Package: penalized (via r-universe)

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Title L1 (Lasso and Fused Lasso) and L2 (Ridge) Penalized Estimation in GLMs and in the Cox Model

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Imports Rcpp

LinkingTo Rcpp, RcppArmadillo

Suggests globaltest

Description Fitting possibly high dimensional penalized regression models. The penalty structure can be any combination of an L1 penalty (lasso and fused lasso), an L2 penalty (ridge) and a positivity constraint on the regression coefficients. The supported regression models are linear, logistic and Poisson regression and the Cox Proportional Hazards model. Cross-validation routines allow optimization of the tuning parameters.

License GPL (>= 2)

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2 breslow object

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breslow object

Breslow estimator object

Description

Stores one or more survival stepfunctions of the Kaplan-Meier and Breslow type.

Details

Index

Breslow objects are generally created by the penalized function and related functions.

Slots

time: Object of class "vector". The time points at which the function starts, jumps or ends. curves: Object of class "matrix". The values of the curve at each time point. Note that the function is left-continuous. Curves are stored as a matrix of dimension (\# curves) x (\# timepoints).

Methods

```
"[" (breslow): Coerces the object to a matrix (as as.matrix) and selects rows and/or columns.
```

"[[" (breslow): Selects a subset of the curves.

as.data.frame (breslow): Returns the "curves" slot together with the "time" slot in a data.frame.

as.list (breslow): Coerces the object to a list.

as.matrix (breslow): Returns the "curves" slot with the "time" slot as column names.

plot (breslow): Straightforward plotting (all curves in one plot).

show (breslow): Summarizes the dimensions of the object.

survival (breslow): Takes a second argument (time). Extracts the value of the survival curve(s) at any time point.

Author(s)

```
Jelle Goeman: <j.j.goeman@lumc.nl>
```

See Also

penalized.

Cross-validation in penalized generalized linear models

Cross-validated penalized regression

Description

Cross-validating generalized linear models with L1 (lasso or fused lasso) and/or L2 (ridge) penalties, using likelihood cross-validation.

Usage

```
cvl (response, penalized, unpenalized, lambda1 = 0, lambda2= 0, positive = FALSE,
    fusedl = FALSE, data, model = c("cox", "logistic", "linear", "poisson"),
    startbeta, startgamma, fold, epsilon = 1e-10, maxiter, standardize = FALSE,
    trace = TRUE, approximate = FALSE)
optL1 (response, penalized, unpenalized, minlambda1, maxlambda1, base1, lambda2 = 0,
  fusedl = FALSE, positive = FALSE, data,
 model = c("cox", "logistic", "linear", "poisson"), startbeta, startgamma, fold,
 epsilon = 1e-10, maxiter = Inf, standardize = FALSE, tol = .Machine$double.eps^0.25,
  trace = TRUE)
optL2 (response, penalized, unpenalized, lambda1 = 0, minlambda2, maxlambda2, base2,
fused1 = FALSE ,positive = FALSE, data,
 model = c("cox", "logistic", "linear", "poisson"), startbeta, startgamma,
 fold, epsilon = 1e-10, maxiter, standardize = FALSE, tol = .Machine$double.eps^0.25,
  trace = TRUE, approximate = FALSE)
profL1 (response, penalized, unpenalized, minlambda1, maxlambda1, base1, lambda2 = 0,
  fused1 = FALSE, positive = FALSE, data,
 model = c("cox", "logistic", "linear", "poisson"), startbeta, startgamma, fold,
 epsilon = 1e-10, maxiter = Inf, standardize = FALSE, steps = 100, minsteps = steps/3,
  log = FALSE, save.predictions = FALSE, trace = TRUE, plot = FALSE)
profL2 (response, penalized, unpenalized, lambda1 = 0, minlambda2, maxlambda2, base2,
  fused1 = FALSE, positive = FALSE, data,
 model = c("cox", "logistic", "linear", "poisson"), startbeta, startgamma, fold,
 epsilon = 1e-10, maxiter, standardize = FALSE, steps = 100, minsteps = steps/2,
 log = TRUE, save.predictions = FALSE, trace = TRUE, plot = FALSE, approximate = FALSE)
```

Arguments

response

The response variable (vector). This should be a numeric vector for linear regression, a Surv object for Cox regression and factor or a vector of 0/1 values for logistic regression.

penalized The penalized covariates. These may be specified either as a matrix or as a

(one-sided) formula object. See also under data.

