

Package ‘graper’

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Type Package

Title Adaptive penalization in high-dimensional regression and classification with external covariates using variational Bayes

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License GPL (>= 2)

Description This package enables regression and classification on high-dimensional data with different relative strengths of penalization for different feature groups, such as different assays or omic types. The optimal relative strengths are chosen adaptively. Optimisation is performed using a variational Bayes approach.

Depends R (>= 3.6)

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coef.graper	<i>Get estimated coefficients from a graper object</i>
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Description

Function to obtain estimated coefficients from a fitted graper model.

Usage

```
## S3 method for class 'graper'
coef(object, include_intercept = TRUE, ...)
```

Arguments

object	fitted graper model as obtained from <code>graper</code>
include_intercept	whether to include the estimated intercept value in the output
...	other arguments

Value

1-Column matrix of estimated coefficients.

Examples

```
# create data
dat <- makeExampleData()
# fit the graper model to the data
fit <- graper(dat$X, dat$y, dat$annot)
# extract the model coefficients
coef(fit)
```

`getPIPs` *Get posterior inclusion probabilities per feature*

Description

Function to obtain estimated posterior inclusion probabilities per feature from a fitted graper model.

Usage

getPIPs(object)

Arguments

object fitted graper model as obtained from [graper](#)

Value

1-Column matrix of estimated posterior inclusion probabilities.

Examples

```
# create data
dat <- makeExampleData()
# fit the graper model to the data
fit <- graper(dat$X, dat$y, dat$annot)
# extract the posterior inclusion probabilities from the fitted model
getPIPs(fit)
```

graper *Fit a regression model with graper*

Description

Fit a regression model with `graper` given a matrix of predictors (X), a response vector (y) and a vector of group memberships for each predictor in X (`annot`). For each group a different strength of penalization is determined adaptively.

Usage

```
graper(X, y, annot, factoriseQ = TRUE, spikeslab = TRUE,
  intercept = TRUE, family = "gaussian", standardize = TRUE,
  n_rep = 1, max_iter = 3000, th = 0.01, d_tau = 0.001,
  r_tau = 0.001, d_gamma = 0.001, r_gamma = 0.001, r_pi = 1,
  d_pi = 1, calcELB = TRUE, verbose = TRUE, freqELB = 1,
  nogamma = FALSE, init_psi = 1)
```

Arguments

X	design matrix of size n (samples) x p (features)
y	response vector of size n
annot	factor of length p indicating group membership of each feature (column) in X
factoriseQ	if set to TRUE, the variational distribution is assumed to fully factorize across features (faster, default). If FALSE, a multivariate variational distribution is used.
spikeslab	if set to TRUE, a spike and slab prior on the coefficients (default).
intercept	whether to include an intercept into the model
family	Likelihood model for the response, either "gaussian" for linear regression or "binomial" for logistic regression
standardize	whether to standardize the predictors to unit variance
n_rep	number of repetitions with different random initializations to be fit
max_iter	maximum number of iterations
th	convergence threshold for the evidence lower bound (ELB)
d_tau	hyper-parameters for prior of tau (noise precision)
r_tau	hyper-parameters for prior of tau (noise precision)
d_gamma	hyper-parameters for prior of gamma (coefficients' prior precision)
r_gamma	hyper-parameters for prior of gamma (coefficients' prior precision)
r_pi	hyper-parameters for Beta prior of the mixture probabilities in the spike and slab prior
d_pi	hyper-parameters for Beta prior of the mixture probabilities in the spike and slab prior
calcELB	whether to calculate the evidence lower bound (ELB)
verbose	whether to print out intermediate messages during fitting
freqELB	frequency at which the evidence lower bound (ELB) is to be calculated, i.e. each freqELB-th iteration
nogamma	if TRUE, the normal prior will have same variance for all groups (only relevant for spikeslab = TRUE)
init_psi	initial value for the spike variables

Details

The function trains the graper model given a matrix of predictors (X), a response vector (y) and a vector of group memberships for each predictor in X (annot). For each feature group as specified in annot a penalty factor and sparsity level is learnt.

