Package ‘crs’

February 19, 2015

Version 0.15-24
Date 2014-12-18
Imports boot, stats, np, quantreg, rgl
Suggests logspline, npRmpi, quadprog
Title Categorical Regression Splines
Description

Regression splines that handle a mix of continuous and categorical (discrete) data often encountered in applied settings. I would like to gratefully acknowledge support from the Natural Sciences and Engineering Research Council of Canada (NSERC:www.nserc.ca), the Social Sciences and Humanities Research Council of Canada (SSHRC:www.sshrc.ca), and the Shared Hierarchical Academic Research Computing Network (SHARCNET:www.sharcnet.ca).

License GPL
URL https://github.com/JeffreyRacine/R-Package-crs/
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NeedsCompilation yes
Repository CRAN
Date/Publication 2014-12-18 18:37:00

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Nonparametric Regression Splines with Continuous and Categorical Predictors

Description

This package provides a method for nonparametric regression that combines the (global) approximation power of regression splines for continuous predictors ('x') with the (local) power of kernel methods for categorical predictors ('z'). The user also has the option of instead using indicator bases for the categorical predictors. When the predictors contain both continuous and categorical (discrete) data types, both approaches offer more efficient estimation than the traditional sample-splitting (i.e. 'frequency') approach where the data is first broken into subsets governed by the categorical z.

To cite the crs package type: ‘citation("crs")’ (without the single quotes).

For a listing of all routines in the crs package type: ‘library(help="crs")’.

For a listing of all demos in the crs package type: ‘demo(package="crs")’.

For a ‘vignette’ that presents an overview of the crs package type: ‘vignette("crs")’.

Details

For the continuous predictors the regression spline model employs the B-spline basis matrix using the B-spline routines in the GNU Scientific Library (http://www.gnu.org/software/gsl/).

The tensor.prod.model.matrix function is used to construct multivariate tensor spline bases when basis="tensor" and uses additive B-splines otherwise (i.e. when basis="additive").

For the discrete predictors the product kernel function is of the ‘Li-Racine’ type (see Li and Racine (2007) for details) which is formed by constructing products of one of the following univariate kernels:

\( l(z_i, z, \lambda) = 1 \) if \( z_i = z \), and \( \lambda \) if \( z_i \neq z \). Note that \( \lambda \) must lie between 0 and 1.

\( \lambda |z_i - z| \) if \( |z_i - z| \geq 1 \). Note that \( \lambda \) must lie between 0 and 1.
Alternatively, for the ordinal/nominal predictors the regression spline model will use indicator basis functions.

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I would like to gratefully acknowledge support from the Natural Sciences and Engineering Research Council of Canada (http://www.nserc.ca), the Social Sciences and Humanities Research Council of Canada (http://www.sshrc.ca), and the Shared Hierarchical Academic Research Computing Network (http://www.sharcnet.ca).

References


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clsd

*Categorical Log spline Density*

**Description**

clsd computes the log spline density, density derivative, distribution, and smoothed quantiles for a one (1) dimensional continuous variable using the approach of Racine (2013).

**Usage**

```r
clsd(x = NULL,
    beta = NULL,
    xeval = NULL,
    degree = NULL,
    segments = NULL,
    degree.min = 2,
    degree.max = 25,
    segments.min = 1,
    segments.max = 100,
    lbound = NULL,
    ubound = NULL,
    basis = "tensor",
    knots = "quantiles",
    penalty = NULL,
    deriv.index = 1,
```
deriv = 1,
elastic.max = TRUE,
elastic.diff = 3,
do.gradient = TRUE,
er = NULL,
monotone = TRUE,
monotone.lb = -250,
n.integrate = 500,
nmulti = 1,
method = c("L-BFGS-B", "Nelder-Mead", "BFGS", "CG", "SANN"),
verbose = FALSE,
quantile.seq = seq(.01,.99,by=.01),
random.seed = 42,
maxit = 10^5,
max.attempts = 25,
NOMAD = FALSE)

Arguments

x a numeric vector of training data
beta a numeric vector of coefficients (default NULL)
xeval a numeric vector of evaluation data
degree integer/vector specifying the polynomial degree of the B-spline basis for each dimension of the continuous x (default degree=2)
segments integer/vector specifying the number of segments of the B-spline basis for each dimension of the continuous x (i.e. number of knots minus one) (default segments=1, i.e. Bezier curve)
segments.min,segments.max when elastic.max=FALSE, the minimum/maximum segments of the B-spline basis for each of the continuous predictors (default segments.min=1, segments.max=100)
degree.min,degree.max when elastic.max=FALSE the minimum/maximum degree of the B-spline basis for each of the continuous predictors (default degree.min=2, degree.max=25)
lbound,ubound lower/upper bound for the support of the density. For example, if there is a priori knowledge that the density equals zero to the left of 0, and has a discontinuity at 0, the user could specify lbound = 0. However, if the density is essentially zero near 0, one does not need to specify lbound
basis a character string (default basis="tensor") indicating whether the additive or tensor product B-spline basis matrix for a multivariate polynomial spline or generalized B-spline polynomial basis should be used
knots a character string (default knots="quantiles") specifying where knots are to be placed. ‘quantiles’ specifies knots placed at equally spaced quantiles (equal number of observations lie in each segment) and ‘uniform’ specifies knots placed at equally spaced intervals
deriv an integer 1 (default deriv=1) specifying whether to compute the univariate 1th partial derivative for each continuous predictor (and difference in levels for each
clsd

