Package 'BCBCSF'

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Title Bias-Corrected Bayesian Classification with Selected Features
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Depends R (>= 2.13.1), abind
Description Fully Bayesian Classification with a subset of high-dimensional features, such as expression levels of genes. The data are modeled with a hierarchical Bayesian models using heavytailed t distributions as priors. When a large number of features are available, one may like to select only a subset of features to use, typically those features strongly correlated with the response in training cases. Such a feature selection procedure is however invalid since the relationship between the response and the features has be exaggerated by feature selection. This package provides a way to avoid this bias and yield better-calibrated predictions for future cases when one uses F-statistic to select features.
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2 d1:bcbcsfexamples

d1:bcbcsfexamples	Examples of fitting models, predicting class labels, evaluating predic-
u. 12 02 00 1 0 1 a mp 2 0 0	tion, and analyzing fitting results

Description

These examples demonstrate how to use BCBCSF package. They use all prior and Markov chain sampling settings by default (except no_rmc as noted below). The methods for setting others can be found from documents for specific functions. However, the default settings may work well for a wide range of gene expression data.

References

Li, L. (2012), Bias-corrected Hierarchical Bayesian Classification with a Selected Subset of Highdimensional Features, *Journal of American Statistical Association*, 107:497,120-134

See Also

bcbcsf_fitpred, bcbcsf_pred, cross_vld, eval_pred, reload_fit_bcbcsf, bcbcsf_sumfit, bcbcsf_plotsumfit

Examples

```
##\dontrun{
## load lymphoma microarray data
data (lymphoma)
## select some cases as testing data set
ts <- c (sort(sample (1:42,5)), 43:44, 61:62)
## training data
X_tr <- lymph.X[-ts,]</pre>
y_tr <- lymph.y[-ts]
## test data
X_ts <- lymph.X[ts,]</pre>
y_ts <- lymph.y[ts]</pre>
####################### training and prediction #################################
## fitting training data with top features selected by F-statistic
out_fit <- bcbcsf_fitpred (X_tr = X_tr, y_tr = y_tr, nos_fsel = c(20, 50),
                       no\_rmc = 100)
## note 1: if 'X_ts' is given above, prediction is made after fitting
## note 2: no_rmc = 100 is too small, omit it and use the default
## predicting class labels of test cases
out_pred <- bcbcsf_pred (X_ts = X_ts, out_fit = out_fit)</pre>
```

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```
## evaluate prediction given true labels
eval_pred (out_pred = out_pred, y_ts = y_ts)
## reload one bcbcsf fit result from hardrive
fit_bcbcsf <- reload_fit_bcbcsf (out_fit$fitfiles[1])</pre>
## the fitting result for no_fsel = 50 can be retrieved directly from
## out_fit:
fit_bcbcsf_fsel50 <- out_fit$fit_bcbcsf</pre>
## summarize the fitting result
sum_fit <- bcbcsf_sumfit (fit_bcbcsf)</pre>
## visualize fitting result
bcbcsf_plotsumfit (sum_fit)
## doing cross validation with bcbcsf_fitpred on lymphoma data
cv_pred <- cross_vld (</pre>
    fitpred_func = bcbcsf_fitpred, X = lymph.X, y = lymph.y, nfold = 2,
    ############ all other arguments passed classifier ############
    nos_fsel = c(20,50), no_rmc = 100)
## note: no_rmc = 100 is too small, omit it and use the default in practice
## evaluate prediction given true labels
eval_pred (out_pred = cv_pred, y_ts = lymph.y)
## warning: this function is slow if nfold is large; if you have a
## computer cluster, you better parallel the cross validation folds.
##}
```

d2:fitpred

Functions for fitting models with MCMC, predicting class labels of test cases, and finding predictive probabilities with cross-validation

Description

bcbcsf_fitpred trains models with Gibbs sampling for each number of retained features. The results are saved in files. This function also makes predictions for test cases if they are provided.

bcbcsf_pred uses the posterior samples saved by bcbcsf_fitpred to predict the class labels of test cases. Prediction results are an array of predictive probabilities array_probs_pred, whose rows for test cases, columns for classes, and the 3rd dimension for different numbers of retained features.

cross_vld uses cross-validation to obtain predictive probabilities for all cases of a data set. This generic function can be used with bcbcsf_fitpred and other classifiers.

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Usage

