Package 'mlt'

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mlt-package

General Information on the mlt Package

Description

The **mlt** package implements maximum likelihood estimation in conditional transformation models as introduced by Hothorn et al. (2020).

An introduction to the package is available in the mlt package vignette from package mlt.docreg (Hothorn, 2020).

A short talk on most likely transformations is available from https://channel9.msdn.com/Events/useR-international-R-User-conference/useR2016/Most-Likely-Transformations.

Novice users might find the high(er) level interfaces offered by package tram more convenient.

Author(s)

This package is authored by Torsten Hothorn <Torsten.Hothorn@R-project.org>.

References

Torsten Hothorn, Lisa Moest, Peter Buehlmann (2018), Most Likely Transformations, *Scandinavian Journal of Statistics*, **45**(1), 110–134, doi:10.1111/sjos.12291.

Torsten Hothorn (2020), Most Likely Transformations: The mlt Package, *Journal of Statistical Software*, **92**(1), 1–68, doi:10.18637/jss.v092.i01

confband

Confidence Bands

Description

Confidence bands for transformation, distribution, survivor or cumulative hazard functions

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Arguments

object an object of class mlt

newdata a data frame of observations

level the confidence level

type the function to compute the confidence band for

K number of grid points the function is evaluated at

cheat number of grid points the function is evaluated at when using the quantile obtained for K grid points

... additional arguments to confint.glht

Details

The function is evaluated at K grid points and simultaneous confidence intervals are then interpolated in order to construct the band.

A smoother band can be obtained by setting cheat to something larger than K: The quantile is obtained for K grid points but the number of evaluated grid points cheat can be much larger at no additional cost. Technically, the nominal level is not maintained in this case but the deviation will be small for reasonably large K.

Value

For each row in newdata the function and corresponding confidence band evaluated at the K (or cheat) grid points is returned.

ctm

Conditional Transformation Models

Description

Specification of conditional transformation models

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Arguments

response a basis function, ie, an object of class basis

interacting a basis function, ie, an object of class basis

shifting a basis function, ie, an object of class basis

scaling a basis function, ie, an object of class basis

scale_shift a logical choosing between two different model types in the presence of a scaling term

data either a data. frame containing the model variables or a formal description of these variables in an object of class vars

todistr a character vector describing the distribution to be transformed

sumconstr a logical indicating if sum constraints shall be applied ... arguments to as.basis when shifting is a formula

Details

Specification of a transformation model of the form

$$P(Y \le y \mid X = x) = F_Z(\sqrt{\exp(s(x)^{\top}\gamma)}[(a(y) \otimes b(x))^{\top}\vartheta] + d(x)^{\top}\beta)$$

(scale_shift = FALSE) or

$$P(Y \le y \mid X = x) = F_Z(\sqrt{\exp(s(x)^{\top}\gamma)}[(a(y) \otimes b(x))^{\top}\vartheta + d(x)^{\top}\beta])$$

(scale_shift = TRUE) with bases a(y) (response), b(x) (interacting), d(x) (shifting), and s(x) (scaling). All except response can be missing (in this case an unconditional distribution is estimated).

This function only specifies the model which can then be fitted using mlt. The shift term is positive by default.

Possible choices of the distributions the model transforms to (the inverse link functions F_Z) include the standard normal ("Normal"), the standard logistic ("Logistic"), the standard minimum extreme value ("MinExtrVal", also known as Gompertz distribution), and the standard maximum extreme value ("MaxExtrVal", also known as Gumbel distribution) distributions. The exponential distribution ("Exponential") can be used to fit Aalen additive hazard models. Laplace and Cauchy distributions are also available.

Value

An object of class ctm.

References

Torsten Hothorn, Lisa Moest, Peter Buehlmann (2018), Most Likely Transformations, *Scandinavian Journal of Statistics*, **45**(1), 110–134, doi:10.1111/sjos.12291.

