

Package: penaltyLearning (via r-universe)

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Title Penalty Learning

Description Implementations of algorithms from Learning Sparse Penalties for Change-point Detection using Max Margin Interval Regression, by Hocking, Rigaiil, Vert, Bach
<<http://proceedings.mlr.press/v28/hocking13.html>> published in proceedings of ICML2013.

Suggests neuroblastoma, jointseg, testthat, future, future.apply, PeakSegDP, PeakError, PeakSegOptimal, directlabels (>= 2017.03.31)

Depends R (>= 2.10)

URL <https://github.com/tdhock/penaltyLearning>

BugReports <https://github.com/tdhock/penaltyLearning/issues>

Imports data.table (>= 1.9.8), ggplot2

Repository <https://tdhock.r-universe.dev>

RemoteUrl <https://github.com/tdhock/penaltylearning>

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change.colors	<i>change colors</i>
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Description

character vector of change-point label colors, to be used with `ggplot2::scale*_manual`

Usage

"change.colors"

change.labels	<i>change labels</i>
---------------	----------------------

Description

data.table of meta-data for label types.

Usage

"change.labels"

changeLabel	<i>changeLabel</i>
-------------	--------------------

Description

Describe an annotated region label for supervised change-point detection.

Usage

```
changeLabel(annotation,  
            min.changes, max.changes,  
            color)
```

Arguments

annotation	annotation
min.changes	min.changes
max.changes	max.changes
color	color

Author(s)

Toby Dylan Hocking

check_features_targets

check features targets

Description

stop with an informative error if there is a problem with the feature or target matrix.

Usage

```
check_features_targets(feature.mat,  
                       target.mat)
```

Arguments

feature.mat	n x p numeric input feature matrix.
target.mat	n x 2 matrix of target interval limits.

Value

number of observations/rows.

Author(s)

Toby Dylan Hocking

check_target_pred

check target pred

Description

stop with an informative error if there are problems with the target matrix or predicted values.

Usage

```
check_target_pred(target.mat,  
                  pred)
```

Arguments

target.mat	target.mat
pred	pred

Value

number of observations.

Author(s)

Toby Dylan Hocking

```
coef.IntervalRegression
      coef IntervalRegression
```

Description

Get the learned coefficients of an IntervalRegression model.

Usage

```
## S3 method for class 'IntervalRegression'
coef(object,
      ...)
```

Arguments

object	object
...	...

Value

numeric matrix [features x regularizations] of learned weights (on the original feature scale), can be used for prediction via `cbind(1,features) %*% weights`.

Author(s)

Toby Dylan Hocking

```
demo8      PeakSegFPOP demo data set
```

Description

PeakSegFPOP demo data set with 8 observations

Usage

```
data("demo8")
```

Format

A list of two objects: `feature.mat` is an 8 x 36 input feature matrix, and `target.mat` is a 8 x 2 output limit matrix.

featureMatrix	<i>featureMatrix</i>
---------------	----------------------

Description

Compute a feature matrix (segmentation problems x features).

Usage

```
featureMatrix(data.sequences,  
              problem.vars, data.var)
```

Arguments

`data.sequences` data.frame of sorted sequences of data to segment.
`problem.vars` character vector of columns of `data.sequences` to treat as segmentation problem IDs.
`data.var` character vector of length 1 (column of `data.sequences` to treat as data to segment).

Value

Numeric feature matrix. Some entries may be missing or infinite; these columns should be removed before model training.

Author(s)

Toby Dylan Hocking

Examples

```
test.df <- data.frame(  
  id=rep(1:2, each=10),  
  x=rnorm(20))  
penaltyLearning::featureMatrix(test.df, "id", "x")  
if(requireNamespace("neuroblastoma")){  
  data(neuroblastoma, package="neuroblastoma", envir=environment())  
  one <- subset(neuroblastoma$profiles, profile.id %in% c(1,2))  
  f.mat <- penaltyLearning::featureMatrix(  
    one, c("profile.id", "chromosome"), "logratio")  
}
```

featureVector	<i>featureVector</i>
---------------	----------------------

Description

Compute a feature vector of constant length which can be used as an input for supervised penalty learning. The output is a target interval of log(penalty) values that achieve minimum incorrect labels (see [targetIntervals](#)).

Usage

```
featureVector(data.vec)
```

Arguments

data.vec numeric vector of ordered data.

Value

Numeric vector of features.

Author(s)

Toby Dylan Hocking

Examples

```
x <- rnorm(10)
penaltyLearning::featureVector(x)
if(requireNamespace("neuroblastoma")){
  data(neuroblastoma, package="neuroblastoma", envir=environment())
  one <- subset(neuroblastoma$profiles, profile.id=="1" & chromosome=="1")
  (f.vec <- penaltyLearning::featureVector(one$logratio))
}
```

GeomTallRect	<i>GeomTallRect</i>
--------------	---------------------

Description

ggproto object for [geom_tallrect](#)

Usage

```
"GeomTallRect"
```

geom_tallrect	<i>geom_tallrect</i>
---------------	----------------------

Description

ggplot2 geom with xmin and xmax aesthetics that covers the entire y range, useful for clickSelects background elements.

