),times=length(Idx_Pathway1)), 2))

# edges between drugs: Group2 ("Nilotinib","Axitinib") indexed as (6:7)
# delete gene ABL2
Idx_Pathway2 <- which( c(colnames(X1),name_genes_duplicate) %like% "BCR" |
                      c(colnames(X1),name_genes_duplicate) %like% "ABL" )[-c(3,5)]
Gmrf_Group2Pathway2 <- t(combn(rep(Idx_Pathway2,each=length(6:7)) +
                              rep((6:7-1)*sum(p),times=length(Idx_Pathway2)), 2))

```

```

# edges between the common gene in different data sources
Gmrf_CommonGene <- NULL
list_CommonGene <- list(0)
k <- 1
for(i in 1:length(name_genes)){
  Idx_CommonGene <- which( c(colnames(X1),name_genes_duplicate) == name_genes[i] )
  if(length(Idx_CommonGene) > 1){
    Gmrf_CommonGene <- rbind(Gmrf_CommonGene,t(combn(rep(Idx_CommonGene,each=length(name_drugs))
      + rep((1:length(name_drugs)-1)*sum(p),times=length(Idx_CommonGene)), 2)))
    k <- k+1
  }
}
Gmrf_duplicate <- rbind( Gmrf_Group1Pathway1, Gmrf_Group2Pathway2, Gmrf_CommonGene )
Gmrf <- Gmrf_duplicate[!duplicated(Gmrf_duplicate),]
example_GDSC$mrfG <- Gmrf

# create the target gene names of the two groups of drugs
targetGenes1 <- matrix(Idx_Pathway1,nrow=1)
colnames(targetGenes1) <- colnames(example_GDSC$data)[seq_along(targetGene$group1)]
targetGenes2 <- matrix(Idx_Pathway2,nrow=1)
colnames(targetGenes2) <- colnames(example_GDSC$data)[seq_along(targetGene$group2)]

targetGene <- list(group1=targetGenes1, group2=targetGenes2)

## Write data file example_GDSC.rda to the user's directory by save()

## End(Not run)

```

fitted.BayesSUR

fitted response values corresponds to the posterior mean estimates

Description

Return the fitted response values that correspond to the posterior mean estimates from a "BayesSUR" class object.

Usage

```

## S3 method for class 'BayesSUR'
fitted(object, Pmax = 0, ...)

```

Arguments

object	an object of class "BayesSUR"
Pmax	threshold that truncates the estimated coefficients based on thresholding the estimated latent indicator variable. Default is 0.
...	other arguments

Value

Fitted values extracted from an object of class "BayesSUR". If the BayesSUR specified data standardization, the fitted values are base based on standardized data.

Examples

```
data("example_eQTL", package = "BayesSUR")
hyperpar <- list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/" )

## check fitted values
fitted.val <- fitted(fit)
```

<code>get.estimate</code>	<i>extract the posterior mean of the parameters</i>
---------------------------	---

Description

Extract the posterior mean of the parameters of a "BayesSUR" class object.

Usage

```
get.estimate(object, estimator = "gamma", Pmax = 0)
```

Arguments

<code>object</code>	an object of class "BayesSUR"
<code>estimator</code>	the name of one estimator. Default is the latent indicator estimator "gamma". Other options "beta", "Gy", "CPO" and "logP" correspond the posterior means of coefficient matrix, response graph and conditional predictive ordinate (CPO) respectively
<code>Pmax</code>	threshold that truncate the estimator. Default is 0. If the estimator is beta, then beta is truncated based on the latent indicator matrix shresholding at Pmax

Value

Return the one estimator from an object of class "BayesSUR". It is the posterior mean of the latent indicator variable if `estimator="gamma"`, posterior mean of the regression coefficients if `estimator="beta"`, posterior mean of the response graph if `estimator="Gy"` and the CPO if `estimator="CPO"`,

Examples

```

data("example_eQTL", package = "BayesSUR")
hyperpar <- list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/" )

