

Package ‘mlt’

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Title Most Likely Transformations

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Description Likelihood-based estimation of conditional transformation models via the most likely transformation approach described in Hothorn et al. (2018) <[DOI:10.1111/sjos.12291](https://doi.org/10.1111/sjos.12291)> and Hothorn (2020) <[DOI:10.18637/jss.v092.i01](https://doi.org/10.18637/jss.v092.i01)>.

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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](https://doi.org/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](https://doi.org/10.18637/jss.v092.i01)

 confband

 Confidence Bands

Description

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

Usage

```
confband(object, newdata, level = 0.95, ...)
## S3 method for class 'mlt'
confband(object, newdata, level = 0.95,
         type = c("trafo", "distribution", "survivor", "cumhazard"),
         K = 20, cheat = K, ...)
```

Arguments

object	an object of class <code>mlt</code>
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 <code>confint.glt</code>

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

Usage

```
ctm(response, interacting = NULL, shifting = NULL, scaling = NULL,
     scale_shift = FALSE, data = NULL,
     todistr = c("Normal", "Logistic", "MinExtrVal", "MaxExtrVal", "Exponential"),
     sumconstr = inherits(interacting, c("formula", "formula_basis")), ...)
```

Arguments

response	a basis function, ie, an object of class <code>basis</code>
interacting	a basis function, ie, an object of class <code>basis</code>
shifting	a basis function, ie, an object of class <code>basis</code>
scaling	a basis function, ie, an object of class <code>basis</code>

scale_shift	a logical choosing between two different model types in the presence of a scaling term
data	either a <code>data.frame</code> containing the model variables or a formal description of these variables in an object of class <code>vars</code>
todistr	a character vector describing the distribution to be transformed
sumconstr	a logical indicating if sum constraints shall be applied
...	arguments to <code>as.basis</code> when <code>shifting</code> is a formula

Details

Specification of a transformation model of the form

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

(`scale_shift = FALSE`) or

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

(`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.

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](https://doi.org/10.1111/sjos.12291).

Description

Methods for objects of class `ctm`

Usage

```
## S3 method for class 'ctm'
variable.names(object,
               which = c("all", "response", "interacting",
                        "shifting", "scaling"),
               ...)
## S3 method for class 'ctm'
coef(object, ...)
```

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	<i>Most Likely Transformations</i>
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Description

Likelihood-based model estimation in conditional transformation models

Usage

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

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
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](https://doi.org/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](https://doi.org/10.18637/jss.v092.i01)

Examples

```
### set-up conditional transformation model for conditional
### distribution of dist given speed
dist <- numeric_var("dist", support = c(2.0, 100), bounds = c(0, Inf))
speed <- numeric_var("speed", support = c(5.0, 23), bounds = c(0, Inf))
ctmm <- ctm(response = Bernstein_basis(dist, order = 4, ui = "increasing"),
            interacting = Bernstein_basis(speed, order = 3))

### fit model
mltm <- mlt(ctmm, data = cars)

### plot data
plot(cars)
### predict quantiles and overlay data with model via a "quantile sheet"
q <- predict(mltm, newdata = data.frame(speed = 0:24), type = "quantile",
            p = 2:8 / 10, K = 500)
tmp <- apply(q, 1, function(x) lines(0:24, x, type = "l"))
```

Description

Methods for objects of class `mlt`

Usage

```

## S3 method for class 'mlt'
coef(object, fixed = TRUE, ...)
coef(object) <- value
## 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(object, parm = coef(object, fixed = FALSE),
        w = NULL, newdata, ...)
## 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),
        ...)
## S3 method for class 'mlt'
as.mlt(object)

```

Arguments

object	a fitted conditional transformation model as returned by <code>mlt</code>
fixed	a logical indicating if only estimated coefficients (<code>fixed = FALSE</code>) should be returned
value	coefficients to be assigned to the model
parm	model parameters
w	model weights
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 <code>parm</code> and <code>w</code> 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	<i>Control Optimisation</i>
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Description

Define optimisers and their control parameters

Usage

```
mltoptim(auglag = list(maxtry = 5, kkt2.check = FALSE),
         spg = list(maxit = 10000, quiet = TRUE, checkGrad = FALSE),
         nloptr = NULL, trace = FALSE)
```

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 BBoptim optimiser (calling spg internally).
nloptr	A list with control parameters for the nloptr optimiser. This is still experimental and thus switched off (defaulting to NULL).
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.

