Package 'peperr'

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Type Package

Title Parallelised Estimation of Prediction Error

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Description Designed for prediction error estimation through resampling techniques, possibly accelerated by parallel execution on a compute cluster. Newly developed model fitting routines can be easily incorporated.
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Description

Evaluate the Brier score, i.e. prediction error, for a fitted model on new data. To be used as argument aggregation. fun in peperr call.

Usage

```
aggregation.brier(full.data=NULL, response, x, model, cplx=NULL, type=c("apparent", "noinf"),
  fullsample.attr = NULL, ...)
```

Arguments

full.data	passed from peperr, but not used for calculation of the Brier score.
response	vector of binary response.
X	n*p matrix of covariates.
model	model fitted as returned by a fit.fun, as used in a call to peperr.
cplx	passed from peperr, but not necessary for calculation of the Brier score.
type	character.
fullsample.att	r
	passed from peperr, but not necessary for calculation of the Brier score.
	additional arguments, passed to predict function.

Details

The empirical Brier score is the mean of the squared difference of the risk prediction and the true value of all observations and takes values between 0 and 1, where small values indicate good prediction performance of the risk prediction model.

Value

Scalar, indicating the empirical Brier score.

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aggregation.misclass Determine the missclassification rate for a fitted model

Description

Evaluate the misclassification rate, i.e. prediction error, for a fitted model on new data. To use as argument aggregation. fun in peperr call.

Usage

```
aggregation.misclass(full.data=NULL, response, x, model, cplx=NULL, type=c("apparent", "noinf"),
  fullsample.attr = NULL, ...)
```

Arguments

full.data passed from peperr, but not used for calculation of the misclassification rate.

response vector of binary response.

x n*p matrix of covariates.

model model fitted with fit.fun.

cplx passed from peperr, but not necessary for calculation of the misclassification

rate.

type character.

fullsample.attr

passed from peperr, but not necessary for calculation of the misclassification

rate.

... additional arguments, passed to predict function.

Details

Misclassification rate is the ratio of observations for which prediction of response is wrong.

Value

Scalar, indicating the misclassification rate.

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Determine the prediction error curve for a fitted model

Description

Interface to pmpec, for conforming to the structure required by the argument aggregation. fun in peperr call. Evaluates the prediction error curve, i.e. the Brier score tracked over time, for a fitted survival model.

Usage

```
aggregation.pmpec(full.data, response, x, model, cplx=NULL, times = NULL,
    type=c("apparent", "noinf"), fullsample.attr = NULL, ...)
```

Arguments

full.data data frame with full data set.	
--	--

response Either a survival object (with Surv(time, status), where time is an n-vector

of censored survival times and status an n-vector containing event status, coded with 0 and 1) or a matrix with columns time containing survival times and status containing integers, where 0 indicates censoring, 1 the interesting event

and larger numbers other competing risks.

x n*p matrix of covariates.

model survival model as returned by fit. fun as used in call to peperr.

cplx numeric, number of boosting steps or list, containing number of boosting steps

in argument stepno.

times vector of evaluation time points. If given, used as well as in calculation of

full apparent and no-information error as in resampling procedure. Not used if

fullsample.attr is specified.

type character.

fullsample.attr

vector of evaluation time points, passed in resampling procedure. Either user-defined, if times were passed as args.aggregation, or the determined time

points from the aggregation. fun call with the full data set.

... additional arguments passed to pmpec call.

Details

If no evaluation time points are passed, they are generated using all uncensored time points if their number is smaller than 100, or 100 time points up to the 95% quantile of the uncensored time points are taken.

pmpec requires a predictProb method for the class of the fitted model, i.e. for a model of class class predictProb.class.

Value

A matrix with one row. Each column represents the estimated prediction error of the fit at the time points.

See Also

```
peperr, predictProb, pmpec
```

```
complexity.ipec.CoxBoost
```

Interface function for complexity selection for CoxBoost via integrated prediction error curve and the bootstrap

Description

Determines the number of boosting steps for a survival model fitted by CoxBoost via integrated prediction error curve (IPEC) estimates, conforming to the calling convention required by argument complexity in peperr call.

Usage

```
complexity.ipec.CoxBoost(response, x, boot.n.c = 10, boost.steps = 100,
    eval.times = NULL, smooth = FALSE, full.data, ...)

complexity.ripec.CoxBoost(response, x, boot.n.c = 10, boost.steps = 100,
    eval.times = NULL, smooth = FALSE, full.data, ...)
```

Arguments

response	a survival object (with Surv(time, status)).
X	n*p matrix of covariates.
boot.n.c	number of bootstrap samples.
boost.steps	maximum number of boosting steps, i.e. number of boosting steps is selected out of interval (1, boost.steps).
eval.times	vector of evaluation time points.
smooth	logical. Shall prediction error curve be smoothed by local polynomial regression before integration?
full.data	Data frame containing response and covariates of the full data set.
	additional arguments passed to CoxBoost call.

Details

Plotting the .632+ estimator for each time point given in eval.times results in a prediction error curve. A summary measure can be obtained by integrating over time. complexity.ripec.CoxBoost computes a Riemann integral, while complexity.ipec.CoxBoost uses a Lebesgue-like integral taking Kaplan-Meier estimates as weights. The number of boosting steps of the interval (0, boost.steps), for which the minimal IPEC is obtained, is returned.

complexity.LASSO

Value

Scalar value giving the number of boosting steps.

See Also

```
peperr, CoxBoost
```

complexity.LASSO

Interface for selection of optimal parameter for lasso fit

Description

Determines the optimal value for tuning parameter lambda for a regression model with lasso penalties via cross-validation. Conforming to the calling convention required by argument complexity in peperr call.