## check output
# extract the posterior mean of the coefficients matrix
beta_hat <- get.estimate(fit, estimator="beta")

```

plot.BayesSUR

create a selection of plots for a "BayesSUR" class object

Description

Convenience function to create a selection of plots for a "BayesSUR" class object. They are plots of estimators, response graph, network, manhattan and MCMC diagnosis indexed by numbers 1:5.

Usage

```

## S3 method for class 'BayesSUR'
plot(x, which = c(1L:4L), ...)

```

Arguments

x	an object of class "BayesSUR".
which	if a subset of the plots is required, specify a subset of the numbers 1:5 which are plots of estimators, response graph, network, manhattan and MCMC diagnosis, respectively. Default is c(1L:4L) Only c(1, 4, 5) is valid for the HRR models.
...	other arguments

Examples

```

data("example_eQTL", package = "BayesSUR")
hyperpar = list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 0, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/" )

```

```
## check output
# Show the interactive plots. Note that it needs at least 2000*(nbloc+1) iterations
# for the diagnosis plots where nbloc=3 by default

plot(fit)
```

plot.CPO

plot the conditional predictive ordinate

Description

Plot the conditional predictive ordinate (CPO) for each individual of a fitted model generated by BayesSUR which is a "BayesSUR" object. CPO is a handy posterior predictive check because it may be used to identify outliers, influential observations, and for hypothesis testing across different non-nested models (Gelfand 1996).

Usage

```
## S3 method for class 'CPO'
plot(
  x,
  outlier.mark = TRUE,
  outlier.thresh = 0.01,
  scale.CPO = TRUE,
  x.loc = FALSE,
  axis.label = NULL,
  las = 0,
  cex.axis = 1,
  mark.pos = c(0, -0.01),
  mark.color = 2,
  mark.cex = 0.8,
  xlab = "Observations",
  ylab = NULL,
  ...
)
```

Arguments

x	an object of class <code>get.estimate</code> with <code>estimator="CPO"</code>
<code>outlier.mark</code>	mark the outliers with the response names. The default is <code>FALSE</code>
<code>outlier.thresh</code>	threshold for the CPOs. The default is <code>0.01</code> .
<code>scale.CPO</code>	scaled CPOs which is divided by their maximum. The default is <code>TRUE</code>
<code>x.loc</code>	a vector of features distance

axis.label	a vector of predictor names which are shown in CPO plot. The default is NULL only showing the indices. The value "auto" show the predictor names from the original data.
las	graphical parameter of plot.default
cex.axis	graphical parameter of plot.default
mark.pos	the location of the marked text relative to the point
mark.color	the color of the marked text. The default color is red.
mark.cex	the fontsize of the marked text. The default fontsize is 0.8.
xlab	a title for the x axis
ylab	a title for the y axis
...	other arguments

Details

The default threshold for the CPOs to detect the outliers is 0.01 by Congdon (2005). It can be tuned by the argument `outlier.thresh`.

References

- Statisticat, LLC (2013). *Bayesian Inference*. Farmington, CT: Statisticat, LLC.
- Gelfand A. (1996). *Model Determination Using Sampling Based Methods*. In Gilks W., Richardson S., Spiegelhalter D. (eds.), *Markov Chain Monte Carlo in Practice*, pp. 145–161. Chapman & Hall, Boca Raton, FL.
- Congdon P. (2005). *Bayesian Models for Categorical Data*. John Wiley & Sons, West Sussex, England.

Examples

```
data("example_eQTL", package = "BayesSUR")
hyperpar <- list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/", output_CPO=TRUE)

## check output
# plot the conditional predictive ordinate (CPO)
CPO <- get.estimate(fit, estimator="CPO")
plot(CPO)
```

plot.estimator *plot the posterior mean estimators*

Description

Plot the posterior mean estimators from a "BayesSUR" class object, including the coefficients beta, latent indicator variable gamma and graph of responses.

Usage