Examples

```
### set-up linear transformation model for conditional
### distribution of dist given speed
dist <- numeric_var("dist", support = c(2.0, 100), bounds = c(0, Inf))
ctmm <- ctm(response = Bernstein_basis(dist, order = 4, ui = "increasing"),
            shifting = ~ speed, data = cars)

### use auglag with kkt2.check = TRUE => the numerically determined
### hessian is returned as "optim_hessian" slot
op <- mltoptim(auglag = list(maxtry = 5, kkt2.check = TRUE))[1]
mltm <- mlt(ctmm, data = cars, scale = FALSE, optim = op)

### compare analytical and numerical hessian
all.equal(c(Hessian(mltm)), c(mltm$optim_hessian), tol = 1e-4)
```

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", "survivor", "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",
                                "survivor", "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 '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 <code>mlt</code> or an unfitted conditional transformation model as returned by <code>ctm</code>
x	a fitted conditional transformation model as returned by <code>mlt</code>
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 (<code>type = "quantile"</code>)
terms	terms to evaluate for the predictions, corresponds to the argument response, interacting and shifting in <code>ctm</code>
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 linearly. 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 <code>nsim</code> elements is returned, each element is of length <code>nrow(newdata)</code> and contains one sample from the conditional distribution for each row of <code>newdata</code> . If FALSE, a list of length <code>nrow(newdata)</code> is returned, its <code>i</code> th element of length <code>nsim</code> contains <code>nsim</code> samples from the conditional distribution given <code>newdata[i,]</code> .
...	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](https://doi.org/10.18637/jss.v092.i01)

Examples

```
library("survival")
op <- options(digits = 2)

### GBSG2 dataset
data("GBSG2", package = "TH.data")

### right-censored response
GBSG2$y <- with(GBSG2, Surv(time, cens))

### 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),
                   support = c(100, 2000))
rb <- Bernstein_basis(rvar, order = 6, ui = "increasing")
### dummy coding of menopausal status
hb <- as.basis(~ 0 + menostat, data = GBSG2)
### treatment contrast of hormonal treatment
xb <- as.basis(~ horTh, data = GBSG2, remove_intercept = TRUE)

### set-up and fit Cox model, stratified by menopausal status
m <- ctm(rb, interacting = hb, shifting = xb, todistr = "MinExtrVal")
fm <- mlt(m, data = GBSG2)

### generate grid for all three variables
### note that the response grid ranges between 1 (bounds[1])
### and 2000 (support[2])
(d <- mkgrid(m, n = 10))
### data.frame of menopausal status and treatment
nd <- do.call("expand.grid", d[-1])
```

```

### plot model on different scales, for all four combinations
### of menopausal status and hormonal treatment
typ <- c("distribution", "survivor", "density", "hazard",
        "cumhazard", "odds")
layout(matrix(1:6, nrow = 2))
nl <- sapply(typ, function(tp)
  ### 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
### => 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)
cd$surv <- c(S <- predict(fm, newdata = d, type = "survivor"))

### 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 <- c(list(prob = 1:9/10), d[-1])
np <- do.call("expand.grid", p)
(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))
### convert to Surv
sapply(s, as.Surv)

### generate 3 parametric bootstrap samples from the model
tmp <- GBSG2[, c("menostat", "horTh")]
s <- simulate(fm, newdata = tmp, nsim = 3)
### refit the model using the simulated response
lapply(s, function(y) {
  tmp$y <- y
  coef(mlt(m, data = tmp))
})

options(op)

```

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, ...)
## 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.Surv(object)
## S3 method for class 'response'
as.Surv(object)
## S3 method for class 'response'
as.double(x, ...)

```

Arguments

<code>object</code>	A vector of (conceptually) exact measurements or an object of class <code>response</code> (for <code>as.Surv</code>) or a list.
<code>x</code>	same as <code>object</code> .
<code>cleft</code>	A vector of left borders of censored measurements
<code>cright</code>	A vector of right borders of censored measurements
<code>tleft</code>	A vector of left truncations
<code>tright</code>	A vector of right truncations
<code>tol</code>	Tolerance for checking if <code>cleft < cright</code>
<code>bounds</code>	Range of possible values for integers
<code>as.R.ordered</code>	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.
<code>...</code>	other arguments, ignored except for <code>tleft</code> and <code>tright</code> to <code>R.ordered</code> and <code>R.integer</code>

Details

R is basically an extension 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](https://doi.org/10.18637/jss.v092.i01)

Examples

```
library("survival")

### randomly right-censored continuous observations
time <- as.double(1:9)
event <- rep(c(FALSE, TRUE), length = length(time))

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)
lt <- c(NA, NA, 7, 8)
rt <- c(NA, 9, NA, 10)
x <- c(3, NA, NA, NA)
rc <- as.double(11:14)
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 <- gl(5, 2, labels = LETTERS[1:5], ordered = TRUE)
R(x)
### interval-censoring (ie, observations can have multiple levels)
lx <- ordered(c("A", "A", "B", "C", "D", "E"),
             levels = LETTERS[1:5], labels = LETTERS[1:5])
rx <- ordered(c("B", "D", "E", "D", "D", "E"),
             levels = LETTERS[1:5], labels = LETTERS[1:5])
R(rx, cleft = lx, cright = rx)

### facilitate nonparametric maximum likelihood
(y <- round(runif(10), 1))
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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