```
bcbcsf_fitpred (
  ## arguments specifying info of data sets
 X_{tr}, y_{tr}, nos_{sel} = ncol(X_{tr}),
 X_ts = NULL, standardize = FALSE, rankf = FALSE,
  ## arguments for prediction
 burn = NULL, thin = 1, offset_sdxj = 0.5,
 ## arguments for Markov chain sampling
 no_rmc = 1000, no_imc = 5, no_mhwmux = 10,
  fit_bcbcsf_filepre = ".fitbcbcsf_",
 ## arguments specifying priors for parameters and hyerparameters
 w0_mu = 0.05, alpha0_mu = 0.5, alpha1_mu = 3,
 w0_x = 1.00, alpha0_x = 0.5, alpha1_x = 10,
 w0_nu = 0.05, alpha0_nu = 0.5, prior_psi = NULL,
  ## arguments for metropolis sampling for wmu, wx
  stepadj_mhwmux = 1, diag_mhwmux = FALSE,
  ## arguments for computing adjustment factor
 bcor = 1, cut_qf = exp(-10), cut_dpoi = exp(-10), nos_sim = 1000,
 ## whether look at progress
 monitor = TRUE)
bcbcsf_pred (X_ts, out_fit, burn = NULL, thin = 1, offset_sdxj = 0.5)
cross_vld (X, y, nfold = 10, folds = NULL,
           fitpred_func = bcbcsf_fitpred, ...)
```

Arguments

matrices containing gene expression data; rows should be for the cases, and X_tr, X_ts, X columns for different genes; X_tr are training data, X_ts are test data or future data for which prediction are needed, X are a data set used for cross-validation.

class labels in training or test data set, or just a data set. y_tr,y

nos_fsel a vector of numbers of features to be retained.

burn, thin burn of Markov chain (super)iterations will be discarded for prediction, and only every thinth are used; by default, 20% of (super)iterations are burned, and

thin=1.

offset_sdxj a value between 0 and 1; 100*offset_sdxj% quantile of the samples of all standard deviations $\sqrt{w_i^x}$ is added to the all standard deviations; this is to rem-

edy the non-normality in real gene expression data sets, and especially offset

some very small standard deviations; by default, median is used.

no_rmc, no_imc no_rmc of super Markov chain transitions are run, with no_imc Markov chain iterations for each; only the last state of each super transition is saved.

fit_bcbcsf_filepre

a string added to the names of files saving Markov chain fitting results; the actual file names contain also the data dimension and number of retained features; d2:fitpred 5

when fit_bcbcsf_filepre is set to NULL, no fitting file will be created, and bcbcsf_fitpred returns only the fitting result corresponding to the last number of retained features in nos_fsel, which is always returned regardless of the value of fit_bcbcsf_filepre.

w0_mu,alpha0_mu,alpha1_mu,w0_x,alpha0_x,alpha1_x,w0_nu,alpha0_nu

settings of priors for means and variances of genes; they are denoted by w_0^{μ} , α_1^{μ} , α_1^{μ} , α_1^{μ} , α_0^{μ} , α_0^{τ} , α_1^{τ} , α_0^{τ} , in the reference.

prior_psi a vector of length the number of classes, specifying the Dirichlet prior distribu-

tion for probabilities of classes; it is denoted by $c_{1:G}$ in the reference; by default,

they are all equal to 1.

no_mhwmux, stepadj_mhwmux, diag_mhwmux

arguments specifying Metropolis sampling for $\log(w^{\mu})$ and $\log(w^x)$; respectively the number of iterations, stepsize adjustment, and an indicator represent-

ing whether one wants to pause and look into this sampling.

bcor taking value 0 or 1, indicating whether bias-correction is to be applied.

cut_qf, cut_dpoi,nos_sim

arguments specifying approximation of adjustment factor; cut_qf is f_ℓ in the reference, cut_dpoi is the threshold below which Poisson probabilities are omitted the number of readon.

ted, nos_sim is the number of random Λ .

nfold, folds folds should be a list of test cases for different folds; if folds is NULL (by de-

fault), folds will be generated by the software, with nfold is set to the smaller

value of the given value and the smallest number of cases in all classes.

out_fit a list returned by bcbcsf_fitpred, which are used to make prediction for test

cases.

standardize if it is set to TRUE, the original gene expression values are centralized and

divided by the pooled standard deviation; by default, it is FALSE.

rankf if it is set to TRUE, the original features will be re-ordered by F-statistic; by

default, it is FALSE.

monitor if it is set to TRUE, progress of fitting is shown on screen

fitpred_func an R function that can fit with training data, and predict for test data; the ar-

guments of fitpred_func must include X_tr, y_tr, X_ts, and the outputs of

fitpred_func must include array_probs_pred

... arguments passed to classifier fitpred_func

Value

nos_fsel a vector of numbers of features retained.

fitfiles a string vector of length nos_fsel, each saving file name of Markov chain fitting

result for a number of retained features in nos_fsel; the fitfiles returned by

cross_vld is for the training in the last fold.

array_probs_pred

an array of predictive probabilities, whose rows for test cases, columns for classes, and the 3rd dimension for different numbers of retained features.

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fit_bcbcsf

a list of Markov chain sampling results from the fitting with number of retained features equal to the last number in nos_fsel. Note that, the fitting results for other numbers (including the last one) of retained feature are saved in harddrive files if fit_bcbcsf_filepre isn't empty, and can be retrieved using function reload_fit_bcbcsf. Particularly, the list component of fit_bcbcsf has fsel saving the indice of features selected by F-statistic.

d3:evalpred

A function for evaluating arrays of predictive probabilities with the true class labels of test cases

Description

This function is used to find error rate, amlp, loss and predictive probabilities at true labels.

Usage