```
## S3 method for class 'estimator'
plot(
  x,
  estimator = NULL,
  colorScale.gamma = grey((100:0)/100),
  colorScale.beta = c("blue", "white", "red"),
  legend.cex.axis = 1,
  name.responses = NA,
  name.predictors = NA,
  xlab = "",
  ylab = "",
  fig.tex = FALSE,
  output = "ParamEstimator",
  header = "",
  header.cex = 2,
  tick = FALSE,
  mgp = c(2.5, 1, 0),
  title.beta = paste("Estimator", "$\\hat{\\mathbf{B}}$"),
  title.gamma = paste("Estimator", "$\\hat{\\mathbf{\\Gamma}}$"),
  title.Gy = paste("Estimator", "$\\hat{\\mathcal{G}}$"),
  cex.main = 1.5,
  ...
)
```

Arguments

x	an object of class <code>get.estimator</code> with <code>estimator=c("beta", "gamma", "Gy")</code>
estimator	print the heatmap of estimators. The value "beta" is for the estimated coefficients matrix, "gamma" for the latent indicator matrix and "Gy" for the graph of responses
colorScale.gamma	value palette for gamma
colorScale.beta	a vector of three colors for diverging color schemes
legend.cex.axis	magnification of axis annotation relative to cex

`name.responses` a vector of the response names. The default is "NA" only to show the locations. The value "auto" show the response names from the original data.
`name.predictors` a vector of the predictor names. The default is "NA" only to show the locations. The value "auto" show the predictor names from the original data.
`xlab` a title for the x axis
`ylab` a title for the y axis
`fig.tex` print the figure through LaTeX. Default is "FALSE"
`output` the file name of printed figure
`header` the main title
`header.cex` size of the main title for all estimators
`tick` a logical value specifying whether tickmarks and an axis line should be drawn. Default is "FALSE"
`mgp` the margin line (in mex units) for the axis title, axis labels and axis line
`title.beta` a title for the printed "beta" if `fig.tex=TRUE`
`title.gamma` a title for the printed "gamma" if `fig.tex=TRUE`
`title.Gy` a title for the printed "Gy" if `fig.tex=TRUE`
`cex.main` size of the title for each estimator
`...` other arguments

Examples

```

data("example_eQTL", package = "BayesSUR")
hyperpar <- list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/" )

## check output
# Plot the estimators from the fitted object
## Not run:
estimators <- get.estimator(fit, estimator = c("beta", "gamma", "Gy"))
plot(estimators)

#Set up temporary work directory for saving a pdf figure
td <- tempdir()
oldwd <- getwd()
setwd(td)

# Produce authentic math formulas in the graph
plot(estimators, fig.tex = TRUE)
system(paste(getOption("pdfviewer"), "ParamEstimator.pdf"))
  
```



```
setwd(oldwd)

## End(Not run)
```

plot.Manhattan	<i>plot Manhattan-like plots for marginal posterior inclusion probabilities (mPIP) and numbers of responses of association for predictors</i>
----------------	---

Description

Plot Manhattan-like plots for marginal posterior inclusion probabilities (mPIP) and numbers of responses of association for predictors of a "BayesSUR" class object.

Usage

```
## S3 method for class 'Manhattan'
plot(
  x,
  which = c(1, 2),
  x.loc = FALSE,
  axis.label = "auto",
  mark.responses = NULL,
  xlab1 = "Predictors",
  ylab1 = "mPIP",
  xlab2 = "Predictors",
  ylab2 = "No. of responses",
  threshold = 0.5,
  las = 0,
  cex.axis = 1,
  mark.pos = c(0, 0),
  mark.color = 2,
  mark.cex = 0.8,
  header = "",
  ...
)
```

Arguments

x	an object of class <code>get.estimator</code> with <code>estimator="gamma"</code>
which	if it's value "1" showing the Manhattan-like plot of the marginal posterior inclusion probabilities (mPIP). If it's value "2" showing the Manhattan-like plot of the number of responses. The default is to show both figures.
x.loc	a vector of features distance
axis.label	a vector of predictor names which are shown in the Manhattan-like plot. The value "NULL" only showing the indices. The default "auto" show the predictor names from the original data.

mark.responses	a vector of response names which are shown in the Manhattan-like plot for the mPIP
xlab1	a title for the x axis of Manhattan-like plot for the mPIP
ylab1	a title for the y axis of Manhattan-like plot for the mPIP
xlab2	a title for the x axis of Manhattan-like plot for the numbers of responses
ylab2	a title for the y axis of Manhattan-like plot for the numbers of responses
threshold	threshold for showing number of response variables significantly associated with each feature
las	graphical parameter of plot.default
cex.axis	graphical parameter of plot.default
mark.pos	the location of the marked text relative to the point
mark.color	the color of the marked text. The default color is red.
mark.cex	the fontsize of the marked text. The default fontsize is 0.8.
header	the main title
...	other arguments

Examples