Usage

```
complexity.LASSO(response, x, full.data, ...)
```

Arguments

response a survival object (Surv(time, status)).

x n*p matrix of covariates.

full.data data frame containing response and covariates of the full data set.
... additional arguments passed to optL1 of package **penalized** call.

Details

Function is basically a wrapper around optL1 of package **penalized**. Calling peperr, default arguments of optL1 can be changed by passing a named list containing these as argument args.complexity.

Value

Scalar value giving the optimal value for lambda.

See Also

```
peperr, optL1
```

```
complexity.mincv.CoxBoost
```

Interface for CoxBoost selection of optimal number of boosting steps via cross-validation

Description

Determines the number of boosting steps for a survival model fitted by CoxBoost via cross-validation, conforming to the calling convention required by argument complexity in peperr call.

Usage

```
complexity.mincv.CoxBoost(response, x, full.data, ...)
```

Arguments

```
response a survival object (Surv(time, status)).

x n*p matrix of covariates.

full.data data frame containing response and covariates of the full data set.

additional arguments passed to cv.CoxBoost call.
```

Details

Function is basically a wrapper around cv.CoxBoost of package CoxBoost. A K-fold cross-validation (default K=10) is performed to search the optimal number of boosting steps, per default in the interval (0, maxstepno=100). The number of boosting steps with minimum mean partial log-likelihood is returned. Calling peperr, the default arguments of cv.CoxBoost can be changed by passing a named list containing these as argument args.complexity.

Value

Scalar value giving the optimal number of boosting steps.

See Also

```
peperr, cv.CoxBoost
```

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extract.fun	Extract functions, libraries and global variables to be loaded onto a
	compute cluster

Description

Automatic extraction of functions, libraries and global variables employed passed functions. Designed for peperr call, see Details section there.

Usage

```
extract.fun(funs = NULL)
```

Arguments

funs list of function names.

Details

This function is necessary for compute cluster situations where for computation on nodes required functions, libraries and variables have to be loaded explicitly on each node. Avoids loading of whole global environment which might include the unnecessary loading of huge data sets.

It might have problems in some cases, especially it is not able to extract the library of a function that has no namespace. Similarly, it can only extract a required library if it is loaded, or if the function contains a require or library call.

Value

list containing

packages vector containing quoted names of libraries

functions vector containing quoted names of functions

variables vector containing quoted names of global variables

See Also

peperr

Examples

```
# 1. Simplified example for illustration
## Not run:
library(CoxBoost)
a <- function(){
# some calculation
}
b<-function(){</pre>
```

fit.CoxBoost

```
# some other calculation
x <- cv.CoxBoost()
# z is global variable
y <- a(z)
}
# list with packages, functions and variables required for b:
extract.fun(list(b))
# 2. As called by default in peperr example
extract.fun(list(fit.CoxBoost, aggregation.pmpec))
## End(Not run)</pre>
```

fit.CoxBoost

Interface function for fitting a CoxBoost model

Description

Interface for fitting survival models by CoxBoost, conforming to the requirements for argument fit.fun in peperr call.

Usage

```
fit.CoxBoost(response, x, cplx, ...)
```

Arguments

response a survival object (with Surv(time, status)).

x n*p matrix of covariates.

cplx number of boosting steps or list, containing number of boosting steps in argument stepno and penalty factor in argument penalty.factor.

... additional arguments passed to CoxBoost call.

Details

Function is basically a wrapper around CoxBoost of package **CoxBoost**. A Cox proportional hazards model is fitted by componentwise likelihood based boosting, especially suited for models with many covariates and few observations.

Value

CoxBoost object

See Also

```
peperr, CoxBoost
```

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fit.coxph

Interface function for fitting a Cox proportional hazards model

Description

Interface for fitting survival models by Cox proporional hazards model, conforming to the requirements for argument fit. fun in peperr call.

Usage

```
fit.coxph(response, x, cplx, ...)
```

Arguments

response a survival object (with Surv(time, status)).

x n*p matrix of covariates.

cplx not used.

... additional arguments passed to coxph call.

Details

Function is basically a wrapper around coxph of package survival.

Value

CoxBoost object

See Also

```
peperr, coxph
```

fit.LASSO

Interface function for fitting a generalised linear model with the lasso

Description

Interface for fitting survival models with the lasso, conforming to the requirements of argument fit.fun in peperr call.

Usage

```
fit.LASSO(response, x, cplx, ...)
```

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Arguments

response response. Could be numeric vector for linear regression, Surv object for Cox

regression or a binary vector for logistic regression.

x n*p matrix of covariates.

cplx LASSO penalty. lambda1 of penalized call.
... additional arguments passed to penalized call.

Details

Function is basically a wrapper around function penalized of package penalized.

Value

penfit object

See Also

peperr, penalized

ipec Integrated prediction error curve

Description

Summary measures of prediction error curves

Usage

```
ipec(pe, eval.times, type=c("Riemann", "Lebesgue", "relativeLebesgue"), response=NULL)
```

Arguments

pe prediction error at different time points. Vector of length of eval.times or ma-

trix (columns correspond to evaluation time points, rows to different prediction

error estimates)

eval.times evalutation time points

type type of integration. 'Riemann' estimates Riemann integral, 'Lebesgue' uses the

probability density as weights, while 'relativeLebesgue' delivers the difference

to the null model (using the same weights as for 'Lebesgue').

response survival object (Surv(time, status)), required only if type is 'Lebesgue' or

'relativeLebesgue'

Details

For survival data, prediction error at each evaluation time point can be extracted of a peperr object by function perr. A summary measure can then be obtained via integrating over time. Note that the time points used for evaluation are stored in list element attribute of the peperr object.