unpenalized Additional unpenalized covariates. Specified as under penalized. Note that an unpenalized intercept is included in the model by default (except in the cox

model). This can be suppressed by specifying unpenalized = ~ 0 .

lambda1, lambda2

The fixed values of the tuning parameters for L1 and L2 penalization. Each must be either a single positive numbers or a vector with length equal to the number of covariates in penalized argument. In the latter case, each covariate is given its own penalty weight.

minlambda1, minlambda2, maxlambda1, maxlambda2

The values of the tuning parameters for L1 or L2 penalization between which the cross-validated likelihood is to be profiled or optimized. For fused lasso penalty minlambda2 and maxlambda2 are the tuning parameters for L1 penalty on the differences of the coefficients between which the cross-validated likelihood is to

be optimized.

base1, base2 An optional vector of length equal to the number of covariates in penalized. If

supplied, profiling or optimization is performed between base1*minlambda1

and base1*maxlambda1; analogous for base2.

fusedl If TRUE or a vector, the penalization method used is fused lasso. The value for

> lambda1 is used as the tuning parameter for L1 penalization on the coefficients and the value for lambda2 is used as the tuning parameter for L1 penalization

on the differences of the coefficients. Default value is FALSE.

If TRUE, constrains the estimated regression coefficients of all penalized covaripositive

> ates to be non-negative. If a logical vector with the length of the number of covariates in penalized, constrains the estimated regression coefficients of a

subset of the penalized covariates to be non-negative.

data A data frame used to evaluate response, and the terms of penalized or

unpenalized when these have been specified as a formula object.

model The model to be used. If missing, the model will be guessed from the response

startbeta Starting values for the regression coefficients of the penalized covariates. These

starting values will be used only for the first values of lambda1 and lambda2.

Starting values for the regression coefficients of the unpenalized covariates. startgamma

These starting values will be used only for the first values of lambda1 and

lambda2.

fold The fold for cross-validation. May be supplied as a single number (between 2

and n) giving the number of folds, or, alternatively, as a length n vector with values in 1: fold, specifying exactly which subjects are assigned to which fold. The default is fold = 1:n, resulting in leave-one-out (n-fold) cross-validation.

epsilon The convergence criterion. As in glm. Convergence is judged separately on the

likelihood and on the penalty.

The maximum number of iterations allowed in each fitting of the model. Set by

default at 25 when only an L2 penalty is present, infinite otherwise.

maxiter

standardize If TRUE, standardizes all penalized covariates to unit central L2-norm before

applying penalization.

steps The maximum number of steps between minlambda1 and maxlambda1 or minlambda2

and maxlambda2 at which the cross-validated likelihood is to be calculated.

minsteps The minimum number of steps between minlambda1 and maxlambda1 or minlambda2

and maxlambda2 at which the cross-validated likelihood is to be calculated. If minsteps is smaller than steps, the algorithm will automatically stop when the cross-validated likelihood drops below the cross-validated likelihood of the null

model, provided it has done at least minsteps steps.

log If FALSE, the steps between minlambda1 and maxlambda1 or minlambda2 and

maxlambda2 are equidistant on a linear scale, if TRUE on a logarithmic scale. Please note the different default between optL1 (FALSE) and optL2 (TRUE).

tol The tolerance of the Brent algorithm used for minimization. See also optimize.

save.predictions

Controls whether or not to save cross-validated predictions for all values of

lambda.

trace If TRUE, prints progress information. Note that setting trace=TRUE may slow

down the algorithm (but it often feels quicker)

approximate If TRUE, the cross-validated likelihood values are approximated rather than fully

calculated. Note that this option is only available for ridge models.

plot If TRUE, makes a plot of cross-validated likelihood versus lambda.

Details

All five functions return a list with the following named elements:

lambda: For optL1 and optL2 lambda gives the optimal value of the tuning parameters found. For profL1 and profL2 lambda is the vector of values of the tuning parameter for which the cross-validated likelihood has been calculated. Absent in the output of cv1.

cvl: The value(s) of the cross-validated likelihood. For optL1, optL2 this is the cross-validated likelihood at the optimal value of the tuning parameter.

fold: Returns the precise allocation of the subjects into the cross-validation folds. Note that the same allocation is used for all cross-validated likelihood calculations in each call to optL1, optL2, profL1, profL2.

predictions: The cross-validated predictions for the left-out samples. The precise format of the cross-validated predictions depends on the type of generalized linear model (see breslow for survival models. The functions profL1 and profL2 return a list here (only if save.predictions = TRUE), whereas optL1, optL2 return the predictions for the optimal value of the tuning parameter only.

fullfit: The fitted model on the full data. The functions profL1 and profL2 return a list of penfit objects here, whereas optL1, optL2 return the full data fit (a single penfit object) for the optimal value of the tuning parameter only.