```
data("example_eQTL", package = "BayesSUR")
hyperpar <- list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/" )

## check output
# show the Manhattan-like plots
gamma <- get.estimator(fit, estimator="gamma")
plot(gamma)
```

plot.MCMCdiag *show trace plots and diagnostic density plots*

Description

Show trace plots and diagnostic density plots of a fitted model object of class "BayesSUR".

Usage

```
## S3 method for class 'MCMCdiag'
plot(x, nbloc = 3, HIWg = NULL, header = "", ...)
```

Arguments

x	an object of class <code>get.estimate</code> with <code>estimator="logP"</code>
nbloc	number of splits for the last half iterations after subtracting burn-in length
HIWg	diagnostic plot of the response graph. Default is NULL. <code>HIW="degree"</code> prints the diagnostic of the degrees of response nodes. <code>HIW="edges"</code> prints the diagnostic of every edge between two responses. <code>HIW="lik"</code> prints the diagnostic of the posterior likelihoods of the hyperparameters related to the response relationships
header	the main title
...	other arguments for the plots of the log-likelihood and model size

Examples

```
data("example_eQTL", package = "BayesSUR")
hyperpar <- list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/" )

## check output
MCMCdiag <- get.estimate(fit, estimator = "logP")
plot(MCMCdiag)
```

plot.network	<i>plot the network representation of the associations between responses and predictors</i>
--------------	---

Description

Plot the network representation of the associations between responses and predictors, based on the estimated gamma matrix and graph of responses from a "BayesSUR" class object.

Usage

```
## S3 method for class 'network'
plot(
  x,
  includeResponse = NULL,
  excludeResponse = NULL,
  includePredictor = NULL,
  excludePredictor = NULL,
  MatrixGamma = NULL,
```

```

PmaxPredictor = 0.5,
PmaxResponse = 0.5,
nodesizePredictor = 2,
nodesizeResponse = 15,
no.isolates = FALSE,
lineup = 1.2,
gray.alpha = 0.6,
edgewith.response = 5,
edgewith.predictor = 2,
edge.weight = FALSE,
label.predictor = NULL,
label.response = NULL,
color.predictor = NULL,
color.response = NULL,
name.predictors = NULL,
name.responses = NULL,
vertex.frame.color = NA,
layoutInCircle = FALSE,
header = "",
...
)

```

Arguments

x	an object of class <code>get.estimator</code> with <code>estimator=c("gamma", "Gy")</code>
includeResponse	A vector of the response names which are shown in the network
excludeResponse	A vector of the response names which are not shown in the network
includePredictor	A vector of the predictor names which are shown in the network
excludePredictor	A vector of the predictor names which are not shown in the network
MatrixGamma	A matrix or dataframe of the latent indicator variable. Default is NULL and to extrate it from object of class inheriting from an object of class "BayesSUR"
PmaxPredictor	cutpoint for thresholding the estimated latent indicator variable. Default is 0.5
PmaxResponse	cutpoint for thresholding the learning structure matrix of multiple response variables. Default is 0.5
nodesizePredictor	node size of Predictors in the output graph. Default is 15
nodesizeResponse	node size of response variables in the output graph. Default is 25
no.isolates	remove isolated nodes from responses graph and Full graph, may get problem if there are also isolated Predictors
lineup	A ratio of the heights between responses' area and Predictors'
gray.alpha	the opacity. The default is 0.6