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ctm-methods

Methods for ctm Objects

Description

Methods for objects of class ctm

Usage

Arguments

object an unfitted conditional transformation model as returned by ctm which a character specifying which names shall be returned additional arguments

Details

coef can be used to get and set model parameters.

mlt

Most Likely Transformations

Description

Likelihood-based model estimation in conditional transformation models

```
mlt(model, data, weights = NULL, offset = NULL, fixed = NULL, theta = NULL,
    pstart = NULL, scale = FALSE, dofit = TRUE, optim = mltoptim())
```

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Arguments

model	a conditional transformation model as specified by ctm
data	a data.frame containing all variables specified in model
weights	an optional vector of case weights
offset	an optional vector of offset values; offsets are not added to an optional scaling term (see link{ctm})
fixed	a named vector of fixed regression coefficients; the names need to correspond to column names of the design matrix
theta	optional starting values for the model parameters
pstart	optional starting values for the distribution function evaluated at the data
scale	a logical indicating if (internal) scaling shall be applied to the model coefficients
dofit	a logical indicating if the model shall be fitted to the data (TRUE) or not. If theta is given, a model of class mlt (a full "fitted" model) featuring these parameters is returned. Otherwise, an unfitted model of class ctm is returned
optim	a list of functions implementing suitable optimisers

Details

This function fits a conditional transformation model by searching for the most likely transformation as described in Hothorn et al. (2018) and Hothorn (2020).

Value

An object of class mlt with corresponding methods.

References

Torsten Hothorn, Lisa Moest, Peter Buehlmann (2018), Most Likely Transformations, *Scandinavian Journal of Statistics*, **45**(1), 110–134, doi:10.1111/sjos.12291.

Torsten Hothorn (2020), Most Likely Transformations: The mlt Package, *Journal of Statistical Software*, **92**(1), 1–68, doi:10.18637/jss.v092.i01

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```
q \leftarrow predict(mltm, newdata = data.frame(speed = 0:24), type = "quantile", p = 2:8 / 10, K = 500)

tmp \leftarrow apply(q, 1, function(x) lines(0:24, x, type = "l"))
```

mlt-methods

Methods for mlt Objects

Description

Methods for objects of class mlt

```
## S3 method for class 'mlt'
coef(object, fixed = TRUE, ...)
coef(object) <- value</pre>
## S3 method for class 'mlt'
weights(object, ...)
## S3 method for class 'mlt'
logLik(object, parm = coef(object, fixed = FALSE), w = NULL, newdata, ...)
## S3 method for class 'mlt'
vcov(object, parm = coef(object, fixed = FALSE), complete = FALSE, ...)
Hessian(object, ...)
## S3 method for class 'mlt'
Hessian(object, parm = coef(object, fixed = FALSE), ...)
Gradient(object, ...)
## S3 method for class 'mlt'
Gradient(object, parm = coef(object, fixed = FALSE), ...)
## S3 method for class 'mlt'
estfun(x, parm = coef(x, fixed = FALSE),
       w = NULL, newdata, ...)
## S3 method for class 'mlt'
residuals(object, parm = coef(object, fixed = FALSE),
       w = NULL, newdata, what = c("shifting", "scaling"), ...)
## S3 method for class 'mlt'
mkgrid(object, n, ...)
## S3 method for class 'mlt'
bounds(object)
## S3 method for class 'mlt'
variable.names(object, ...)
## S3 method for class 'mlt_fit'
update(object, weights = stats::weights(object),
      subset = NULL, offset = object$offset, theta = coef(object, fixed = FALSE),
       fixed = NULL, ...)
## S3 method for class 'mlt'
as.mlt(object)
```

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Arguments

object, x a fitted conditional transformation model as returned by mlt

fixed a logical indicating if only estimated coefficients (fixed = FALSE) should be

returned OR (for update) a named vector of fixed regression coefficients; the

names need to correspond to column names of the design matrix

value coefficients to be assigned to the model

parm model parameters
w model weights

what type of residual: shifting means score with respect to a constant intercept for

the shift term and scaling means score with respect to a constant intercept in the scaling term. This works whether or not such terms are actually present in

the model

weights model weights

newdata an optional data frame of new observations. Allows evaluation of the log-

likelihood for a given model object on these new observations. The parameters

parm and w are ignored in this situation.

n number of grid points

subset an optional integer vector indicating the subset of observations to be used for

fitting.

offset an optional vector of offset values

theta optional starting values for the model parameters

complete currently ignored
... additional arguments

Details

coef can be used to get and set model parameters, weights and logLik extract weights and evaluate the log-likelihood (also for parameters other than the maximum likelihood estimate). Hessian returns the Hessian and vcov the inverse thereof. Gradient gives the negative gradient (sum of the score contributions) and estfun the negative score contribution by each observation. mkgrid generates a grid of all variables (as returned by variable.names) in the model. update allows refitting the model with alternative weights and potentially different starting values. bounds gets bounds for bounded variables in the model.

mltoptim Control Optimisation

Description

Define optimisers and their control parameters

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Usage

Arguments

auglag	A list with control parameters for the auglag optimiser. maxtry is the number of times the algorithm is started on random starting values in case it failed with the precomputed ones.
spg	A list with control parameters for the ${\tt BBoptim}$ optimiser (calling ${\tt spg}$ internally).
nloptr	A list with control parameters for the nloptr family of optimisers.
trace	A logical switching trace reports by the optimisers off.

Details

This function sets-up functions to be called in mlt internally.

Value

A list of functions with arguments theta (starting values), f (log-likelihood), g (scores), ui and ci (linear inequality constraints). Adding further such functions is a way to add more optimisers to mlt. The first one in this list converging defines the resulting model.

plot-predict-simulate Plots, Predictions and Samples from mlt Objects

Description

Plot, predict and sample from objects of class mlt

Usage