Usage

```
geom_tallrect(mapping = NULL,
              data = NULL, stat = "identity",
              position = "identity",
              ..., na.rm = FALSE,
              show.legend = NA,
              inherit.aes = TRUE)
```

Arguments

mapping	mapping
data	data
stat	stat
position	position
...	...
na.rm	na.rm
show.legend	show.legend
inherit.aes	inherit.aes

Author(s)

Toby Dylan Hocking

IntervalRegressionCV	<i>IntervalRegressionCV</i>
----------------------	-----------------------------

Description

Use cross-validation to fit an L1-regularized linear interval regression model by optimizing margin and/or regularization parameters. This function repeatedly calls [IntervalRegressionRegularized](#), and by default assumes that margin=1. To optimize the margin, specify the margin.vec parameter manually, or use [IntervalRegressionCVmargin](#) (which takes more computation time but yields more accurate models). If the future package is available, two levels of future_lapply are used to parallelize on validation.fold and margin.

Usage

```
IntervalRegressionCV(feature.mat,
  target.mat, n.folds = ifelse(nrow(feature.mat) <
    10, 3L, 5L),
  fold.vec = sample(rep(1:n.folds,
    l = nrow(feature.mat))),
  verbose = 0, min.observations = 10,
  reg.type = "min",
  incorrect.labels.db = NULL,
  initial.regularization = 0.001,
  margin.vec = 1, LAPPLY = NULL,
  check.unlogged = TRUE,
  ...)
```

Arguments

<code>feature.mat</code>	Numeric feature matrix, n observations x p features.
<code>target.mat</code>	Numeric target matrix, n observations x 2 limits. These should be real-valued (possibly negative). If your data are interval censored positive-valued survival times, you need to log them to obtain <code>target.mat</code> .
<code>n.folds</code>	Number of cross-validation folds.
<code>fold.vec</code>	Integer vector of fold id numbers.
<code>verbose</code>	numeric: 0 for silent, bigger numbers (1 or 2) for more output.
<code>min.observations</code>	stop with an error if there are fewer than this many observations.
<code>reg.type</code>	Either "1sd" or "min" which specifies how the regularization parameter is chosen during the internal cross-validation loop. <code>min</code> : first take the mean of the K-CV error functions, then minimize it (this is the default since it tends to yield the least test error). <code>1sd</code> : take the most regularized model with the same margin which is within one standard deviation of that minimum (this model is typically a bit less accurate, but much less complex, so better if you want to interpret the coefficients).
<code>incorrect.labels.db</code>	either <code>NULL</code> or a <code>data.table</code> , which specifies the error function to compute for selecting the regularization parameter on the validation set. <code>NULL</code> means to minimize the squared hinge loss, which measures how far the predicted $\log(\text{penalty})$ values are from the target intervals. If a <code>data.table</code> is specified, its first key should correspond to the rownames of <code>feature.mat</code> , and columns <code>min.log.lambda</code> , <code>max.log.lambda</code> , <code>fp</code> , <code>fn</code> , <code>possible.fp</code> , <code>possible.fn</code> ; these will be used with ROChange to compute the AUC for each regularization parameter, and the maximum will be selected (in the plot this is <code>negative.auc</code> , which is minimized). This <code>data.table</code> can be computed via <code>labelError(modelSelection(. . .),...)\$model.errors</code> – see example(ROChange). In practice this makes the computation longer, and it should only result in more accurate models if there are many labels per data sequence.
<code>initial.regularization</code>	Passed to IntervalRegressionRegularized .

margin.vec	numeric vector of margin size hyper-parameters. The computation time is linear in the number of elements of margin.vec – more values takes more computation time, but yields slightly more accurate models (if there is enough data).
LAPPLY	Function to use for parallelization, by default <code>future_lapply</code> if it is available, otherwise <code>lapply</code> . For debugging with <code>verbose>0</code> it is useful to specify <code>LAPPLY=lapply</code> in order to interactively see messages, before all parallel processes end.
check.unlogged	If TRUE, stop with an error if target matrix is non-negative and has any big difference in successive quantiles (this is an indicator that the user probably forgot to log their outputs).
...	passed to <code>IntervalRegressionRegularized</code> .

Value

List representing regularized linear model.

Author(s)

Toby Dylan Hocking

Examples

```
if(interactive()){
  library(penaltyLearning)
  data("neuroblastomaProcessed", package="penaltyLearning", envir=environment())
  if(require(future)){
    plan(multiprocess)
  }
  set.seed(1)
  i.train <- 1:100
  fit <- with(neuroblastomaProcessed, IntervalRegressionCV(
    feature.mat[i.train,], target.mat[i.train,],
    verbose=0))
  ## When only features and target matrices are specified for
  ## training, the squared hinge loss is used as the metric to
  ## minimize on the validation set.
  plot(fit)
  ## Create an incorrect labels data.table (first key is same as
  ## rownames of feature.mat and target.mat).
  library(data.table)
  errors.per.model <- data.table(neuroblastomaProcessed$errors)
  errors.per.model[, pid.chr := paste0(profile.id, ".", chromosome)]
  setkey(errors.per.model, pid.chr)
  set.seed(1)
  fit <- with(neuroblastomaProcessed, IntervalRegressionCV(
    feature.mat[i.train,], target.mat[i.train,],
    ## The incorrect.labels.db argument is optional, but can be used if
    ## you want to use AUC as the CV model selection criterion.
    incorrect.labels.db=errors.per.model))
  plot(fit)
}
```

IntervalRegressionCVmargin

IntervalRegressionCVmargin

Description

Use cross-validation to fit an L1-regularized linear interval regression model by optimizing both margin and regularization parameters. This function just calls [IntervalRegressionCV](#) with a `margin.vec` parameter that is computed based on the finite target interval limits. If default parameters are used, this function should be about 10 times slower than [IntervalRegressionCV](#) (since this function computes `n.margin=10` models per regularization parameter whereas [IntervalRegressionCV](#) only computes one). On large ($N > 1000$ rows) data sets, this function should yield a model which is a little more accurate than [IntervalRegressionCV](#) (since the margin parameter is optimized).