```

edgewidth.response
    the edge width between response nodes
edgewidth.predictor
    the edge width between the predictor and response node
edge.weight    draw weighted edges after thresholding at 0.5. The default value FALSE is not to
                draw weighed edges
label.predictor
    A vector of the names of predictors
label.response A vector of the names of response variables
color.predictor
    color of the predictor nodes
color.response color of the reponse nodes
name.predictors
    a subtitle for the predictors
name.responses a subtitle for the responses
vertex.frame.color
    The color of the frame of the vertices. If you don't want vertices to have a frame,
    supply NA as the color name
layoutInCircle place vertices on a circle, in the order of their vertex ids. The default is FALSE
header         the main title
...           other arguments

```

Examples

```

data("example_eQTL", package = "BayesSUR")
hyperpar <- list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/" )

## check output
# show the Network representation of the associations between responses and features
network <- get.estimate(fit, estimator = c("gamma", "Gy"))
plot(network)

```

plot.response.graph *plot the estimated graph for multiple response variables*

Description

Plot the estimated graph for multiple response variables from a "BayesSUR" class object.

Usage

```
## S3 method for class 'response.graph'
plot(
  x,
  PmaxResponse = 0.5,
  PtrueResponse = NULL,
  name.responses = NA,
  edge.weight = FALSE,
  label.color = "black",
  node.size = 30,
  node.color = "dodgerblue",
  ...
)
```

Arguments

x	an object of class <code>get.estimator</code> with <code>estimator="Gy"</code>
PmaxResponse	cutpoint for thresholding the learning structure matrix of multiple response variables. Default is 0.5
PtrueResponse	true adjacency matrix for the structure of multiple response variables
name.responses	A vector for the node names. The default is "NA" only to show the locations. Value "auto" show the response names from the original data.
edge.weight	draw weighted edges after thresholding at 0.5. The default value "FALSE" is not to draw weighted edges
label.color	label color. Default is "black"
node.size	node size. Default is 30
node.color	node color. Default is "dodgerblue"
...	other arguments

Examples

```
data("example_eQTL", package = "BayesSUR")
hyperpar <- list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
```

```

data = example_eQTL[["data"]], outFilePath = tempdir(),
nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
hyperpar = hyperpar, tmpFolder = "tmp/" )

## check output
# show the graph relationship between responses
Gy <- get.estimate(fit, estimator = "Gy")
plot(Gy)

```

predict.BayesSUR	<i>predict responses corresponding to the posterior mean of the coefficients, return posterior mean of coefficients or indices of nonzero coefficients</i>
------------------	--

Description

Predict responses corresponding to the posterior mean of the coefficients, return posterior mean of coefficients or indices of nonzero coefficients of a "BayesSUR" class object.

Usage

```

## S3 method for class 'BayesSUR'
predict(
  object,
  newx,
  type = c("response", "coefficients", "nonzero"),
  Pmax = 0,
  ...
)

```

Arguments

object	an object of class "BayesSUR"
newx	Matrix of new values for x at which predictions are to be made. Must be a matrix
type	Type of prediction required. Type "response" gives the fitted responses. Type "coefficients" computes the coefficients truncated the estimated coefficients based on thresholding the estimated latent indicator variable at Pmax. Type "nonzero" returns a list of the indices of the nonzero coefficients corresponding to the estimated latent indicator variable thresholding at Pmax
Pmax	threshold that truncates the estimated coefficients based on thresholding the estimated latent indicator variable. Default is 0.
...	other arguments

Value

Predicted values extracted from an object of class "BayesSUR". If the BayesSUR specified data standardization, the fitted values are base based on standardized data.

Examples

```

data("example_eQTL", package = "BayesSUR")
hyperpar <- list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/" )

## check prediction
predict.val <- predict(fit, newx=example_eQTL[["blockList"]][[2]])

```

print.BayesSUR	<i>print a short summary of the Bayesian Seemingly Unrelated Regressions Fits</i>
----------------	---

Description

Print a short summary of a "BayesSUR" class object. It includes the argument matching information, number of selected predictors based on thresholding the posterior mean of the latent indicator variable at 0.5 by default.

Usage