Value

ipec

Value of integrated prediction error curve. Integer or vector, if pe is vector or matrix, respectively, i.e. one entry per row of the passed matrix.

See Also

perr

Examples

```
## Not run:
n <- 200
p <- 100
beta <- c(rep(1,10), rep(0,p-10))
x <- matrix(rnorm(n*p),n,p)</pre>
real.time <- -(\log(\text{runif}(n)))/(10*\exp(\text{drop}(x \%*\% \text{ beta})))
cens.time <- rexp(n,rate=1/10)</pre>
status <- ifelse(real.time <= cens.time,1,0)</pre>
time <- ifelse(real.time <= cens.time,real.time,cens.time)</pre>
# Example:
# Obtain prediction error estimate fitting a Cox proportional hazards model
# using CoxBoost
# through 10 bootstrap samples
# with fixed complexity 50 and 75
# and aggregate using prediction error curves
peperr.object <- peperr(response=Surv(time, status), x=x,</pre>
   fit.fun=fit.CoxBoost, complexity=c(50, 75),
   indices=resample.indices(n=length(time), method="sub632", sample.n=10))
# 632+ estimate for both complexity values at each time point
prederr <- perr(peperr.object)</pre>
# Integrated prediction error curve for both complexity values
ipec(prederr, eval.times=peperr.object$attribute, response=Surv(time, status))
## End(Not run)
```

peperr

Parallelised Estimation of Prediction Error

Description

Prediction error estimation for regression models via resampling techniques. Potentially parallelised, if compute cluster is available.

Usage

```
peperr(response, x,
indices = NULL,
fit.fun, complexity = NULL, args.fit = NULL, args.complexity = NULL,
```

Arguments

response

Either a survival object (with Surv(time, status), where time is an n-vector of censored survival times and status an n-vector containing event status, coded with 0 and 1) or a matrix with columns time containing survival times and status containing integers, where 0 indicates censoring, 1 the interesting event and larger numbers other competing risks. In case of binary response, vector with entries 0 and 1.

X

n*p matrix of covariates.

indices

named list, with two elements (both expected to be lists) sample.index, containing the vector of indices of observations used to fit the model, and list not.in.sample, containing the vector of indices of observations used for assessment. One list entry per split. Function resample.indices provides the most common resampling methods. If argument indices is not specified (default), the indices are determined as follows: If number of observations in the passed data matrix is smaller than number of covariates, 500 bootstrap samples without replacement are generated ("subsampling"), else 500 bootstrap samples with replacement.

fit.fun

function returning a fitted model, see Details.

complexity

if the choice of a complexity parameter is necessary, for example the number of boosting steps in boosting techniques, a function returning complexity parameter for model fitted with fit.fun, see Details. Alternatively, one explicit value for the complexity or a vector of values can be passed. In the latter case, the model fit is carried out for each of the complexity parameters. Alternatively, a named list can be passed, if complexity is a tuple of different parameter values.

args.fit

named list of arguments to be passed to the function given in fit.fun.

args.complexity

if complexity is a function, a named list of arguments to be passed to this function.

parallel

the default setting corresponds to the case that sfCluster is used or if R runs sequential, i.e. without any parallelisation. If sfCluster is used, settings from sfCluster commandline call are taken, i.e. the required number of nodes has to be specified as option of the sfCluster call (and not using argument cpus). If another cluster solution (specified by argument clustertype) shall be used, a cluster with cpus CPUs is started if parallel=TRUE. parallel=FALSE switches back to sequential execution. See Details.

number of nodes, i.e., number of parallel running R processes, to be set up in a cpus cluster, if not specified by commandline call. Only needed if parallel=TRUE. clustertype type of cluster, character. 'SOCK' for socket cluster, 'MPI', 'PVM' or 'NWS'. Only considered if parallel=TRUE. If so, a socket cluster, which does not require any additional installation, is started as default. clusterhosts host list for socket and NWS clusters, if parallel=TRUE. Has to be specified only if using more than one machine. if function is used in already parallelised code. If set to TRUE, no cluster is noclusterstart initialised even if a compute cluster is available and function works in sequential mode. Additionally usable if calls on the slaves should be executed before calling function peperr, for example to load data on slaves, see Details. noclusterstop if TRUE, cluster stop is suppressed. Useful for debugging of sessions on slaves. Note that the next peperr call forces cluster stop, except if called with nocluster start=TRUE. aggregation.fun function that evaluates the prediction error for a model fitted by the function given in fit. fun, see Details. If not specified, function aggregation.pmpec is taken if response is survival object, in case of binary response function aggregation.brier. args.aggregation named list of arguments to be passed to the function given in argument aggregation. fun. load.list a named list with element packages, functions and variables containing quoted names of libraries, functions and global variables required for computation on cluster nodes. The default extracts automatically the libraries, functions and global variables of the, potentially user-defined, functions fit.fun, complexity and aggregation. fun, see function extract. fun. Can be set to NULL, e.g. if no libraries, functions and variables are needed. Alternatively, use argument load. all. See Details. load.vars a named list with global variables required for computation on cluster nodes. See Details. Relict, global variabels can now be passed as list element variables of argument load.list. load.all logical. If set to TRUE, all variables, functions and libraries of the current global environment are loaded on cluster nodes. See Details. logical. If TRUE, output about the current execution step is printed (if running trace parallel: printed on nodes, that means not visible in master R process, see Details). if TRUE, information concerning export of variables is given. debug peperr.lib.loc location of package **peperr** if not in standard library search path (.libPaths()), to be specified for loading **peperr** onto the cluster nodes. RNG type of RNG. "fixed" requires a specified seed. "RNGstream" and "SPRNG" use default seeds, if not specified. See Details. seed seed to allow reproducibility of results. Only considered if argument RNG is not "none". See Details.

if TRUE and a compute cluster is used, computation of slaves is executed load

balanced. See Details.