```
## S3 method for class 'ctm'
plot(x, newdata, type = c(
         "distribution", "logdistribution",
         "survivor", "logsurvivor",
"density", "logdensity",
"hazard", "loghazard",
         "cumhazard", "logcumhazard",
         "odds", "logodds",
         "quantile", "trafo"),
     q = NULL, prob = 1:(K - 1) / K, K = 50, col = rgb(.1, .1, .1, .1), lty = 1,
     add = FALSE, ...)
## S3 method for class 'mlt'
plot(x, ...)
## S3 method for class 'ctm'
predict(object, newdata, type = c("trafo",
         "distribution", "logdistribution",
         "survivor", "logsurvivor",
         "density", "logdensity",
         "hazard", "loghazard",
         "cumhazard", "logcumhazard",
         "odds", "logodds",
         "quantile"),
         terms = c("bresponse", "binteracting", "bshifting"),
         q = NULL, prob = NULL, K = 50, interpolate = FALSE, ...)
## S3 method for class 'mlt'
predict(object, newdata = object$data, ...)
## S3 method for class 'ctm'
simulate(object, nsim = 1, seed = NULL, newdata, K = 50, q = NULL,
         interpolate = FALSE, bysim = TRUE, ...)
## S3 method for class 'mlt'
simulate(object, nsim = 1, seed = NULL, newdata = object$data, bysim = TRUE, ...)
```

Arguments

object a fitted conditional transformation model as returned by mlt or an unfitted conditional transformation model as returned by ctm

x a fitted conditional transformation model as returned by mlt

newdata an optional data frame of observations
type type of prediction or plot to generate
q quantiles at which to evaluate the model

prob probabilities for the evaluation of the quantile function (type = "quantile")

terms to evaluate for the predictions, corresponds to the argument response,

interacting and shifting in $\operatorname{\mathsf{ctm}}$

K number of grid points to generate (in the absence of q)

col color for the lines to plot

lty line type for the lines to plot

add logical indicating if a new plot shall be generated (the default)

interpolate logical indicating if quantiles shall be interpolated linearily. This unnecessary

option is no longer implemented (starting with 1.2-1).

nsim number of samples to generate

seed optional seed for the random number generator

bysim logical, if TRUE a list with nsim elements is returned, each element is of length

nrow(newdata) and contains one sample from the conditional distribution for each row of newdata. If FALSE, a list of length nrow(newdata) is returned, its ith element of length nsim contains nsim samples from the conditional distribu-

tion given newdata[i,].

. . . additional arguments

Details

plot evaluates the transformation function over a grid of q values for all observations in newdata and plots these functions (according to type). predict evaluates the transformation function over a grid of q values for all observations in newdata and returns the result as a matrix (where _columns_ correspond to _rows_ in newdata, see examples). Lack of type = "mean" is a feature and not a bug.

Argument type defines the scale of the plots or predictions: type = "distribution" means the cumulative distribution function, type = "survivor" is the survivor function (one minus distribution function), type = "density" the absolute continuous or discrete density (depending on the response), type = "hazard", type = "cumhazard", and type = "odds" refers to the hazard (absolute continuous or discrete), cumulative hazard (defined as minus log-survivor function in both the absolute continuous and discrete cases), and odds (distribution divided by survivor) functions. The quantile function can be evaluated for probabilities prob by type = "quantile".

Note that the predict method for ctm objects requires all model coefficients to be specified in this unfitted model. simulate draws samples from object by numerical inversion of the quantile function.

Note that offsets are ALWAYS IGNORED when computing predictions. If you want the methods to pay attention to offsets, specify them as a variable in the model with fixed regression coefficient using the fixed argument in mlt.

More examples can be found in Hothorn (2018).

References

Torsten Hothorn (2020), Most Likely Transformations: The mlt Package, *Journal of Statistical Software*, **92**(1), 1–68, doi:10.18637/jss.v092.i01