Value

A named list. See details.

Note

The optL1 and optL2 functions use Brent's algorithm for minimization without derivatives (see also optimize). There is a risk that these functions converge to a local instead of to a global optimum. This is especially the case for optL1, as the cross-validated likelihood as a function of lambda1 quite often has local optima. It is recommended to use optL1 in combination with profL1 to check whether optL1 has converged to the right optimum.

See also the notes under penalized.

Author(s)

```
Jelle Goeman: <j.j.goeman@lumc.nl>
```

References

Goeman J.J. (2010). L-1 Penalized Estimation in the Cox Proportional Hazards Model. Biometrical Journal 52 (1) 70-84.

See Also

```
penalized, penfit, plotpath.
```

Examples

Netherlands Cancer Institute 70 gene signature

The 70 gene signature of the Netherlands Cancer Institute for prediction of metastasis-free survival, measured on 144 independent lymph node positive patients.

Description

A data.frame of 144 lymph node positive breast cancer patients on metastasis-free survival, 5 clinical risk factors, and gene expression measurements of 70 genes found to be prognostic for metastasis-free survival in an earlier study. The included variables are

time Metastasis-free follow-up time (months).

event Event indicator. 1 = metastasis or death; 0 = censored.

Diam Diameter of the tumor (two levels).

N Number of affected lymph nodes (two levels).

ER Estrogen receptor status (two levels).

Grade Grade of the tumor (three ordered levels).

Age Patient age at diagnosis (years).

TSPYL5...C20orf46 Gene expression measurements of 70 prognostic genes.

Usage

data(nki70)

Format

A data.frame.

Note

The 70 gene signature was trained on lymph node negative patients only.

References

M.J. van de Vijver, Y.D. He, L.J. van 't Veer, H. Dai, A.A.M. Hart, D.W. Voskuil, G.J. Schreiber, J.L. Peterse, C. Roberts, M.J. Marton, M. Parrish, D. Atsma, A. Witteveen, A. Glas, L. Delahaye, T. van der Velde, H. Bartelink, S. Rodenhuis, E.T. Rutgers, S.H. Friend, and R. Bernards (2002). A gene-expression signature as a predictor of survival in breast cancer. New England Journal of Medicine 347 (25), 1999–2009.

Penalized generalized linear models

Penalized regression

Description

Fitting generalized linear models with L1 (lasso and fused lasso) and/or L2 (ridge) penalties, or a combination of the two.

Usage

```
penalized (response, penalized, unpenalized, lambda1=0,
  lambda2=0, positive = FALSE, data, fusedl=FALSE,
  model = c("cox", "logistic", "linear", "poisson"),
  startbeta, startgamma, steps =1, epsilon = 1e-10,
  maxiter, standardize = FALSE, trace = TRUE)
```

Arguments

response The response variable (vector). This should be a numeric vector for linear re-

gression, a Surv object for Cox regression and factor or a vector of 0/1 values

for logistic regression.

penalized The penalized covariates. These may be specified either as a matrix or as a

(one-sided) formula object. See also under data.

unpenalized Additional unpenalized covariates. Specified as under penalized. Note that

an unpenalized intercept is included in the model by default (except in the \mbox{Cox}

model). This can be suppressed by specifying unpenalized = \sim 0.

lambda1, lambda2

The tuning parameters for L1 and L2 penalization. Each must be either a single positive numbers or a vector with length equal to the number of covariates in penalized argument. In the latter case, each covariate is given its own penalty

weight.

positive If TRUE, constrains the estimated regression coefficients of all penalized covari-

ates to be non-negative. If a logical vector with the length of the number of covariates in penalized, constrains the estimated regression coefficients of a

subset of the penalized covariates to be non-negative.

data A data.frame used to evaluate response, and the terms of penalized or

unpenalized when these have been specified as a formula object.

fusedl If TRUE or a vector, the penalization method used is fused lasso. The value for

lambda1 is used as the tuning parameter for L1 penalization on the coefficients and the value for lambda2 is used as the tuning parameter for L1 penalization

on the differences of the coefficients. Default value is FALSE.

model The model to be used. If missing, the model will be guessed from the response

input.

startbeta Starting values for the regression coefficients of the penalized covariates.

starting values for the regression coefficients of the unpenalized covariates.