1b

sr if TRUE, intermediate results are saved. If execution is interrupted, they can be

restored by setting argument sr.restore to TRUE. See documentation of package

snowfall for details

sr. name if sr is set to TRUE and more than one computation runs simultaneously, unique

names need to be used.

sr.restore if sr is set to TRUE, an interrupted computation is restarted.

Details

Validation of new model fitting approaches requires the proper use of resampling techniques for prediction error estimation. Especially in high-dimensional data situations the computational demand might be huge. peperr accelerates computation through automatically parallelisation of the resampling procedure, if a compute cluster is available. A noticeable speed-up is reached even when using a dual-core processor.

Resampling based prediction error estimation requires for each split in training and test data the following steps: a) selection of model complexity (if desired), using the training data set, b) fitting the model with the selected (or a given) complexity on the training set and c) measurement of prediction error on the corresponding test set.

Functions for fitting the model, determination of model complexity, if required by the fitting procedure, and aggregating the prediction error are passed as arguments fit.fun, complexity and aggregation.fun. Already available functions are

for model fit: fit.CoxBoost, fit.coxph, fit.LASSO, fit.rsf_mtry

to determine complexity: complexity.mincv.CoxBoost, complexity.ipec.CoxBoost, complexity.LASSO, complexity.ipec.rsf_mtry

to aggregate prediction error: aggregation.pmpec, aggregation.brier, aggregation.misclass

Function peperr is especially designed for evaluation of newly developed model fitting routines. For that, own routines can be passed as arguments to the peperr call. They are incorporated as follows (also compare existing functions, as named above):

- Model fitting techniques, which require selection of one or more complexity parameters, often provide routines based on cross-validation or similar to determine this parameter. If this routine is already at hand, the complexity function needed for the peperr call is not more than a wrapper around that, which consists of providing the data in the required way, calling the routine and return the selected complexity value(s).
- 2. For a given model fitting routine the fitting function, which is passed to the peperr call as argument fit.fun, is not more than a wrapper around that. Explicitly, response and matrix of covariates have to be transformed to the required form, if necessary, the routine is called with the passed complexity value, if required, and the fitted prediction model is returned.
- 3. Prediction error is estimated using a fitted model and a data set, by any kind of comparison of the true and the predicted response values. In case of survival response, apparent error (type apparent), which means that the prediction error is estimated in the same data set as used for model fitting, and no-information error (type noinf), which calculates the prediction error in permuted data, have to be provided. Note that the aggregation function returns the error with an additional attribute called addattr. The evaluation time points have to be stored there to allow later access.

4. In case of survival response, the user may additionally provide a function for partial log likelihood calculation, if he uses an own function for model fit, called PLL.class. If prediction error curves are used for aggregation (aggregation.pmpec), a predictProb method has to be provided, i.e. for each model of class class predictProb.class, see there.

Concerning parallelisation, there are three possibilities to run peperr:

- Start R on commandline with sfCluster and preferred options, for example number of cpus. Leave the three arguments parallel, clustertype and nodes unchanged.
- Use any other cluster solution supported by **snowfall**, i.e. LAM/MPI, socket, PVM, NWS (set argument clustertype). Argument parallel has to be set to TRUE and number of cpus can be chosen by argument nodes)
- If no cluster is used, R works sequentially. Keep parallel=NULL. No parallelisation takes place and therefore no speed up can be obtained.

In general, if parallel=NULL, all information concerning the cluster set-up is taken from commandline, else, it can be specified using the three arguments parallel, clustertype, nodes, and, if necessary, clusterhosts.

sfCluster is a Unix tool for flexible and comfortable managment of parallel R processes. It is available at www.imbi.uni-freiburg.de/parallel, together with detailed information. However, peperr is usable with any other cluster solution supported by snowfall, i.e. sfCluster has not to be installed to use package peperr. Note that this may require cluster handling by the user, e.g. manually shut down with 'lamhalt' on commandline for type="MPI". But, using a socket cluster (argument parallel=TRUE and clustertype="SOCK"), does not require any extra installation.

Note that the run time cannot speed up anymore if the number of nodes is chosen higher than the number of passed training/test samples plus one, as parallelisation takes place in the resampling procedure and one additional run is used for computation on the full sample.

If not running in sequential mode, a specified number of R processes called nodes is spawned for parallel execution of the resampling procedure (see above). This requires to provide all variables, functions and libraries necessary for computation on each of these R processes, so explicitly all variables, functions and libraries required by the, potentially user-defined, functions fit.fun, complexity and aggregation.fun. The simplest possibility is to load the whole content of the global environment on each node and all loaded libraries. This is done by setting argument load.all=TRUE. This is not the default, as a huge amount of data is potentially loaded to each node unnecessarily. Function extract.fun is provided to extract the functions and libraries needed, automatically called at each call of function peperr. Note that all required libraries have to be located in the standard library search path (obtained by .libPaths()). Another alternative is to load required data manually on the slaves, using snowfall functions sfLibrary, sfExport and sfExportAll. Then, argument noclusterstart has to be switched to TRUE. Additionally, argument load.list could be set to NULL, to avoid potentially overwriting of functions and variables loaded to the cluster nodes automatically.