```
library("survival")
op <- options(digits = 2)
### GBSG2 dataset
data("GBSG2", package = "TH.data")
### right-censored response
GBSG2$y <- with(GBSG2, Surv(time, cens))</pre>
### define Bernstein(log(time)) parameterisation
### of transformation function. The response
### is bounded (log(0) doesn't work, so we use log(1))
### support defines the support of the Bernstein polynomial
### and add can be used to make the grid wider (see below)
rvar <- numeric_var("y", bounds = c(0, Inf),</pre>
                    support = c(100, 2000))
rb <- Bernstein_basis(rvar, order = 6, ui = "increasing")</pre>
### dummy coding of menopausal status
hb <- as.basis(~ 0 + menostat, data = GBSG2)</pre>
### treatment contrast of hormonal treatment
xb <- as.basis(~ horTh, data = GBSG2, remove_intercept = TRUE)</pre>
### set-up and fit Cox model, stratified by menopausal status
m <- ctm(rb, interacting = hb, shifting = xb, todistr = "MinExtrVal")</pre>
fm <- mlt(m, data = GBSG2)</pre>
### generate grid for all three variables
### note that the response grid ranges between 1 (bounds[1])
### and 2000 (support[2])
(d \leftarrow mkgrid(m, n = 10))
### data.frame of menopausal status and treatment
nd <- do.call("expand.grid", d[-1])</pre>
### plot model on different scales, for all four combinations
### of menopausal status and hormonal treatment
typ <- c("distribution", "survivor", "density", "hazard",</pre>
         "cumhazard", "odds")
layout(matrix(1:6, nrow = 2))
nl <- sapply(typ, function(tp)</pre>
    ### K = 500 makes densities and hazards smooth
    plot(fm, newdata = nd, type = tp, col = 1:nrow(nd), K = 500))
legend("topleft", lty = 1, col = 1:nrow(nd),
       legend = do.call("paste", nd), bty = "n")
### plot calls predict, which generates a grid with K = 50
### response values
```

```
### note that a K x nrow(newdata) matrix is returned
### (for reasons explained in the next example)
predict(fm, newdata = nd, type = "survivor")
### newdata can take a list, and evaluates the survivor
### function on the grid defined by newdata
### using a linear array model formulation and is
### extremely efficient (wrt computing time and memory)
### d[1] (the response grid) varies fastest
\#\#\# \Rightarrow the first dimension of predict() is always the response,
### not the dimension of the predictor variables (like one
### might expect)
predict(fm, newdata = d, type = "survivor")
### owing to this structure, the result can be quickly stored in
### a data frame as follows
cd <- do.call("expand.grid", d)</pre>
cd$surv <- c(S <- predict(fm, newdata = d, type = "survivor"))</pre>
### works for distribution functions
all.equal(1 - S, predict(fm, newdata = d, type = "distribution"))
### cumulative hazard functions
all.equal(-log(S), predict(fm, newdata = d, type = "cumhazard"))
### log-cumulative hazard functions (= trafo, for Cox models)
all.equal(log(-log(S)), predict(fm, newdata = d, type = "logcumhazard"))
all.equal(log(-log(S)), predict(fm, newdata = d, type = "trafo"))
### densities, hazards, or odds functions
predict(fm, newdata = d, type = "density")
predict(fm, newdata = d, type = "hazard")
predict(fm, newdata = d, type = "odds")
### and quantiles (10 and 20%)
predict(fm, newdata = d[-1], type = "quantile", prob = 1:2 / 10)
### note that some quantiles are only defined as intervals
### (> 2000, in this case). Intervals are returned as an "response"
### object, see ?R. Unfortunately, these can't be stored as array, so
### a data.frame is returned where the quantile varies first
p \leftarrow c(list(prob = 1:9/10), d[-1])
np <- do.call("expand.grid", p)</pre>
(Q <- predict(fm, newdata = d[-1], type = "quantile", prob = 1:9 / 10))
np$Q <- Q
np
\#\#\# simulating from the model works by inverting the distribution
### function; some obs are right-censored at 2000
(s <- simulate(fm, newdata = nd, nsim = 3))</pre>
### convert to Surv
sapply(s, as.Surv)
### generate 3 parametric bootstrap samples from the model
tmp <- GBSG2[, c("menostat", "horTh")]</pre>
s <- simulate(fm, newdata = tmp, nsim = 3)</pre>
### refit the model using the simulated response
```

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```
lapply(s, function(y) {
  tmp$y <- y
  coef(mlt(m, data = tmp))
})
options(op)</pre>
```