Usage

```
IntervalRegressionCVmargin(feature.mat,
    target.mat, log10.diff = 2,
    n.margin = 10L, ...)
```

Arguments

<code>feature.mat</code>	Numeric feature matrix, n observations \times p features.
<code>target.mat</code>	Numeric target matrix, n observations \times 2 limits.
<code>log10.diff</code>	Numeric scalar: factors of 10 below the largest finite limit difference to use as a minimum margin value (difference on the \log_{10} scale which is used to generate margin parameters). Bigger values mean a grid of margin parameters with a larger range. For example if the largest finite limit in <code>target.mat</code> is 26 and the smallest finite limit is -4 then the largest limit difference is 30, which will be used as the maximum margin parameter. If <code>log10.diff</code> is the default of 2 then that means the smallest margin parameter will be 0.3 (two factors of 10 smaller than 30).
<code>n.margin</code>	Integer scalar: number of margin parameters, by default 10.
<code>...</code>	Passed to IntervalRegressionCV .

Value

Model fit list from [IntervalRegressionCV](#).

Author(s)

Toby Dylan Hocking

Examples

```

if(interactive()){
  library(penaltyLearning)
  data(
    "neuroblastomaProcessed",
    package="penaltyLearning",
    envir=environment())
  if(require(future)){
    plan(multiprocess)
  }
  set.seed(1)
  fit <- with(neuroblastomaProcessed, IntervalRegressionCVmargin(
    feature.mat, target.mat, verbose=1))
  plot(fit)
  print(fit$plot.heatmap)
}

```

IntervalRegressionInternal

IntervalRegressionInternal

Description

Solve the squared hinge loss interval regression problem for one regularization parameter: $w^* = \operatorname{argmin}_w L(w) + \text{regularization} * \|w\|_1$ where $L(w)$ is the average squared hinge loss with respect to the targets, and $\|w\|_1$ is the L1-norm of the weight vector (excluding the first element, which is the un-regularized intercept or bias term). This function performs no scaling of input features, and is meant for internal use only! To learn a regression model, try [IntervalRegressionCV](#) or [IntervalRegressionUnregularized](#).

Usage

```

IntervalRegressionInternal(features,
  targets, initial.param.vec,
  regularization, threshold = 0.001,
  max.iterations = 1000,
  weight.vec = NULL,
  Lipschitz = NULL,
  verbose = 2, margin = 1,
  biggest.crit = 100)

```

Arguments

features	Scaled numeric feature matrix (problems x features). The first column/feature should be all ones and will not be regularized.
targets	Numeric target matrix (problems x 2).
initial.param.vec	initial guess for weight vector (features).

regularization	Degree of L1-regularization.
threshold	When the stopping criterion gets below this threshold, the algorithm stops and declares the solution as optimal.
max.iterations	If the algorithm has not found an optimal solution after this many iterations, increase Lipschitz constant and max.iterations.
weight.vec	A numeric vector of weights for each training example.
Lipschitz	A numeric scalar or NULL, which means to compute Lipschitz as the mean of the squared L2-norms of the rows of the feature matrix.
verbose	Cat messages: for restarts and at the end if ≥ 1 , and for every iteration if ≥ 2 .
margin	Margin size hyper-parameter, default 1.
biggest.crit	Restart FISTA with a bigger Lipschitz (smaller step size) if crit gets larger than this.

Value

Numeric vector of scaled weights w of the affine function $f_w(X) = X \%*\% w$ for a scaled feature matrix X with the first row entirely ones.

Author(s)

Toby Dylan Hocking

IntervalRegressionRegularized
IntervalRegressionRegularized

Description

Repeatedly use [IntervalRegressionInternal](#) to solve interval regression problems for a path of regularization parameters. This function does not perform automatic selection of the regularization parameter; instead, it returns regression models for a range of regularization parameters, and it is up to you to select which one to use. For automatic regularization parameter selection, use [IntervalRegressionCV](#).

Usage

```
IntervalRegressionRegularized(feature.mat,
  target.mat, initial.regularization = 0.001,
  factor.regularization = 1.2,
  verbose = 0, margin = 1,
  ...)
```

Arguments

<code>feature.mat</code>	Numeric feature matrix.
<code>target.mat</code>	Numeric target matrix.
<code>initial.regularization</code>	Initial regularization parameter.
<code>factor.regularization</code>	Increase regularization by this factor after finding an optimal solution. Or NULL to compute just one model (<code>initial.regularization</code>).
<code>verbose</code>	Print messages if ≥ 1 .
<code>margin</code>	Non-negative margin size parameter, default 1.
<code>...</code>	Other parameters to pass to IntervalRegressionInternal .

Value

List representing fit model. You can do `fit$predict(feature.matrix)` to get a matrix of predicted log penalty values. The `param.mat` is the `n.features * n.regularization` numeric matrix of optimal coefficients (on the original scale).