Note that a set.seed call before calling function peperr is not sufficient to allow reproducibility of results when running in parallel mode, as the slave R processes are not affected as they are own R instances. peperr provides two possibilities to make results reproducible:

 Use RNG="RNGstream" or RNG="SPRNG". Independent parallel random number streams are initialized on the cluster nodes, using function sfClusterSetupRNG of package snowfall. A

seed can be specified using argument seed, else the default values are taken. A set. seed call on the master is required additionally and argument 1b=FALSE, see below.

• If RNG="fixed", a seed has to be specified. This can be either an integer or a vector of length number of samples +2. In the second case, the first entry is used for the main R process, the next number of samples ones for each sample run (in parallel execution mode on slave R processes) and the last one for computation on full sample (as well on slave R process in parallel execution mode). Passing integer x is equivalent to passing vector x+(0:(number of samples+1)). This procedure allows reproducibility in any case, i.e. also if the number of parallel processes changes as well as in sequential execution.

Load balancing (argument 1b) means, that a slave gets a new job immediately after the previous is finished. This speeds up computation, but may change the order of jobs. Due to that, results are only reproducible, if RNG="fixed" is used.

Value

Object of class peperr

indices list of resampling indices.

complexity passed complexity. If argument complexity not specified, 0.

selected.complexity

selected complexity for the full data set, if complexity was passed as function.

Else equal to value complexity.

response passed response.

full.model.fit List, one entry per complexity value. Fitted model of the full data set by passed

fit.fun.

full apparent full apparent error of the full data set. Matrix: One row per complexity value. In

case of survival response, columns correspond to evaluation timepoints, which

are returned in value attribute.

noinf.error No information error of the full data set, i. e. evaluation in permuted data.

Matrix: One row per complexity value. Columns correspond to evaluation time-

points, which are returned in attribute.

attribute if response is survival: Evaluation time points. Passed in args.aggregation or

automatically determined by aggregation function. Otherwise, if available, extra

attribute returned by aggregation function, else NULL, see Details.

sample.error list. Each entry contains matrix of prediction error for one resampling test sam-

ple. One row per complexity value.

sample.complexity

vector of complexity values. Equals value complexity, if complexity value was passed explicitly, otherwise by function complexity selected complexity value

for each resampling sample. If argument complexity not specified, 0.

sample.lipec only, if response is survival. Lebesgue integrated prediction error curve for each

sample. List with one entry per sample, each a matrix with one row per com-

plexity value.

sample.pll only, if response is survival and PLL.class function available. Predictive partial

log likelihood for each sample. List with one entry per sample, each a matrix

with one row per complexity value.

```
null.model.fit only, if response is survival or binary. Fit of null model, i.e. fit without information of covariates. In case of survival response Kaplan-Meier, else logistic regression model.

null.model only, if response is survival or binary. Vector or scalar: Prediction error of the null model, in case of survival response at each evaluation time point.

sample.null.model
```

list. Prediction error of the null model for one resampling test sample. Matrix, one row per complexity value.

Author(s)

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References

Binder, H. and Schumacher, M. (2008) Adapting prediction error estimates for biased complexity selection in high-dimensional bootstrap samples. Statistical Applications in Genetics and Molecular Biology, 7:1.

Porzelius, C., Binder, H., Schumacher, M. (2008) Parallelised prediction error estimation for evaluation of high-dimensional models. Manuscript.

See Also

```
perr, resample.indices, extract.fun
```

Examples

```
# Generate survival data with 10 informative covariates
## Not run:
n <- 200
p <- 100
beta <- c(rep(1,10), rep(0,p-10))
x <- matrix(rnorm(n*p),n,p)</pre>
real.time <- -(log(runif(n)))/(10*exp(drop(x %*% beta)))</pre>
cens.time <- rexp(n,rate=1/10)</pre>
status <- ifelse(real.time <= cens.time,1,0)</pre>
time <- ifelse(real.time <= cens.time,real.time,cens.time)</pre>
# A: R runs sequential or R is started on commandline with desired options
# (for example using sfCluster: sfCluster -i --cpus=5)
# Example A1:
# Obtain prediction error estimate fitting a Cox proportional hazards model
# using CoxBoost
# through 10 bootstrap samples
# with fixed complexity 50 and 75
# and aggregate using prediction error curves (default setting)
peperr.object1 <- peperr(response=Surv(time, status), x=x,</pre>
   fit.fun=fit.CoxBoost, complexity=c(50, 75),
   indices=resample.indices(n=length(time), method="sub632", sample.n=10))
peperr.object1
```

```
# Diagnostic plots
plot(peperr.object1)
# Extraction of prediction error curves (.632+ prediction error estimate),
# blue line corresponds to complexity 50,
# red one to complexity 75
plot(peperr.object1$attribute,
  perr(peperr.object1)[1,], type="l", col="blue",
  xlab="Evaluation time points", ylab="Prediction error")
lines(peperr.object1$attribute,
  perr(peperr.object1)[2,], col="red")
# Example A2:
# As Example A1, but
# with complexity selected through a cross-validation procedure
# and extra argument 'penalty' passed to fit function and complexity function
peperr.object2 <- peperr(response=Surv(time, status), x=x,</pre>
   fit.fun=fit.CoxBoost, args.fit=list(penalty=100),
   complexity=complexity.mincv.CoxBoost, args.complexity=list(penalty=100),
   indices=resample.indices(n=length(time), method="sub632", sample.n=10),
   trace=TRUE)
peperr.object2
# Diagnostic plots
plot(peperr.object2)
# Example A3:
# As Example A2, but
# with extra argument 'times', specifying the evaluation times passed to aggregation.fun
# and seed, for reproducibility of results
# Note: set.seed() is required additional to argument 'seed',
# as function 'resample.indices' is used in peperr call.
set.seed(123)
peperr.object3 <- peperr(response=Surv(time, status), x=x,</pre>
   fit.fun=fit.CoxBoost, args.fit=list(penalty=100),
   complexity=complexity.mincv.CoxBoost, args.complexity=list(penalty=100),
   indices=resample.indices(n=length(time), method="sub632", sample.n=10),
  args.aggregation=list(times=seq(0, quantile(time, probs=0.9), length.out=100)),
   trace=TRUE, RNG="fixed", seed=321)
peperr.object3
# Diagnostic plots
plot(peperr.object3)
# B: R is started sequential, desired cluster options are given as arguments
# Example B1:
# As example A1, but using a socket cluster and 3 CPUs
peperr.object4 <- peperr(response=Surv(time, status), x=x,</pre>
   fit.fun=fit.CoxBoost, complexity=c(50, 75),
   indices=resample.indices(n=length(time), method="sub632", sample.n=10),
   parallel=TRUE, clustertype="SOCK", cpus=3)
```