By default it uses a Spike-and-Slab prior on the coefficients and uses a fully factorized variational distribution in the inference. This provides a fast way to train the model. Using spikeslab=FALSE a ridge regression like model can be fitted using a normal instead of the spike and slab prior. Setting factoriseQ = FALSE gives a more exact inference scheme based on a multivariate variational distribution, but can be much slower.

As the optimization is non-convex is can be helpful to use multiple random initializations by setting n_rep to a value larger 1. The returned model is then chosen as the optimal fit with respect to the evidence lower bound (ELB).

Depending on the response vector a linear regression model (family = "gaussian") or a logistic regression model (family = "binomial") is fitted. Note, that the implementation of logistic regression is still experimental.

Value

A graper object containing

- EW_beta** estimated model coefficients in liner/logistic regression
- EW_s** estimated posterior-inclusion probabilities for each feature
- intercept** estimated intercept term
- annot** annotation vector of features to the groups as specified when calling [graper](#)
- EW_gamma** estimated penalty factor per group
- EW_pi** estimated sparsity level per group (from 1 (dense) to 0 (sparse))
- EW_tau** estimated noise precision
- sigma2_tildebeta_s1, EW_tildebeta_s1, alpha_gamma, alpha_tau, beta_tau, Sigma_beta, alpha_pi, beta_pi**
parameters of the variational distributions of beta, gamma, tau and pi
- ELB** final value of the evidence lower bound
- ELB_trace** values of the evidence lower bound for all iterations
- Options** other options used when calling [graper](#)

Examples

```
# create data
dat <- makeExampleData()

# fit a sparse model with spike and slab prior
fit <- graper(dat$X, dat$y, dat$annot)
fit # print fitted object
beta <- coef(fit, include_intercept=FALSE) # model coefficients
pips <- getPIPs(fit) # posterior inclusion probabilities
pf <- fit$EW_gamma # penalty factors per group
sparsities <- fit$EW_pi # sparsity levels per group

# fit a dense model without spike and slab prior
fit <- graper(dat$X, dat$y, dat$annot, spikeslab=FALSE)

# fit a dense model using a multivariate variational distribution
fit <- graper(dat$X, dat$y, dat$annot, factoriseQ=TRUE,
              spikeslab=FALSE)
```

makeExampleData

*Simulate example data from the graper model***Description**

Simulate data from the graper model with groups of equal size and pre-specified parameters gamma, pi and tau.

Usage

```
makeExampleData(n = 100, p = 200, g = 4, gammas = c(0.1, 1, 10,
100), pis = c(0.5, 0.5, 0.5, 0.5), tau = 1, rho = 0,
response = "gaussian", intercept = 0)
```

Arguments

n	number of samples
p	number of features
g	number of groups
gammas	vector of length g, specifying the slab precision of the prior on beta per group
pis	vector of length g, specifying the probability of s to be 1 (slab)
tau	noise precision
rho	correlation of design matrix (Toeplitz structure)
response	"gaussian" for continuous response from a linear regression model, "bernoulli" for a binary response from a logistic regression model.
intercept	model intercept (default: 0)

Value

list containing the design matrix X, the response y, the feature annotation to groups annot as well as the different parameters in the Bayesian model and the correlation strength rho

Examples

```
dat <- makeExampleData()
```

makeExampleDataWithUnequalGroups

Simulate example data from the graper model with groups of unequal size

Description

Simulate data from the graper model with groups of unequal size and pre-specified parameters gamma, pi and tau.

Usage

```
makeExampleDataWithUnequalGroups(n = 100, pg = c(100, 100, 10, 10),
                                 gammas = c(0.1, 10, 0.1, 10), pis = c(0.5, 0.5, 0.5, 0.5), tau = 1,
                                 rho = 0, response = "gaussian", intercept = 0)
```

Arguments

n	number of samples
pg	vector of length g (desired number of groups) with number of features per group
gammas	vector of length g, specifying the slab precision of the prior on beta per group
pis	vector of length g, specifying the probability of s to be 1 (slab)
tau	noise precision (only relevant for gaussian response)
rho	correlation of design matrix (Toeplitz structure)
response	"gaussian" for continuous response from a linear regression model, "bernoulli" for a binary response from a logistic regression model.
intercept	model intercept (default: 0)

Value

list containin the design matrix X, the response y, the feature annotation to groups annot as well as the different parameters in the Bayesian model and the correlation strength rho

Examples

```
dat <- makeExampleDataWithUnequalGroups()
```

plotELBO*Plot evidence lower bound*

Description

Function to plot the evidence lower bound (ELBO) over iterations to monitor the convergence of the algorithm.

