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` *Get estimated coefficients from a graper object*

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 `graper`
`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$annot)
fit # print fitted object
beta <- coef(fit, include_intercept=FALSE) # model coeffients
pips <- getPIPs(fit) # posterior inclusion probabilities
pf <- fit$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 *Predict response on new data*

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: • **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

`x`	fitted graper model as obtained from `graper`
`...`	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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