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```
## End(Not run)
```

perr

Prediction error estimates

Description

Extracts prediction error estimates from peperr objects.

Usage

```
perr(peperrobject,
    type = c("632p", "632", "apparent", "NoInf", "resample", "nullmodel"))
```

Arguments

peperrobject peperr object obtained by call to function peperr.

type "632p" for the .632+ prediction error estimate (default), "632" for the .632 pre-

diction error estimate. "apparent", "NoInf", "resample" and "nullmodel" return the apparent error, the no-information error, the mean sample error and

the nullmodel fit, see Details.

Details

The .632 and the .632+ prediction error estimates are weighted combinations of the apparent error and bootstrap cross-validation error estimate, for survival data at given time points.

Value

If type="632p" or type="632": Prediction error: Matrix, with one row per complexity value.

If type="apparent": Apparent error of the full data set. Matrix: One row per complexity value. In case of survival response, columns correspond to evaluation timepoints, which are given in attribute addattr.

If type="NoInf": No-information error of the full data set, i. e. evaluation in permuted data. Matrix: One row per complexity value. Columns correspond to evaluation timepoints, which are given in attribute addattr.

If type="resample": Matrix. Mean prediction error of resampling test samples, one row per complexity value.

If type="nullmodel": Vector or scalar: Null model prediction error, i.e. of fit without information of covariates. In case of survival response Kaplan-Meier estimate at each time point, if response is binary logistic regression model, else not available.

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References

Binder, H. and Schumacher, M. (2008) Adapting prediction error estimates for biased complexity selection in high-dimensional bootstrap samples. Statistical Applications in Genetics and Molecular Biology, 7:1.

Gerds, T. and Schumacher, M. (2007) Efron-type measures of prediction error for survival analysis. Biometrics, 63, 1283–1287.

Schumacher, M. and Binder, H., and Gerds, T. (2007) Assessment of Survival Prediction Models in High-Dimensional Settings. Bioinformatics, 23, 1768-1774.

See Also

```
peperr, ipec
```

Examples

```
## Not run:
n <- 200
p <- 100
beta <- c(rep(1,10),rep(0,p-10))
x <- matrix(rnorm(n*p),n,p)</pre>
real.time <- -(log(runif(n)))/(10*exp(drop(x %*% beta)))</pre>
cens.time <- rexp(n,rate=1/10)</pre>
status <- ifelse(real.time <= cens.time,1,0)</pre>
time <- ifelse(real.time <= cens.time,real.time,cens.time)</pre>
# Example:
# Obtain prediction error estimate fitting a Cox proportional hazards model
# using CoxBoost
# through 10 bootstrap samples
# with fixed complexity 50 and 75
# and aggregate using prediction error curves
peperr.object <- peperr(response=Surv(time, status), x=x,</pre>
   fit.fun=fit.CoxBoost, complexity=c(50, 75),
   indices=resample.indices(n=length(time), method="sub632", sample.n=10))
# 632+ estimate for both complexity values at each time point
perr(peperr.object)
## End(Not run)
```

PLL

Generic function for extracting the predictive partial log-likelihood

Description

Generic function for extracting th predictive partial log-likelihood from a fitted survival model.

PLL.CoxBoost

Usage

```
PLL(object, newdata, newtime, newstatus, ...)
```

Arguments

object fitted model of class class.

newdata n_new*p matrix of covariates.

newtime n_new-vector of censored survival times.

newstatus n_new-vector of event status, coded with 0 for censoring and 1, if an event oc-

curred.

... additional arguments, for example complexity value, if necessary.

Details

The predictive partial log-likelihood measures the prediction performance of each model fitted in a boostrap sample, using the data not in this sample. Multiplying by (-2) leads to a deviance-like measure, which means that small values indicate good prediction performance.

peperr requires function PLL. class in case of survival response, for each model fit of class class. At the time, PLL. CoxBoost is available.

Value

Vector of length n_new

PLL.CoxBoost Predictive partial log-likelihood for CoxBoost model fit

Description

Extracts the predictive partial log-likelihood from a CoxBoost model fit.

Usage