steps If greater than 1, the algorithm will fit the model for a range of steps lambda1-

values, starting from the maximal value down to the value of lambda1 specified. This is useful for making plots as in plotpath. With steps = "Park" it is possible to choose the steps in such a way that they are at the approximate value at

which the active set changes, following Park and Haste (2007).

epsilon The convergence criterion. As in glm. Convergence is judged separately on the

likelihood and on the penalty.

maxiter The maximum number of iterations allowed. Set by default at 25 when only an

L2 penalty is present, infinite otherwise.

standardize If TRUE, standardizes all penalized covariates to unit central L2-norm before

applying penalization.

trace If TRUE, prints progress information. Note that setting trace=TRUE may slow

down the algorithm up to 30 percent (but it often feels quicker)

Details

The penalized function fits regression models for a given combination of L1 and L2 penalty parameters.

Value

penalized returns a penfit object when steps = 1 or a list of such objects if steps > 1.

Note

The response argument of the function also accepts formula input as in lm and related functions. In that case, the right hand side of the response formula is used as the penalized argument or, if that is already given, as the unpenalized argument. For example, the input penalized(y^x) is equivalent to penalized(y^x) and penalized(y^x , z) to penalized(y^x , z).

In case of tied survival times, the function uses Breslow's version of the partial likelihood.

Author(s)

```
Jelle Goeman: <j.j.goeman@lumc.nl>
```

References

Goeman J.J. (2010). L-1 Penalized Estimation in the Cox Proportional Hazards Model. Biometrical Journal 52 (1) 70-84.

See Also

penfit for the penfit object returned, plotpath for plotting the solution path, and cvl for cross-validation and optimizing the tuning parameters.

Examples

```
# More examples in the package vignette:
# type vignette("penalized")

data(nki70)

# A single lasso fit predicting survival
pen <- penalized(Surv(time, event), penalized = nki70[,8:77],
    unpenalized = ~ER+Age+Diam+N+Grade, data = nki70, lambda1 = 10)
show(pen)
coefficients(pen)</pre>
```

Penalized regression contrasts

Contrast functions for penalized regression

Description

Contrast functions for factors that are appropriate for penalized regression.

Usage

```
contr.none(n, contrasts)
contr.diff(n, contrasts = TRUE)
```

Arguments

n A vector of levels for a factor, or the number of levels.

contrasts A logical indicating whether contrasts should be computed. This argument is

ignored in contr.none.

Details

These functions are used for creating contrast matrices for use in fitting penalized analysis of variance and regression models. The columns of the resulting matrices contain contrasts which can be used for coding a factor with n levels. The returned value contains the computed contrasts.

contr.none returns an identity matrix except when the number of levels is 2, in which case it returns a single contrast. contr.none ensures that all levels of an unordered factor are treated symmetrically in a penalized regression model.

penfit object 11

contr.diff returns a lower triangular matrix of ones if contrasts=FALSE and the same matrix without its first column if contrasts=TRUE. This makes sure that penalization is done on the difference between successive levels of an ordered factor. It is not appropriate for unordered factors.

Value

contr.diff returns a matrix with n rows and k columns, with k=n-1 if contrasts is TRUE and k=n if contrasts is FALSE.

contr. none returns a matrix with n rows and n columns, except when n=2 when it returns a matrix with 2 rows and one column.

Author(s)

```
Jelle Goeman: <j.j.goeman@lumc.nl>
```

See Also

```
penalized, contr.treatment, contr.poly, contr.helmert, contr.SAS, contr.sum.
```

Examples

```
# Three levels
levels <- LETTERS[1:3]
contr.none(levels)
contr.diff(levels)

# Two levels
levels <- LETTERS[1:2]
contr.none(levels)</pre>
```

penfit object

Penalized regression object

Description

Stores the result of a call to penalized.

Slots

penalized: Object of class "vector". Regression coefficients for the penalized covariates.

unpenalized: Object of class "vector". Regression coefficients for the unpenalized covariates.

residuals: Object of class "vector". Unstandardized residuals for each subject in the fitted model. Martingale residuals are given for the cox model.

fitted: Object of class "vector". Fitted values (means) for each subject in the fitted model. In the cox model, this slot holds the relative risks.

lin.pred: Object of class "vector". Linear predictors for each subject in the fitted model.