Author(s)

Toby Dylan Hocking

Examples

```
if(interactive()){
  library(penaltyLearning)
  data("neuroblastomaProcessed", package="penaltyLearning", envir=environment())
  i.train <- 1:500
  fit <- with(neuroblastomaProcessed, IntervalRegressionRegularized(
    feature.mat[i.train,], target.mat[i.train,]))
  plot(fit)
}
```

IntervalRegressionUnregularized

IntervalRegressionUnregularized

Description

Use [IntervalRegressionRegularized](#) with `initial.regularization=0` and `factor.regularization=NULL`, meaning fit one un-regularized interval regression model.

Usage

```
IntervalRegressionUnregularized(...)
```

Arguments

... passed to [IntervalRegressionRegularized](#).

Value

List representing fit model, see [help\(IntervalRegressionRegularized\)](#) for details.

Author(s)

Toby Dylan Hocking

labelError	<i>Compute incorrect labels</i>
------------	---------------------------------

Description

Compute incorrect labels for several change-point detection problems and models. Use this function after having computed changepoints, loss values, and model selection functions (see [modelSelection](#)). The next step after labelError is typically computing target intervals of log(penalty) values that predict changepoints with minimum incorrect labels for each problem (see [targetIntervals](#)).

Usage

```
labelError(models, labels,
           changes, change.var = "chromStart",
           label.vars = c("min",
                         "max"), model.vars = "n.segments",
           problem.vars = character(0),
           annotations = change.labels)
```

Arguments

models	data.frame with one row per (problem,model) combination, typically the output of modelSelection(...) . There is a row for each changepoint model that could be selected for a particular segmentation problem. There should be columns <code>problem.vars</code> (for problem ID) and <code>model.vars</code> (for model complexity).
labels	data.frame with one row per (problem,region). Each label defines a region in a particular segmentation problem, and a range of predicted changepoints which are consistent in that region. There should be a column "annotation" which takes one of the corresponding values in the annotation column of change.labels (used to determine the range of predicted changepoints which are consistent). There should also be a columns <code>problem.vars</code> (for problem ID) and <code>label.vars</code> (for region start/end).
changes	data.frame with one row per (problem,model,change), for each predicted change-point (in each model and segmentation problem). Should have columns <code>problem.vars</code> (for problem ID), <code>model.vars</code> (for model complexity), and <code>change.var</code> (for changepoint position).

change.var	character(length=1): column name of predicted change-point position in labels. The default "chromStart" is useful for genomic data with segment start/end positions stored in columns named chromStart/chromEnd. A predicted changepoint at position X is interpreted to mean a changepoint between X and X+1.
label.vars	character(length=2): column names of start and end positions of labels, in same units as change-point positions. The default is c("min", "max"). Labeled regions are (start,end] – open on the left and closed on the right, so for example a 0changes annotation between start=10 and end=20 means that any predicted changepoint at 11, ..., 20 is a false positive.
model.vars	character: column names used to identify model complexity. The default "n.segments" is for change-point models such as in the jointseg and changepoint packages.
problem.vars	character: column names used to identify data set / segmentation problem, should be present in all three data tables (models, labels, changes).
annotations	data.table with columns annotation, min.changes, max.changes, possible.fn, possible.fp which is joined to labels in order to determine how to compute false positives and false negatives for each annotation.

Value

list of two data.tables: label.errors has one row for every combination of models and labels, with status column that indicates whether or not that model commits an error in that particular label; model.errors has one row per model, with columns for computing target intervals and ROC curves (see [targetIntervals](#) and [ROChange](#)).

Author(s)

Toby Dylan Hocking

Examples

```
label <- function(annotation, min, max){
  data.frame(profile.id=4, chrom="chr14", min, max, annotation)
}
label.df <- rbind(
  label("1change", 70e6, 80e6),
  label("0changes", 20e6, 60e6))
model.df <- data.frame(chrom="chr14", n.segments=1:3)
change.df <- data.frame(chrom="chr14", rbind(
  data.frame(n.segments=2, changepoint=75e6),
  data.frame(n.segments=3, changepoint=c(75e6, 50e6))))
penaltyLearning::labelError(
  model.df, label.df, change.df,
  problem.vars="chrom", # for all three data sets.
  model.vars="n.segments", # for changes and selection.
  change.var="changepoint", # column of changes with breakpoint position.
  label.vars=c("min", "max")) # limit of labels in ann.
```

```
largestContinuousMinimumC  
  largestContinuousMinimumC
```

Description

Find the run of minimum cost with the largest size. This function use a linear time C implementation, and is meant for internal use. Use [targetIntervals](#) for real data.

Usage

```
largestContinuousMinimumC(cost,  
  size)
```

Arguments

cost	numeric vector of cost values.
size	numeric vector of interval size values.

Value

Integer vector length 2 (start and end of target interval relative to cost and size).

Author(s)

Toby Dylan Hocking

Examples

```
library(penaltyLearning)  
data(neuroblastomaProcessed, envir=environment())  
one.problem.error <-  
  neuroblastomaProcessed$errors[profile.id=="4" & chromosome=="1"]  
indices <- one.problem.error[, largestContinuousMinimumC(  
  errors, max.log.lambda-min.log.lambda)]  
one.problem.error[indices[["start"]]:indices[["end"]],]
```

largestContinuousMinimumR
largestContinuousMinimumR

Description

Find the run of minimum cost with the largest size. This function uses a two pass R implementation, and is meant for internal use. Use [targetIntervals](#) for real data.