```
## S3 method for class 'CoxBoost'
PLL(object, newdata, newtime, newstatus, complexity, ...)
```

Arguments

object fitted model of class CoxBoost.

newdata n_new*p matrix of covariates.

newtime n_new-vector of censored survival times.

newstatus n_new-vector of survival status, coded with 0 and .1

complexity complexity, either one value, which is number of boosting steps, or a list con-

taining number of boosting steps in argument stepno.

... additional arguments, not used.

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Details

Used by function peperr, if function fit. CoxBoost is used for model fit.

Value

Vector of length n_new

PLL.coxph

Predictive partial log-likelihood for Cox poportional hazards model

Description

Extracts the predictive partial log-likelihood from a coxph model fit.

Usage

```
## S3 method for class 'coxph'
PLL(object, newdata, newtime, newstatus, complexity, ...)
```

Arguments

object fitted model of class coxph.

newdata n_new*p matrix of covariates.

 $\label{eq:newtime} \mbox{n_new-vector of censored survival times}.$

newstatus n_new-vector of survival status, coded with 0 and .1

complexity not used.

... additional arguments, not used.

Details

Used by function peperr, if function fit.coxph is used for model fit.

Value

Vector of length n_new

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plot.peperr

Plot method for peperr object

Description

Plots, allowing to get a first impression of the prediction error estimates and to check complexity selection in bootstrap samples.

Usage

```
## S3 method for class 'peperr'
plot(x, y, ...)
```

Arguments

```
x peperr object.y not used.... additional arguments, not used.
```

Details

The plots provide a simple and fast overview of the results of the estimation of the prediction error through resampling. Which plots are shown depends on if complexity was selected, i.e., a function was passed in the peperr call for complexity, or explicitly passed. In case of survival response, prediction error curves are shown. In case of binary response, where one complexity value is passed explicitly, no plot is available. Especially in the case that complexity is selected in each bootstrap sample, these diagnostic plots help to check whether the resampling procedure works adequately and to detect specific problems due to high-dimensional data structures.

Examples

```
## Not run:
n <- 200
p <- 100
beta <- c(rep(1,10),rep(0,p-10))
x <- matrix(rnorm(n*p),n,p)
real.time <- -(log(runif(n)))/(10*exp(drop(x %*% beta)))
cens.time <- rexp(n,rate=1/10)
status <- ifelse(real.time <= cens.time,1,0)
time <- ifelse(real.time <= cens.time,real.time,cens.time)

peperr.object1 <- peperr(response=Surv(time, status), x=x,
    fit.fun=fit.CoxBoost, complexity=c(50, 75),
    indices=resample.indices(n=length(time), method="sub632", sample.n=10))
plot(peperr.object1)

peperr.object2 <- peperr(response=Surv(time, status), x=x,
    fit.fun=fit.CoxBoost, args.fit=list(penalty=100),</pre>
```

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```
complexity=complexity.mincv.CoxBoost, args.complexity=list(penalty=100),
  indices=resample.indices(n=length(time), method="sub632", sample.n=10),
  trace=TRUE)
plot(peperr.object2)

peperr.object3 <- peperr(response=Surv(time, status), x=x,
  fit.fun=fit.CoxBoost, args.fit=list(penalty=100),
  complexity=complexity.mincv.CoxBoost, args.complexity=list(penalty=100),
  indices=resample.indices(n=length(time), method="sub632", sample.n=10),
  args.aggregation=list(times=seq(0, quantile(time, probs=0.9), length.out=100)),
  trace=TRUE)
plot(peperr.object3)

## End(Not run)</pre>
```

pmpec

Calculate prediction error curves

Description

Calculation of prediction error curve from a survival response and predicted probabilities of survival.

Usage

Arguments

object fitted model of a class for which the interface function predictProb.class is

available.

response Either a survival object (with Surv(time, status), where time is an n-vector

of censored survival times and status an n-vector containing event status, coded with 0 and 1) or a matrix with columns time containing survival times and status containing integers, where 0 indicates censoring, 1 the interesting event

and larger numbers other competing risks.

x n*p matrix of covariates.

times vector of time points at which the prediction error is to be estimated.

model.args named list of additional arguments, e.g. complexity value, which are to be

passed to predictProb function.

type type of output: Estimated prediction error (default) or no information error (pre-

diction error obtained by permuting the data).

external.time optional vector of time points, used for censoring distribution.

external.status

optional vector of status values, used for censoring distribution.

26 predictProb

data

Data frame containing n-vector of observed times ('time'), n-vector of event status ('status') and n*p matrix of covariates (remaining entries). Alternatively to response and x, for compatibility to **pec**.

Details

Prediction error of survival data is measured by the Brier score, which considers the squared difference of the true event status at a given time point and the predicted event status by a risk prediction model at that time. A prediction error curve is the weighted mean Brier score as a function of time at time points in times (see References).

pmpec requires a predictProb method for the class of the fitted model, i.e. for a model of class class predictProb.class.

pmpec is implemented to behave similar to function pec of package **pec**, which provides several predictProb methods.

In bootstrap framework, data contains only a part of the full data set. For censoring distribution, the full data should be used to avoid extreme variance in case of small data sets. For that, the observed times and status values can be passed as argument external.time and external.status.

Value

Vector of prediction error estimates at each time point given in time.

Author(s)

Harald Binder

References

Gerds, A. and Schumacher, M. (2006) Consistent estimation of the expected Brier score in general survival models with right-censored event times. Biometrical Journal, 48, 1029–1040.

Schoop, R. (2008) Predictive accuracy of failure time models with longitudinal covariates. PhD thesis, University of Freiburg. http://www.freidok.uni-freiburg.de/volltexte/4995/.