Usage

```
plotELBO(fit)
```

Arguments

fit fit as produced by [graper](#)

Value

a ggplot object

Examples

```
dat <- makeExampleData()
fit <- graper(dat$X, dat$y, dat$annot)
plotELBO(fit)
```

plotGroupPenalties*Plot group-wise penalties*

Description

Function to plot the group-wise penalty factors (gamma) and sparsity levels.

Usage

```
plotGroupPenalties(fit)
```

Arguments

fit fit as produced by [graper](#)

Value

a ggplot object

Examples

```
dat <- makeExampleData()
fit <- graper(dat$X, dat$y, dat$annot)
plotGroupPenalties(fit)
```

plotPosterior

Plot posterior distributions

Description

Function to plot the posterior of the model parameters obtained by graper from the variational inference framework.

Usage

```
plotPosterior(fit, param2plot, beta0 = NULL, gamma0 = NULL,
              tau0 = NULL, pi0 = NULL, s0 = NULL, jmax = 2, range = NULL)
```

Arguments

fit	fit as produced by graper
param2plot	which parameter of the graper model to plot (gamma, beta, tau or s)
beta0	true beta (if known)
gamma0	true gamma (if known)
tau0	true tau (if known)
pi0	true pi (if known)
s0	true s (if known)
jmax	maximal number of components per group to plot (for beta and s)
range	plotting range (x-axis)

Value

a ggplot object

Examples

```
# create data
dat <- makeExampleData()
# fit the graper model
fit <- graper(dat$X, dat$y, dat$annot)
# plot posterior distribution of the gamma parameter
plotPosterior(fit, param2plot="gamma")
```

predict.graper	<i>Predict response on new data</i>
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Description

Function to predict the response on a new data set using a fitted graper model.

Usage

```
## S3 method for class 'graper'
predict(object, newX, type = c("inRange", "response",
"link"), ...)
```

Arguments

object	fitted graper model as obtained from graper
newX	Predictor matrix of size n_test (number of new test samples) x p (number of predictors) (same feature structure as used in graper)
type	type of prediction returned, either: <ul style="list-style-type: none"> • response:returns the linear predictions for linear regression and class probabilities for logistic regression • link:returns the linear predictions • inRange:returns linear predictions for linear and class memberships for logistic regression
...	other arguments

Value

A vector with predictions.

Examples

```
# create data
dat <- makeExampleData()
# split data into train and test sets of equal size
ntrain <- dat$n / 2
# fit the model to the train data
fit <- graper(dat$X[seq_len(ntrain), ],
               dat$y[seq_len(ntrain)], dat$annot)
# make predictions on the test data
ypred <- predict(fit, dat$X[seq_len(ntrain) + dat$n / 2, ])

# create data for logistic regression
dat <- makeExampleData(response="bernoulli")
# split data into train and test sets of equal size
ntrain <- dat$n / 2
# fit the graper model for a logistic model
fit <- graper(dat$X[seq_len(ntrain), ],
               dat$y[seq_len(ntrain)],
               dat$annot, family="binomial")
# make predictions on the test data
ypred <- predict(fit, dat$X[seq_len(ntrain) + dat$n / 2, ], type = "inRange")
```

`print.graper` *Print a graper object*

Description

Function to print a fitted graper model.

Usage

```
## S3 method for class 'graper'  
print(x, ...)
```

Arguments

<code>x</code>	fitted graper model as obtained from <code>graper</code>
<code>...</code>	additional print arguments

Value

Print output.

Examples

```
# create data  
dat <- makeExampleData()  
# fit the graper model  
fit <- graper(dat$X, dat$y, dat$annot)  
# print a summary of the fitted model  
print(fit)
```

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