Usage

```
largestContinuousMinimumR(cost,  
  size)
```

Arguments

cost	numeric vector of cost values.
size	numeric vector of interval size values.

Value

Integer vector length 2 (start and end of target interval relative to cost and size).

Author(s)

Toby Dylan Hocking

Examples

```
library(penaltyLearning)
data(neuroblastomaProcessed, envir=environment())
one.problem.error <-
  neuroblastomaProcessed$errors[profile.id=="4" & chromosome=="1"]
indices <- one.problem.error[, largestContinuousMinimumR(
  errors, max.log.lambda-min.log.lambda)]
one.problem.error[indices[["start"]]:indices[["end"]],]
```

modelSelection	<i>Compute exact model selection function</i>
----------------	---

Description

Given `loss.vec L_i`, `model.complexity K_i`, the model selection function $i^*(\lambda) = \operatorname{argmin}_i L_i + \lambda K_i$, compute all of the solutions $(i, \min.\lambda, \max.\lambda)$ with i being the solution for every λ in $(\min.\lambda, \max.\lambda)$. Use this function after having computed changepoints and loss values for each model, and before using `labelError`. This function uses the linear time algorithm implemented in C code (`modelSelectionC`).

Usage

```
modelSelection(models,
  loss = "loss", complexity = "complexity")
```

Arguments

<code>models</code>	data.frame with one row per model. There must be at least two columns <code>models[[loss]]</code> and <code>models[[complexity]]</code> , but there can also be other meta-data columns.
<code>loss</code>	character: column name of <code>models</code> to interpret as loss L_i .
<code>complexity</code>	character: column name of <code>models</code> to interpret as complexity K_i .

Value

data.frame with a row for each model that can be selected for at least one λ value, and the following columns. $(\min.\lambda, \max.\lambda)$ and $(\min.\log.\lambda, \max.\log.\lambda)$ are intervals of optimal penalty constants, on the original and log scale; the other columns (and rownames) are taken from `models`. This should be used as the `models` argument of `labelError`.

Author(s)

Toby Dylan Hocking

modelSelectionC	<i>Exact model selection function</i>
-----------------	---------------------------------------

Description

Given `loss.vec L_i`, `model.complexity K_i`, the model selection function $i^*(\lambda) = \operatorname{argmin}_i L_i + \lambda K_i$, compute all of the solutions $(i, \min.\lambda, \max.\lambda)$ with i being the solution for every λ in $(\min.\lambda, \max.\lambda)$. This function uses the linear time algorithm implemented in C code. This function is mostly meant for internal use – it is instead recommended to use `modelSelection`.

Usage

```
modelSelectionC(loss.vec,
  model.complexity,
  model.id)
```

Arguments

```
loss.vec      numeric vector: loss  $L_i$ 
model.complexity
              numeric vector: model complexity  $K_i$ 
model.id      vector: indices  $i$ 
```

Value

data.frame with a row for each model that can be selected for at least one lambda value, and the following columns. (min.lambda, max.lambda) and (min.log.lambda, max.log.lambda) are intervals of optimal penalty constants, on the original and log scale; model.complexity are the K_i values; model.id are the model identifiers (also used for row names); and model.loss are the C_i values.

Author(s)

Toby Dylan Hocking

Examples

```
loss.vec <- c(
  -9.9, -12.8, -19.2, -22.1, -24.5, -26.1, -28.5, -30.1, -32.2,
  -33.7, -35.2, -36.8, -38.2, -39.5, -40.7, -41.8, -42.8, -43.9,
  -44.9, -45.8)
seg.vec <- seq_along(loss.vec)
exact.df <- penaltyLearning::modelSelectionC(loss.vec, seg.vec, seg.vec)
## Solve the optimization using grid search.
L.grid <- with(exact.df, {
  seq(min(max.log.lambda)-1,
      max(min.log.lambda)+1,
      l=100)
})
lambda.grid <- exp(L.grid)
kstar.grid <- sapply(lambda.grid, function(lambda){
  crit <- with(exact.df, model.complexity * lambda + model.loss)
  picked <- which.min(crit)
  exact.df$model.id[picked]
})
grid.df <- data.frame(log.lambda=L.grid, segments=kstar.grid)
library(ggplot2)
## Compare the results.
ggplot()+
  ggtitle("grid search (red) agrees with exact path computation (black)") +
  geom_segment(aes(min.log.lambda, model.id,
                  xend=max.log.lambda, yend=model.id),
              data=exact.df)+
```

```
geom_point(aes(log.lambda, segments),
           data=grid.df, color="red", pch=1)+
ylab("optimal model complexity (segments)")+
xlab("log(lambda)")
```

modelSelectionR	<i>Exact model selection function</i>
-----------------	---------------------------------------

Description

Given `loss.vec` L_i , `model.complexity` K_i , the model selection function $i^*(\lambda) = \operatorname{argmin}_i L_i + \lambda K_i$, compute all of the solutions (i , `min.lambda`, `max.lambda`) with i being the solution for every λ in (`min.lambda`, `max.lambda`). This function uses the quadratic time algorithm implemented in R code. This function is mostly meant for internal use and comparison – it is instead recommended to use [modelSelection](#).