See Also

predictProb, pec

predictProb

Generic function for extracting predicted survival probabilities

Description

Generic function for extraction of predicted survival probabilities from a fitted survival model conforming to the interface required by pmpec.

predictProb.CoxBoost 27

Usage

```
predictProb(object, response, x, ...)
```

Arguments

object a fitted survival model.

response Either a survival object (with Surv(time, status), where time is an n-vector

of censored survival times and status an n-vector containing event status, coded with 0 and 1) or a matrix with columns time containing survival times and status containing integers, where 0 indicates censoring, 1 the interesting event and larger numbers other competing risks. In case of binary response, vector

with entries 0 and 1.

x n*p matrix of covariates.

... additional arguments, for example model complexity or, in case of survival re-

sponse, argument times, a vector containing evaluation times.

Details

pmpec requires a predictProb.class function for each model fit of class class. It extracts the predicted probability of survival from this model.

See existing predictProb functions, at the time predictProb.CoxBoost, predictProb.coxph and predictProb.survfit.

If desired predictProb function for class class is not available in **peperr**, but implemented in package **pec** as predictSurvProb.class, it can easily be transformed as predictProb method.

Value

Matrix with predicted probabilities for each evaluation time point in times (columns) and each new observation (rows).

predictProb.CoxBoost Extract predicted survival probabilities from a CoxBoost fit

Description

Extracts predicted survival probabilities from survival model fitted by CoxBoost, providing an interface as required by pmpec.

Usage

```
## S3 method for class 'CoxBoost'
predictProb(object, response, x, times, complexity, ...)
```

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Arguments

object a fitted model of class CoxBoost.

response survival object (with Surv(time, status), where time is an n-vector of cen-

sored survival times and status an n-vector containing survival status, coded with

0 and 1.

x n*p matrix of covariates.

times vector of evaluation time points.

complexity complexity value.

. . . additional arguments, currently not used.

Value

Matrix with probabilities for each evaluation time point in times (columns) and each new observation (rows).

predictProb.coxph

Extract predicted survival probabilities from a coxph object

Description

Extracts predicted survival probabilities for survival models fitted by Cox proportional hazards model, providing an interface as required by pmpec.

Usage

```
## S3 method for class 'coxph'
predictProb(object, response, x, times, ...)
```

Arguments

object a fitted model of class coxph.

response survival object (with Surv(time, status), where time is an n-vector of cen-

sored survival times and status an n-vector containing survival status, coded with

0 and 1.

x n*p matrix of covariates.

times vector of evaluation time points.

... additional arguments, currently not used.

Value

Matrix with probabilities for each evaluation time point in times(columns) and each new observation (rows).

predictProb.survfit 29

predictProb.survfit Extract predicted survival probabilities from a survfit object

Description

Extracts predicted survival probabilities for survival models fitted by survfit, providing an interface as required by pmpec.

Usage

```
## S3 method for class 'survfit'
predictProb(object, response, x, times, train.data, ...)
```

Arguments

object a fitted model of class survfit.

response survival object (with Surv(time, status), where time is an n-vector of cen-

sored survival times and status an n-vector containing survival status, coded with

0 and 1.

x n*p matrix of covariates.

times vector of evaluation time points.

train.data not used.

... additional arguments, currently not used.

Value

Matrix with probabilities for each evaluation time point in times(columns) and each new observation (rows).

resample.indices Generation of indices for resampling Procedure

Description

Generates training and test set indices for use in resampling estimation of prediction error, e.g. cross-validation or bootstrap (with and without replacement).

Usage

```
resample.indices(n, sample.n = 100, method = c("no", "cv", "boot", "sub632"))
```

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Arguments

n number of observations of the full data set.

sample.n the number of bootstrap samples in case of method="boot" and the number

of cross-validation subsets in case of method="cv", e.g. 10 for 10-fold cross-validation. Not considered if method="no", where number of samples is one

(the full data set) by definition.

method by default, the training set indices are the same as the test set indices, i.e. the

model is assessed in the same data as fitted ("no"). "cv": Cross-validation, "boot": Bootstrap (with replacement), "sub632": Boostrap without replacement, also called subsampling. In the latter case, the number of observations in

each sample equals round (0.632 * n), see Details.

Details

As each bootstrap sample should be taken as if new data, complexity selection should be carried out in each bootstrap sample. Binder and Schumacher show that when bootstrap samples are drawn with replacement, often too complex models are obtained in high-dimensional data settings. They recommend to draw bootstrap samples without replacement, each of size $round(0.632 \times n)$, which equals the expected number of unique observations in one bootstrap sample drawn with replacement, to avoid biased complexity selection and improve predictive power of the resulting models.

Value

A list containing two lists of length sample.n:

sample.index contains in each element the indices of observations of one training set.

not.in.sample contains in each element the indices of observations of one test set, correspond-

ing to the training set in listelement sample.index.

References

Binder, H. and Schumacher, M. (2008) Adapting prediction error estimates for biased complexity selection in high-dimensional bootstrap samples. Statistical Applications in Genetics and Molecular Biology, 7:1.

See Also

peperr

Examples

```
# generate dataset: 100 patients, 20 covariates
data <- matrix(rnorm(2000), nrow=100)

# generate indices for training and test data for 10-fold cross-validation
indices <- resample.indices(n=100, sample.n = 10, method = "cv")

# create training and test data via indices</pre>
```

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```
trainingsample1 <- data[indices$sample.index[[1]],]
testsample1 <- data[indices$not.in.sample[[1]],]</pre>
```

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