```

## S3 method for class 'BayesSUR'
print(x, Pmax = 0.5, ...)

```

Arguments

x	an object of class "BayesSUR"
Pmax	threshold that truncates the estimated coefficients based on thresholding the estimated latent indicator variable. Default is 0.5
...	other arguments

Value

Return a short summary from an object of class "BayesSUR", including the number of selected predictors with $mPIP > Pmax$ and the expected log pointwise predictive density estimates (i.e., $elpd.LOO$ and $elpd.WAIC$).

Examples

```

data("example_eQTL", package = "BayesSUR")
hyperpar = list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/", output_CPO=TRUE)

## check output
# show the print information
print(fit)

```

summary.BayesSUR

summarizing Bayesian Seemingly Unrelated Regressions Fits

Description

Summary method for class "BayesSUR". It includes the argument matching information, Top predictors/responses on average mPIP across all responses/predictors, elpd estimates, MCMC specification, model specification and hyper-parameters. The summarized number of the selected variable corresponds to the posterior mean of the latent indicator variable thresholding at 0.5 by default.

Usage

```

## S3 method for class 'BayesSUR'
summary(object, Pmax = 0.5, ...)

```

Arguments

object	an object of class "BayesSUR"
Pmax	threshold that truncates the estimated coefficients based on thresholding the estimated latent indicator variable. Default is 0.5
...	other arguments

Value

Return a result summary from an object of class "BayesSUR", including the CPOs, number of selected predictors with $mPIP > Pmax$, top 10 predictors on average mPIP across all responses, top 10 responses on average mPIP across all predictors, Expected log pointwise predictive density (elpd) estimates, MCMC specification, model specification (i.e., covariance prior and gamma prior) and hyper-parameters.

Examples

```

data(example_eQTL, package = "BayesSUR")
hyperpar = list( a_w = 2 , b_w = 5 )

set.seed(9173)
fit <- BayesSUR(Y = example_eQTL[["blockList"]][[1]],
               X = example_eQTL[["blockList"]][[2]],
               data = example_eQTL[["data"]], outFilePath = tempdir(),
               nIter = 100, burnin = 50, nChains = 2, gammaPrior = "hotspot",
               hyperpar = hyperpar, tmpFolder = "tmp/", output_CPO=TRUE)

## check output
# show the summary information
summary(fit)

```

targetGene

targetGene

Description

Indexes list of target genes corresponding the example_GDSC data set. It has two components representing the gene indexes of the MAPK/ERK pathway and BCR-ABL gene fusion in the example_GDSC data set.

#importFrom plyr mapvalues #importFrom data.table like

Usage

```
targetGene
```

Format

An object of class list of length 2.

Examples

```

# Load the indexes of gene targets from the GDSC sample dataset
data("targetGene", package = "BayesSUR")
str(targetGene)

## Not run:
#=====
# This code below is to do preprocessing of GDSC data and obtain the complete dataset
# "example_GDSC.rda" above. The user needs load the datasets from
# ftp://ftp.sanger.ac.uk/pub4/cancerrxgene/releases/release-5.0/.
# But downloading and transforming the three used datasets below to *.csv files first.
#=====

requireNamespace("plyr", quietly = TRUE)

```

```

requireNamespace("data.table", quietly = TRUE)

features <- data.frame(read.csv("/gdsc_en_input_w5.csv", head=T))
names.fea <- strsplit(rownames(features), ",")
features <- t(features)
p <- c(13321, 13747-13321, 13818-13747)
Cell.Line <- rownames(features)
features <- data.frame(Cell.Line, features)

ic50_00 <- data.frame(read.csv("gdsc_drug_sensitivity_fitted_data_w5.csv", head=T))
ic50_0 <- ic50_00[,c(1,4,7)]
drug.id <- data.frame(read.csv("gdsc_tissue_output_w5.csv", head=T))[,c(1,3)]
drug.id2 <- drug.id[!duplicated(drug.id$drug.id),]
# delete drug.id=1066 since ID1066 and ID156 both correspond drug AZD6482,
# and no ID1066 in the "suppl.Data1" by Garnett et al. (2012)
drug.id2 <- drug.id2[drug.id2$drug.id!=1066,]
drug.id2$drug.name <- as.character(drug.id2$drug.name)
drug.id2$drug.name <- substr(drug.id2$drug.name, 1, nchar(drug.id2$drug.name)-6)
drug.id2$drug.name <- gsub(" ", "-", drug.id2$drug.name)

ic50 <- ic50_0
# mapping the drug_id to drug names in drug sensitivity data set
ic50$drug_id <- plyr::mapvalues(ic50$drug_id, from = drug.id2[,2], to = drug.id2[,1])
colnames(ic50) <- c("Cell.Line", "compound", "IC50")