Usage

```
modelSelectionR(loss.vec,
               model.complexity,
               model.id)
```

Arguments

<code>loss.vec</code>	numeric vector: loss L_i
<code>model.complexity</code>	numeric vector: model complexity K_i
<code>model.id</code>	vector: indices i

Value

data.frame with a row for each model that can be selected for at least one λ value, and the following columns. (`min.lambda`, `max.lambda`) and (`min.log.lambda`, `max.log.lambda`) are intervals of optimal penalty constants, on the original and log scale; `model.complexity` are the K_i values; `model.id` are the model identifiers (also used for row names); and `model.loss` are the C_i values.

Author(s)

Toby Dylan Hocking

Examples

```
loss.vec <- c(
  -9.9, -12.8, -19.2, -22.1, -24.5, -26.1, -28.5, -30.1, -32.2,
  -33.7, -35.2, -36.8, -38.2, -39.5, -40.7, -41.8, -42.8, -43.9,
  -44.9, -45.8)
seg.vec <- seq_along(loss.vec)
penaltyLearning::modelSelectionR(loss.vec, seg.vec, seg.vec)
```

neuroblastomaProcessed

Processed neuroblastoma data set with features and targets

Description

Features are inputs and targets are outputs for penalty learning functions like `penaltyLearning::IntervalRegressionCV`. `data(neuroblastoma, package="neuroblastoma")` was processed by computing optimal Gaussian segmentation models from 1 to 20 segments (`cghseg:::segmeanCO` or `Segmentor3IsBack::Segmentor`), then label error was computed using `neuroblastoma$annotations` (`penaltyLearning::labelError`), then target intervals were computed (`penaltyLearning::targetInterval`). Features were also computed based on `neuroblastoma$profiles`.

Usage

```
data("neuroblastomaProcessed")
```

Format

List of two matrices: `feature.mat` is `n.observations x n.features`, and `target.mat` is `n.observations x 2`, where `n.observations=3418` and `n.features=117`.

notConverging

Interval regression problem that was not converging

Description

A small data set which was diverging using a previous implementation of `IntervalRegressionCV`.

Usage

```
data("notConverging")
```

Format

A list with names: `X.mat` are numeric inputs, `y.mat` are numeric outputs, `fold.vec` is an integer vector of fold ID numbers.

Source

github.com/tdhock/neuroblastoma-data, `data/H3K4me3_TDH_other/cv/equal_labels/testFolds/3/sampleSelectionGP_erf/5/c`

oneSkip	<i>oneSkip</i>
---------	----------------

Description

A loss and model complexity function which never selects one of the models, using a linear penalty.

Usage

```
data("oneSkip")
```

Format

A list of two data.frames (input and output).

Source

example(exactModelSelection) in PeakSegDP package.

plot.IntervalRegression	<i>plot IntervalRegression</i>
-------------------------	--------------------------------

Description

Plot an IntervalRegression model.

Usage

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

Arguments

x	x
...	...

Value

a ggplot.

Author(s)

Toby Dylan Hocking

```
predict.IntervalRegression  
    predict IntervalRegression
```

Description

Compute model predictions.

Usage

```
## S3 method for class 'IntervalRegression'  
predict(object,  
        X, ...)
```

Arguments

object	object
X	X
...	...

Value

numeric matrix of predicted log(penalty) values.

Author(s)

Toby Dylan Hocking

```
print.IntervalRegression  
    print IntervalRegression
```

Description

print learned model parameters.

Usage

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

Arguments

x	x
...	...

Author(s)

Toby Dylan Hocking

ROChange

*ROC curve for changepoints***Description**

Compute a Receiver Operating Characteristic curve for a penalty function.

Usage

```
ROChange(models, predictions,
         problem.vars = character())
```

Arguments

models	data.frame describing the number of incorrect labels as a function of $\log(\lambda)$, with columns <code>min.log.lambda</code> , <code>max.log.lambda</code> , <code>fp</code> , <code>fn</code> , <code>possible.fp</code> , <code>possible.fn</code> , etc. This can be computed via <code>labelError(modelSelection(...), ...) \$model.errors</code> – see examples.
predictions	data.frame with a column named <code>pred.log.lambda</code> , the predicted $\log(\text{penalty})$ value for each segmentation problem.
problem.vars	character: column names used to identify data set / segmentation problem.

Value

named list of results:

roc	a data.table with one row for each point on the ROC curve
thresholds	two rows of roc which correspond to the predicted and minimal error thresholds
auc.polygon	a data.table with one row for each vertex of the polygon used to compute AUC
auc	numeric Area Under the ROC curve
aum	numeric Area Under Min(FP, FN)
aum.grad	data.table with one row for each prediction, and columns <code>hi/lo</code> bound for the aum generalized gradient.

Author(s)