R

Response Variables

Description

Represent a possibly censored or truncated response variable

Usage

```
R(object, ...)
## S3 method for class 'numeric'
R(object = NA, cleft = NA, cright = NA,
   tleft = NA, tright = NA, tol = sqrt(.Machine$double.eps),
   as.R.ordered = FALSE, as.R.interval = FALSE, ...)
## S3 method for class 'ordered'
R(object, cleft = NA, cright = NA, ...)
## S3 method for class 'integer'
R(object, cleft = NA, cright = NA, bounds = c(min(object), Inf), ...)
## S3 method for class 'factor'
R(object, ...)
## S3 method for class 'Surv'
R(object, as.R.ordered = FALSE, as.R.interval = FALSE, ...)
as.Surv(object)
## S3 method for class 'response'
as.Surv(object)
## S3 method for class 'response'
as.double(x, ...)
```

Arguments

object	A vector of (conceptually) exact measurements or an object of class response (for as.Surv) or a list.
X	same as object.
cleft	A vector of left borders of censored measurements
cright	A vector of right borders of censored measurements
tleft	A vector of left truncations
tright	A vector of right truncations
tol	Tolerance for checking if cleft < cright

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bounds	Range of possible values for integers
as.R.ordered	logical, should numeric responses or right-censored (and possible left-truncated survival) times be coded as ordered factor? This leads to a parameterisation allowing to maximise the nonparametric maximum likelihood
as.R.interval	logical, should numeric responses be coded for the nonparametric maximum likelihood
	other arguments, ignored except for tleft and tright to R. ordered and R. integer

Details

R is basically an extention of Surv for the representation of arbitrarily censored or truncated measurements at any scale. The storage.mode of object determines if models are fitted by the discrete likelihood (integers or factors) or the continuous likelihood (log-density for numeric objects). Interval-censoring is given by intervals (cleft, cright], also for integers and factors (see example below). Left- and right-truncation can be defined by the tleft and tright arguments. Existing Surv objects can be converted using R(Surv(...))\$ and, in some cases, an as.Surv() method exists for representing response objects as Surv objects.

R applied to a list calls R for each of the list elements and returns a joint object.

More examples can be found in Hothorn (2018) and in vignette ("tram", package = "tram").

References

Torsten Hothorn (2020), Most Likely Transformations: The mlt Package, *Journal of Statistical Software*, **92**(1), 1–68, doi:10.18637/jss.v092.i01

```
library("survival")
### randomly right-censored continuous observations
time <- as.double(1:9)</pre>
event <- rep(c(FALSE, TRUE), length = length(time))</pre>
Surv(time, event)
R(Surv(time, event))
### right-censoring, left-truncation
ltm <- 1:9 / 10
Surv(ltm, time, event)
R(Surv(ltm, time, event))
### interval-censoring
Surv(ltm, time, type = "interval2")
R(Surv(ltm, time, type = "interval2"))
### interval-censoring, left/right-truncation
lc <- as.double(1:4)</pre>
lt <- c(NA, NA, 7, 8)
rt <- c(NA, 9, NA, 10)
```

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```
x \leftarrow c(3, NA, NA, NA)
rc <- as.double(11:14)</pre>
R(x, cleft = lt, cright = rt)
as.Surv(R(x, cleft = lt, cright = rt))
R(x, tleft = 1, cleft = lt, cright = rt)
R(x, tleft = 1, cleft = lt, cright = rt, tright = 15)
R(x, tleft = lc, cleft = lt, cright = rt, tright = rc)
### discrete observations: counts
x <- 0:9
R(x)
### partially interval-censored counts
rx <- c(rep(NA, 6), rep(15L, 4))
R(x, cright = rx)
### ordered factor
x \leftarrow gl(5, 2, labels = LETTERS[1:5], ordered = TRUE)
### interval-censoring (ie, observations can have multiple levels)
1x <- ordered(c("A", "A", "B", "C", "D", "E"),</pre>
              levels = LETTERS[1:5], labels = LETTERS[1:5])
rx <- ordered(c("B", "D", "E", "D", "D", "E"),</pre>
              levels = LETTERS[1:5], labels = LETTERS[1:5])
R(rx, cleft = lx, cright = rx)
### facilitate nonparametric maximum likelihood
(y <- round(runif(10), 1))</pre>
R(y, as.R.ordered = TRUE)
R(Surv(time, event), as.R.ordered = TRUE)
R(Surv(ltm, time, event), as.R.ordered = TRUE)
```

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