# transform drug sensitivity overall cell lines to a data matrix
y0 <- reshape(ic50, v.names="IC50", timevar="compound", idvar="Cell.Line", direction="wide")
y0$Cell.Line <- gsub("-", ".", y0$Cell.Line)

#####
# select nonmissing pharmacological data
#####
y00 <- y0
m0 <- dim(y0)[2]-1
eps <- 0.05
# r1.na is better to be not smaller than r2.na
r1.na <- 0.3
r2.na <- 0.2
k <- 1
while(sum(is.na(y0[,2:(1+m0)]))>0){
  r1.na <- r1.na - eps/k
  r2.na <- r1.na - eps/k
  k <- k + 1
  ## select drugs with <30% (decreasing with k) missing data overall cell lines
  na.y <- apply(y0[,2:(1+m0)], 2, function(xx) sum(is.na(xx))/length(xx))
  while(sum(na.y<r1.na)<m0){
    y0 <- y0[,-c(1+which(na.y>=r1.na))]
    m0 <- sum(na.y<r1.na)
    na.y <- apply(y0[,2:(1+m0)], 2, function(xx) sum(is.na(xx))/length(xx))
  }
}

## select cell lines with treatment of at least 80% (increasing with k) drugs

```

```

na.y0 <- apply(y0[,2:(1+m0)], 1, function(xx) sum(is.na(xx))/length(xx))
while(sum(na.y0<r2.na)<(dim(y0)[1])){
  y0 <- y0[na.y0<r2.na,]
  na.y0 <- apply(y0[,2:(1+m0)], 1, function(xx) sum(is.na(xx))/length(xx))
}
num.na <- sum(is.na(y0[,2:(1+m0)]))
message("#{NA}=", num.na, "\n", "r1.na =", r1.na, ", r2.na =", r2.na, "\n")
}

#####
# combine drug sensitivity, tissues and molecular features
#####
yx <- merge(y0, features, by="Cell.Line")
names.cell.line <- yx$Cell.Line
names.drug <- colnames(yx)[2:(dim(y0)[2])]
names.drug <- substr(names.drug, 6, nchar(names.drug))
# numbers of gene expression features, copy number features and mutation features
p <- c(13321, 13747-13321, 13818-13747)
num.nonpen <- 13
yx <- data.matrix(yx[,-1])
y <- yx[,1:(dim(y0)[2]-1)]
x <- cbind(yx[,dim(y0)[2]-1+sum(p)+1:num.nonpen], yx[,dim(y0)[2]-1+1:sum(p)])

# delete genes with only one mutated cell line
x <- x[,-c(num.nonpen+p[1]+p[2]+which(colSums(x[,num.nonpen+p[1]+p[2]+1:p[3]])<=1))]
p[3] <- ncol(x) - num.nonpen - p[1] - p[2]

GDSC <- list(y=y, x=x, p=p, num.nonpen=num.nonpen, names.cell.line=names.cell.line,
            names.drug=names.drug)

#####
#####
## select a small set of drugs
#####
#####

name_drugs <- c("Methotrexate","RDEA119","PD-0325901","CI-1040","AZD6244","Nilotinib",
               "Axitinib")

# extract the drugs' pharmacological profiling and tissue dummy
YX0 <- cbind(GDSC$y[,colnames(GDSC$y) %in% paste("IC50.",name_drugs,sep="")]
            [,c(1,3,6,4,7,2,5)], GDSC$x[,1:GDSC$num.nonpen])
colnames(YX0) <- c(name_drugs, colnames(GDSC$x)[1:GDSC$num.nonpen])
# extract the genetic information of CNV & MUT
X23 <- GDSC$x[, GDSC$num.nonpen+GDSC$p[1]+1:(p[2]+p[3])]
colnames(X23)[1:p[2]] <- paste(substr(colnames(X23)[1:p[2]], 1,
                                   nchar(colnames(X23)[1:p[2]])-3), ".CNV", sep="")