Toby Dylan Hocking

Examples

```

library(penaltyLearning)
library(data.table)

data(neuroblastomaProcessed, envir=environment())
## Get incorrect labels data for one profile.
pid <- 11
pro.errors <- neuroblastomaProcessed$errors[
  profile.id==pid][order(chromosome, min.log.lambda)]
dcast(pro.errors, n.segments ~ chromosome, value.var="errors")
## Get the feature that corresponds to the BIC penalty = log(n),
## meaning log(penalty) = log(log(n)).
chr.vec <- paste(c(1:4, 11, 17))
pid.names <- paste0(pid, ".", chr.vec)
BIC.feature <- neuroblastomaProcessed$feature.mat[pid.names, "log2.n"]
pred <- data.table(pred.log.lambda=BIC.feature, chromosome=chr.vec)
## edit one prediction so that it ends up having the same threshold
## as another one, to illustrate an aum sub-differential with
## un-equal lo/hi bounds.
err.changes <- pro.errors[, {
  .SD[c(NA, diff(errors) != 0), .(min.log.lambda)]
}, by=chromosome]
(ch.vec <- err.changes[, structure(min.log.lambda, names=chromosome)])
other <- "11"
(diff.other <- ch.vec[[other]]-pred[other, pred.log.lambda, on=.(chromosome)])
pred["1", pred.log.lambda := ch.vec[["1"]]-diff.other, on=.(chromosome)]
pred["4", pred.log.lambda := 2, on=.(chromosome)]
ch.vec[["1"]]-pred["1", pred.log.lambda, on=.(chromosome)]
result <- ROChange(pro.errors, pred, "chromosome")
library(ggplot2)
## Plot the ROC curves.
ggplot()+
  geom_path(aes(FPR, TPR), data=result$roc)+
  geom_point(aes(FPR, TPR, color=threshold), data=result$thresholds, shape=1)

## Plot the number of incorrect labels as a function of threshold.
ggplot()+
  geom_segment(aes(
    min.thresh, errors,
    xend=max.thresh, yend=errors),
  data=result$roc)+
  geom_point(aes((min.thresh+max.thresh)/2, errors, color=threshold),
    data=result$thresholds,
    shape=1)+
  xlab("log(penalty) constant added to BIC penalty")

## Plot area under Min(FP,FN).
err.colors <- c(
  "fp"="red",
  "fn"="deepskyblue",
  "min.fp.fn"="black")
err.sizes <- c(

```

```

    "fp"=3,
    "fn"=2,
    "min.fp.fn"=1)
roc.tall <- melt(result$roc, measure.vars=names(err.colors))
area.rects <- data.table(
  chromosome="total",
  result$roc[0<min.fp.fn])
(gg.total <- ggplot()+
  geom_vline(
    xintercept=0,
    color="grey")+
  geom_rect(aes(
    xmin=min.thresh, xmax=max.thresh,
    ymin=0, ymax=min.fp.fn),
    data=area.rects,
    alpha=0.5)+
  geom_text(aes(
    min.thresh, min.fp.fn/2,
    label=sprintf(
      "Area Under Min(FP,FN)=%.3f ",
      result$aum)),
    data=area.rects[1],
    hjust=1,
    color="grey50")+
  geom_segment(aes(
    min.thresh, value,
    xend=max.thresh, yend=value,
    color=variable, size=variable),
    data=data.table(chromosome="total", roc.tall))+
  scale_size_manual(values=err.sizes)+
  scale_color_manual(values=err.colors)+
  theme_bw()+
  theme(panel.grid.minor=element_blank()+
  scale_x_continuous(
    "Prediction threshold")+
  scale_y_continuous(
    "Incorrectly predicted labels",
    breaks=0:10))

## Add individual error curves.
tall.errors <- melt(
  pro.errors[pred, on=(chromosome)],
  measure.vars=c("fp", "fn"))
gg.total+
  geom_segment(aes(
    min.log.lambda-pred.log.lambda, value,
    xend=max.log.lambda-pred.log.lambda, yend=value,
    size=variable, color=variable),
    data=tall.errors)+
  facet_grid(chromosome ~ ., scales="free", space="free")+
  theme(panel.spacing=grid::unit(0, "lines"))+
  geom_blank(aes(
    0, errors),

```

```

data=data.table(errors=c(1.5, -0.5))

print(result$aum.grad)
if(interactive()){#this can be too long for CRAN.
  ## Plot how Area Under Min(FP,FN) changes with each predicted value.
  aum.dt <- pred[, {
    data.table(log.pen=seq(0, 4, by=0.5))[, {
      chr <- paste(chromosome)
      new.pred.dt <- data.table(pred)
      new.pred.dt[chr, pred.log.lambda := log.pen, on=.(chromosome)]
      with(
        ROChange(pro.errors, new.pred.dt, "chromosome"),
        data.table(aum))
    }, by=log.pen]
  }, by=chromosome]
  bounds.dt <- melt(
    result$aum.grad,
    measure.vars=c("lo", "hi"),
    variable.name="bound",
    value.name="slope")[pred, on=.(chromosome)]
  bounds.dt[, intercept := result$aum-slope*pred.log.lambda]
  ggplot()+
    geom_abline(aes(
      slope=slope, intercept=intercept),
      size=1,
      data=bounds.dt)+
    geom_text(aes(
      2, 2, label=sprintf("directional derivatives = [%d, %d]", lo, hi)),
      data=result$aum.grad)+
    scale_color_manual(
      values=c(
        predicted="red",
        new="black"))+
    geom_point(aes(
      log.pen, aum, color=type),
      data=data.table(type="new", aum.dt))+
    geom_point(aes(
      pred.log.lambda, result$aum, color=type),
      shape=1,
      data=data.table(type="predicted", pred))+
    theme_bw()+
    theme(panel.spacing=grid::unit(0, "lines"))+
    facet_wrap("chromosome", labeller=label_both)+
    coord_equal()+
    xlab("New log(penalty) value for chromosome")+
    ylab("Area Under Min(FP,FN)
using new log(penalty) for this chromosome
and predicted log(penalty) for others")
  }

```

squared.hinge	<i>squared hinge</i>
---------------	----------------------

Description

The squared hinge loss.