categorical predictor) or not and if so what order. Note that if deriv is higher
than the spline degree of the associated continuous predictor then the derivative
will be zero and a warning issued to this effect.
deriv.index an integer 1 (default deriv.index=1) specifying the index (currently only sup-
ports 1) of the variable whose derivative is requested.
rmulti integer number of times to restart the process of finding extrema of the cross-
validation function from different (random) initial points (default rmulti=1).
penalty the parameter to be used in the AIC criterion. The method chooses the number of
degrees plus number of segments (knots-1) that maximizes 2*log1-penalty*(degree+segments). The default is to use the penalty parameter of log(n)/2 (2 would deliver stan-
ard AIC, log(n) standard BIC).
elastic.max,elastic.diff
  a logical value/integer indicating whether to use ‘elastic’ search bounds such that
  the optimal degree/segment must lie elastic.diff units from the respective
  search bounds.
do.gradient a logical value indicating whether or not to use the analytical gradient during
  optimization (defaults to TRUE).
er a scalar indicating the fraction of data range to extend the tails (default 1/10log(n)),
  see extendrange for further details.
monotone a logical value indicating whether modify the standard B-spline basis function
  so that it is tailored for density estimation (default TRUE).
monotone.lb a negative bound specifying the lower bound on the linear segment coefficients
  used when (monotone=FALSE).
n.integrate the number of evenly spaced integration points on the extended range specified
  by er (defaults to 500).
method see optim for details.
verbose a logical value which when TRUE produces verbose output during optimization
quantile.seq a sequence of numbers lying in [0,1] on which quantiles from the logspline
distribution are obtained.
random.seed seeds the random number generator for initial parameter values when optim is
called.
maxit maximum number of iterations used by optim.
max.attempts maximum number of attempts to undertake if optim fails for any set of initial
  parameters for each value of rmulti.
NOMAD a logical value which when TRUE calls snomadr to determine the optimal degree
  and segments.

Details

Typical usages are (see below for a list of options and also the examples at the end of this help file)

model <- clsd(x)
clsd computes a logspline density estimate of a one (1) dimensional continuous variable. The spline model employs the tensor product B-spline basis matrix for a multivariate polynomial spline via the B-spline routines in the GNU Scientific Library (http://www.gnu.org/software/gsl/) and the tensor.prod.model.matrix function.

When basis="additive" the model becomes additive in nature (i.e. no interaction/tensor terms thus semiparametric not fully nonparametric).
When basis="tensor" the model uses the multivariate tensor product basis.

Value

clsd returns a clsd object. The generic functions coef, fitted, plot and summary support objects of this type (er=FALSE plots the density on the sample realizations (default is ‘extended range’ data), see er above, distribution=TRUE plots the distribution). The returned object has the following components:

- density: estimates of the density function at the sample points
- density.er: the density evaluated on the ‘extended range’ of the data
- density.deriv: estimates of the derivative of the density function at the sample points
- density.deriv.er: estimates of the derivative of the density function evaluated on the ‘extended range’ of the data
- distribution: estimates of the distribution function at the sample points
- distribution.er: the distribution evaluated on the ‘extended range’ of the data
- xer: the ‘extended range’ of the data
- degree: integer/vector specifying the degree of the B-spline basis for each dimension of the continuous x
- segments: integer/vector specifying the number of segments of the B-spline basis for each dimension of the continuous x
- xq: vector of quantiles
- tau: vector generated by quantile.seq or input by the user (lying in [0,1]) from which the quantiles xq are obtained

Usage Issues

This function should be considered to be in ‘beta’ status until further notice.
If smoother estimates are desired and degree=degree.min, increase degree.min to, say, degree.min=3.
The use of ‘regression’ B-splines can lead to undesirable behavior at the endpoints of the data (i.e. when monotone=FALSE). The default ‘density’ B-splines ought to be well-behaved in these regions.