# locate all genes with CNV or MUT information
name_genes_duplicate <- c( substr(colnames(X23)[1:p[2]], 1, nchar(colnames(X23)[1:p[2]])-4),
                        substr(colnames(X23)[p[2]+1:p[3]], 1, nchar(colnames(X23)[p[2]+1:p[3]])-4) )
name_genes <- name_genes_duplicate[!duplicated(name_genes_duplicate)]

```

```

# select the GEX which have the common genes with CNV or MUT
X1 <- GDSC$x[,GDSC$num.nonpen+which(colnames(GDSC$x)[GDSC$num.nonpen+1:p[1]] %in% name_genes)]

p[1] <- ncol(X1)
X1 <- log(X1)

# summary the data information
example_GDSC <- list( data=cbind( YX0, X1, X23 ) )
example_GDSC$blockList <- list(1:length(name_drugs), length(name_drugs)+1:GDSC$num.nonpen,
                               ncol(YX0)+1:sum(p))

#=====
# construct the G matrix: edge potentials in the MRF prior
#=====

# edges between drugs: Group1 ("RDEA119","17-AAG","PD-0325901","CI-1040" and "AZD6244")
# indexed as (2:5)
# http://software.broadinstitute.org/gsea/msigdb/cards/KEGG_MAPK_SIGNALING_PATHWAY
pathway_genes <- read.table("MAPK_pathway.txt")[[1]]
Idx_Pathway1 <- which(c(colnames(X1),name_genes_duplicate) %in% pathway_genes)
Gmrf_Group1Pathway1 <- t(combn(rep(Idx_Pathway1,each=length(2:5)) +
                              rep((2:5-1)*sum(p),times=length(Idx_Pathway1)), 2))

# edges between drugs: Group2 ("Nilotinib","Axitinib") indexed as (6:7)
# delete gene ABL2
Idx_Pathway2 <- which( c(colnames(X1),name_genes_duplicate) %like% "BCR" |
                      c(colnames(X1),name_genes_duplicate) %like% "ABL" )[-c(3,5)]
Gmrf_Group2Pathway2 <- t(combn(rep(Idx_Pathway2,each=length(6:7)) +
                              rep((6:7-1)*sum(p),times=length(Idx_Pathway2)), 2))

# edges between the common gene in different data sources
Gmrf_CommonGene <- NULL
list_CommonGene <- list(0)
k <- 1
for(i in 1:length(name_genes)){
  Idx_CommonGene <- which( c(colnames(X1),name_genes_duplicate) == name_genes[i] )
  if(length(Idx_CommonGene) > 1){
    Gmrf_CommonGene <- rbind(Gmrf_CommonGene,t(combn(rep(Idx_CommonGene,each=length(name_drugs))
                                                    + rep((1:length(name_drugs)-1)*sum(p),times=length(Idx_CommonGene)), 2)))
    k <- k+1
  }
}
Gmrf_duplicate <- rbind( Gmrf_Group1Pathway1, Gmrf_Group2Pathway2, Gmrf_CommonGene )
Gmrf <- Gmrf_duplicate[!duplicated(Gmrf_duplicate),]
example_GDSC$mrfG <- Gmrf

# create the target gene names of the two groups of drugs
targetGenes1 <- matrix(Idx_Pathway1,nrow=1)
colnames(targetGenes1) <- colnames(example_GDSC$data)[seq_along(targetGene$group1)]
targetGenes2 <- matrix(Idx_Pathway2,nrow=1)
colnames(targetGenes2) <- colnames(example_GDSC$data)[seq_along(targetGene$group2)]

```

```
targetGene <- list(group1=targetGenes1, group2=targetGenes2)
## Write data file targetGene.rda to the user's directory by save()

## End(Not run)
```

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