Usage

```
squared.hinge(x, e = 1)
```

Arguments

x	x
e	e

Author(s)

Toby Dylan Hocking

targetIntervalResidual	<i>targetIntervalResidual</i>
------------------------	-------------------------------

Description

Compute residual of predicted penalties with respect to target intervals. This function is useful for visualizing the errors in a plot of log(penalty) versus a feature.

Usage

```
targetIntervalResidual(target.mat,  
  pred)
```

Arguments

target.mat	n x 2 numeric matrix: target intervals of log(penalty) values that yield minimal incorrect labels.
pred	numeric vector: predicted log(penalty) values.

Value

numeric vector of n residuals. Predictions that are too high (above target.mat[,2]) get positive residuals (too few changepoints), and predictions that are too low (below target.mat[,1]) get negative residuals.

Author(s)

Toby Dylan Hocking

Examples

```

library(penaltyLearning)
library(data.table)
data(neuroblastomaProcessed, envir=environment())
## The BIC model selection criterion is lambda = log(n), where n is
## the number of data points to segment. This implies log(lambda) =
## log(log(n)), which is the log2.n feature.
row.name.vec <- grep(
  "^4|520[.]",
  rownames(neuroblastomaProcessed$feature.mat),
  value=TRUE)
feature.mat <- neuroblastomaProcessed$feature.mat[row.name.vec, ]
target.mat <- neuroblastomaProcessed$target.mat[row.name.vec, ]
pred.dt <- data.table(
  row.name=row.name.vec,
  target.mat,
  feature.mat[, "log2.n", drop=FALSE])
pred.dt[, pred.log.lambda := log2.n ]
pred.dt[, residual := targetIntervalResidual(
  cbind(min.L, max.L),
  pred.log.lambda)]
library(ggplot2)
limits.dt <- pred.dt[, data.table(
  log2.n,
  log.penalty=c(min.L, max.L),
  limit=rep(c("min", "max"), each=.N))][is.finite(log.penalty)]
ggplot()+
  geom_abline(slope=1, intercept=0)+
  geom_point(aes(
    log2.n,
    log.penalty,
    fill=limit),
    data=limits.dt,
    shape=21)+
  geom_segment(aes(
    log2.n, pred.log.lambda,
    xend=log2.n, yend=pred.log.lambda-residual),
    data=pred.dt,
    color="red")+
  scale_fill_manual(values=c(min="white", max="black"))

```

Description

Compute a ROC curve using a target interval matrix. A prediction less than the lower limit is considered a false positive (penalty too small, too many changes), and a prediction greater than the upper limit is a false negative (penalty too large, too few changes). **WARNING:** this ROC curve is less detailed than the one you get from [ROChange](#)! Use [ROChange](#) if possible.

Usage

```
targetIntervalROC(target.mat,
  pred)
```

Arguments

target.mat	n x 2 numeric matrix: target intervals of log(penalty) values that yield minimal incorrect labels.
pred	numeric vector: predicted log(penalty) values.

Value

list describing ROC curves, same as [ROChange](#).

Author(s)

Toby Dylan Hocking

Examples

```
library(penaltyLearning)
library(data.table)
data(neuroblastomaProcessed, envir=environment())

pid.vec <- c("1", "4")
chr <- 2
incorrect.labels <-
  neuroblastomaProcessed$errors[profile.id%in%pid.vec & chromosome==chr]
pid.chr <- paste0(pid.vec, ".", chr)
target.mat <- neuroblastomaProcessed$target.mat[pid.chr, , drop=FALSE]
pred.dt <- data.table(profile.id=pid.vec, pred.log.lambda=1.5)
roc.list <- list(
  labels=ROChange(incorrect.labels, pred.dt, "profile.id"),
  targets=targetIntervalROC(target.mat, pred.dt$pred.log.lambda))

err <- data.table(incorrect=names(roc.list))[, {
  roc.list[[incorrect]]$roc
}, by=incorrect]
library(ggplot2)
ggplot()+
  ggtitle("incorrect targets is an approximation of incorrect labels")+
  scale_size_manual(values=c(labels=2, targets=1))+
  geom_segment(aes(
    min.thresh, errors,
```

```

color=incorrect,
size=incorrect,
xend=max.thresh, yend=errors),
  data=err)

```

targetIntervals	<i>Compute target intervals</i>
-----------------	---------------------------------

Description

Compute target intervals of log(penalty) values that result in predicted changepoint models with minimum incorrect labels. Use this function after `labelError`, and before `IntervalRegression*`.

Usage

```
targetIntervals(models,
  problem.vars)
```

Arguments

models	data.table with columns errors, min.log.lambda, max.log.lambda, typically labelError()\$model.errors.
problem.vars	character: column names used to identify data set / segmentation problem.

Value

data.table with columns problem.vars, one row for each segmentation problem. The "min.log.lambda", and "max.log.lambda" columns give the largest interval of log(penalty) values which results in the minimum incorrect labels for that problem. This can be used to create the target.mat parameter of the `IntervalRegression*` functions.

Author(s)

Toby Dylan Hocking

Examples

```

data.table::setDTthreads(1)

library(penaltyLearning)
data(neuroblastomaProcessed, envir=environment())
targets.dt <- targetIntervals(
  neuroblastomaProcessed$errors,
  problem.vars=c("profile.id", "chromosome"))

```

<code>theme_no_space</code>	<i>theme no space</i>
-----------------------------	-----------------------

Description

ggplot2 theme element for no space between panels.

Usage

```
theme_no_space(...)
```

Arguments

... ...

Author(s)

Toby Dylan Hocking

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