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loglik: Object of class "numeric". Log likelihood of the fitted model. For the Cox model, reports the full likelihood rather than the partial likelihood.

penalty: Object of class "vector". L1 and L2 penalties of the fitted model.

iterations: Object of class "numeric". Number of iterations used in the fitting process.

converged: Object of class "logical". Whether the fitting process was judged to be converged.

model: Object of class "character". The name of the generalized linear model used.

lambda1: Object of class "vector". The lambda1 parameter(s) used.

lambda2: Object of class "vector". The lambda2 parameter(s) used.

nuisance: Object of class "list". The maximum likelihood estimates of any nuisance parameters in the model.

weights: Object of class "vector". The weights of the covariates used for standardization.

formula: Object of class "list". A named list containing the unpenalized and penalized formula objects, if present.

Methods

basehaz (penfit): Returns the baseline hazard (a data.frame) if a cox model was fitted, NULL otherwise. An additional argument center (default (TRUE) can be used to give the survival curve at the covariate mean (center = TRUE) rather than at zero.

basesurv (penfit): Returns the baseline survival curve (a breslow object) if a cox model was fitted, NULL otherwise. An additional argument center (default (TRUE) can be used to give the survival curve at the covariate mean (center = TRUE) rather than at zero.

coef (penfit): Returns the regression coefficients. Accepts a second argument "which", that takes values "nonzero" (the default), "all", "penalized" or "unpenalized" for extracting only the nonzero, the penalized or the unpenalized regression coefficients. A third argument "standardize" (default FALSE) can be used to let the method return the regression coefficients for the standardized covariates.

coefficients (penfit): synonym for coef above.

fitted (penfit): Returns the fitted values for each subject (i.e. the predicted means). In the Cox model, this method returns the relative risks for each individual.

fitted.values (penfit): synonym for fitted above.

linear.predictors (penfit): Returns the linear predictors for each subject.

loglik (penfit): Returns the log likelihood of the fitted model.

penalty (penfit): Returns the L1 and L2 penalties of the fitted model.

residuals (penfit): Returns the residuals.

show (penfit): Summarizes the fitted model.

weights (penfit): Returns the weights used for standardization.

predict (penfit): Calculates predictions for new subjects. See predict.

Author(s)

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See Also

```
penalized.
```

```
Plotting the LASSO path
```

Plotting the LASSO path

Description

Plotting a LASSO path fitted using penalized with steps > 1.

Usage

```
plotpath(object, labelsize = 0.6, standardize = FALSE, ...)
```

Arguments

object A list of link{penfit} objects calculated for the same data but different

lambda1 values. This object can be created using the link{penalized} func-

tion using the steps argument.

labelsize Sets the size of the variable labels in the plot. Set to zero for no variable labels.

standardize If TRUE, plots the regression coefficients for the covariates standardize to unit

second central moment. See penalized for details on standardization. Note that the standardization in plotpath can also be used if standardization was not

used in penalized.

... Any other arguments will be forwarded to the plot function.

Author(s)

```
Jelle Goeman: <j.j.goeman@lumc.nl>
```

See Also

```
penalized, penfit.
```

Examples

```
data(nki70)
# Fit the model with the steps argument and plot
pen <- penalized(Surv(time, event), penalized = nki70[,8:77],
    data = nki70, lambda1=1, steps = 20)
plotpath(pen)</pre>
```

```
Prediction from penalized models

Prediction based on penfit objects
```

Description

Predicting a response for new subjects based on a fitted penalized regression model.

Usage

```
## S4 method for signature 'penfit'
predict(object, penalized, unpenalized, data)
```

Arguments

object The fitted model (a penfit object).

penalized The matrix of penalized covariates for the new subjects.

The unpenalized covariates for the new subjects.

data A data. frame used to evaluate the terms of penalized or unpenalized when

these have been specified as a formula object.

Details

The user need only supply those terms from the original call that are different relative to the original call that produced the penfit object. In particular, if penalized and/or unpenalized was specified in matrix form, a matrix must be given with the new subjects' data. The columns of these matrices must be exactly the same as in the matrices supplied in the original call that produced the penfit object. If either penalized or unpenalized was given as a formula in the original call, the user of predict must supply a new data argument. As with matrices, the new data argument must have a similar make-up as the data argument in the original call that produced the penfit object. In particular, any factors in data must have the same levels.

Value

The predictions, either as a vector (logistic and Poisson models), a matrix (linear model), or a breslow object (Cox model).

Examples

```
data(nki70)
pen <- penalized(Surv(time, event), penalized = nki70[1:50,8:77],
    unpenalized = ~ER+Age+Diam+N+Grade, data = nki70[1:50,], lambda1 = 10)
predict(pen, nki70[51:52,8:77], data = nki70[51:52,])</pre>
```

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