Package ‘graper’

Type Package

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

Version 1.20.0

Date 2018-10-26

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)

Encoding UTF-8

LazyData TRUE

Imports Matrix, Rcpp, stats, ggplot2, methods, cowplot, matrixStats

LinkingTo Rcpp, RcppArmadillo, BH

biocViews Regression, Bayesian, Classification

RoxygenNote 6.1.1

Suggests knitr, rmarkdown, BiocStyle, testthat

VignetteBuilder knitr

git_url https://git.bioconductor.org/packages/graper

git_branch RELEASE_3_19

git_last_commit a4dfa52

git_last_commit_date 2024-04-30

Repository Bioconductor 3.19

Date/Publication 2024-05-12

Author Britta Velten [aut, cre], Wolfgang Huber [aut]

Maintainer Britta Velten <britta.velten@gmail.com>


## Description

Function to obtain estimated coefficients from a fitted graper model.

## Usage

```r
## 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

```r
# 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 it can be helpful to use multiple random initializations by setting `n_rep` to a value larger than 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 linear/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**

```r
# 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()
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

```r
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

```r
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
plotPosterior

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

```r
# 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)
Index

coef.graper, 2

getPIPs, 3
graper, 2, 3, 5, 8–11

makeExampleData, 6
makeExampleDataWithUnequalGroups, 7

plotELBO, 8
plotGroupPenalties, 8
plotPosterior, 9
predict.graper, 10
print.graper, 11