```
eval_pred (out_pred, y_ts, Mloss = NULL)
```

Arguments

out_pred a list returned by function bcbcsf_fitpred with X_ts given, or bcbcsf_pred,

or by cross_vld.

y_ts a vector of true class labels.

Mloss a matrix indicting loss function, with element m_{ij} saving the losss from predict-

ing class i with class label j; by default, it is NULL.

Value

probs_at_truelabels

a matrix of predictive probabilities at true labels, with rows for cases, and columns

for different numbers of retained features

summary a data frame, with rows for different numbers of retained features, and columns:

Error.Rate: fraction of cases misclassified with fair threshold, and AMLP: minus average log probabilities at true labels, often called "deviation", and Loss (if

Mloss is given): average loss.

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d4:analyzefit	Functions for analyzing and visualizing a BCBCSF fitting result	

Description

These functions are used to look at the fitting results, especially plot the gene signals.

Usage

Arguments

fit_bcbcsf_afile		
	a string of name of a file saving a Markov chain fitting result; it can be found from the value fitfiles of function bcbcsf_fitpred.	
fit_bcbcsf	a list of Markov chain fitting result, returned by function reload_fit_bcbcsf and bcbcsf_fitpred; if it is NULL, it will be retrieved by running reload_fit_bcbcsf with value in fit_bcbcsf_afile.	
burn, thin	burn of Markov chain (super)iterations will be discarded (burned) for evaluation, and only every thinth are used; by default, 20% of (super)iterations are burned, and thin=1.	
sum_fit	a list returned by function bcbcsf_sumfit	

Value

reload_fit_bcbcsf returns a list of Markov chain fitting results, including how to do feature selection and data preprocessing.

bcbcsf_sumfit returns a list of point estimates of means and variances.

bcbcsf_plotsumfit returns nothing; it plots the normalized means (for each gene, original expression means substracted by their means and divided by the common standard deviation), and overall signals (Euclid distance of normalized means) for the selected features.

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Description

This is one of the microarray data sets used to demonstrate BCBCSF in the reference article. Information about this data set can be found from the reference.

Usage

data(lymphoma)

Value

lymph.X a matrix of gene expression data for p = 4026 genes on n = 62 cases in G=3

classes

lymph.y a vector of class labels coded by 1,2,3.

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