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References


See Also

logspline

Examples

```R
## Not run:
## Old Faithful eruptions data histogram and clsd density

library(MASS)
data(faithful)
attach(faithful)

model <- clsd(eruptions)

ylim <- c(0,max(model$density,hist(eruptions,breaks=20,plot=FALSE)$density))

plot(model,ylim=ylim)

hist(eruptions,breaks=20,freq=FALSE,add=TRUE,lty=2)

rug(eruptions)

summary(model)

coef(model)

## Simulated data

set.seed(42)
require(logspline)

## Example - simulated data

n <- 250
x <- sort(rnorm(n))
f.dgp <- dnorm(x)

model <- clsd(x)

## Standard (cubic) estimate taken from the logspline package
## Compute MSEs

mse.clspd <- mean((fitted(model)-f.dgp)^2)

model.logspline <- logspline(x)

mse.logspline <- mean((dlogspline(x,model.logspline)-f.dgp)^2)
```
```r
ylim <- c(0, max(fitted(model), dlogspline(x, model.logspline), f.dgp))

plot(model,
    ylim=ylim,
    sub=paste("MSE: logspline = ", format(mse.logspline), ", clsd = ",
                format(mse.clsd),
                lty=3,
                col=3)

xer <- model$xer

lines(xer, dlogspline(xer, model.logspline), col=2, lty=2)
lines(xer, dnorm(xer), col=1, lty=1)

rug(x)

legend("topright", c("DGP",
                  paste("Cubic Log spline Density (package 'logspline', knots = ",
                        model.logspline$nknots, "), sep=""),
                  paste("clsd Density (degree = ", model$degree, ", segments = ",
                        model$segments, ", penalty = ", round(model$penalty,2), ")", sep=""),
                  lty=1:3,
                  col=1:3,
                  bty="n",
                  cex=0.75)

summary(model)

coef(model)

## Simulate data with known bounds

set.seed(42)
n <- 10000
x <- runif(n, 0, 1)
model <- clsd(x, lbound=0, ubound=1)

plot(model)

## End(Not run)
```

---

**Description**

Canadian cross-section wage data consisting of a random sample taken from the 1971 Canadian Census Public Use Tapes for male individuals having common education (grade 13). There are 205 observations in total.
Usage

data("cps71")

Format

A data frame with 2 columns, and 205 rows.

logwage  the first column, of type numeric
age  the second column, of type integer

Source

Aman Ullah

References


Examples

```r
## Example - we compare the nonparametric local linear kernel regression
## method with the regression spline for the cps71 data. Note that there
## are no categorical predictors in this dataset so we are merely
## comparing and contrasting the two nonparametric estimates.

data(cps71)
attach(cps71)
require(np)

model.crs <- crs(logwage~age,complexity="degree-knots")
model.np <- npreg(logwage~age,regtype="ll")

plot(age,logwage,cex=0.25,col="grey",
     sub=paste("crs-CV = ",formatC(model.crs$cv.score,format="f",digits=3),
                 ", npreg-CV = ",formatC(model.np$bw$cv.val,format="f",digits=3),sep=""))
lines(age,fitted(model.crs),lty=1,col=1)
lines(age,fitted(model.np),lty=2,col=2)

crs.txt <- paste("crs (R-squared = ",formatC(model.crs$r.squared,format="f",digits=3),"),sep="")
np.txt <- paste("ll-npreg (R-squared = ",formatC(model.np$r2,format="f",digits=3),"),sep="")

legend(22.5,15,c(crs.txt,np.txt),lty=c(1,2),col=c(1,2),bty="n")

summary(model.crs)
summary(model.np)
detach("package:np")
```
**Description**

`crs` computes a regression spline estimate of a one (1) dimensional dependent variable on an \( r \)-dimensional vector of continuous and categorical (factor/ordered) predictors (Ma and Racine (2013), Ma, Racine and Yang (under revision)).

**Usage**

```r
crs(...)  
## Default S3 method:  
crs(xz,  
y,  
degree = NULL,  
segments = NULL,  
include = NULL,  
kernel = TRUE,  
lambda = NULL,  
complexity = c("degree-knots","degree","knots"),  
knots = c("quantiles","uniform","auto"),  
basis = c("additive","tensor","glp","auto"),  
deriv = 0,  
data.return = FALSE,  
prune = FALSE,  
model.return = FALSE,  
tau = NULL,  
weights = NULL,  
...)

## S3 method for class 'formula'  
crs(formula,  
data = list(),  
degree = NULL,  
segments = NULL,  
include = NULL,  
degree.max = 10,  
segments.max = 10,  
degree.min = 0,  
segments.min = 1,  
CV.df.min = 1,  
CV = c("nomad","exhaustive","none"),  
CV.threshold = 1000,  
CV.func = c("CV.ls","CV.gcv","CV.aic"),  
kernel = TRUE,  
lambda = NULL,  
...)
```

The `crs` function is designed to estimate regression splines for both continuous and categorical predictors. It provides flexibility in specifying the degree of the polynomial, the number of segments, and the inclusion of variables. The usage examples demonstrate how to specify these parameters, with default settings for many arguments to allow for straightforward application. Additional arguments like `kernel`, `lambda`, and `complexity` can be adjusted to control the smoothness and complexity of the estimated spline.
Arguments

**xz**  numeric (x) and or nominal/ordinal (factor/ordered) predictors (z)

**y**  a numeric vector of responses.

**degree**  integer/vector specifying the polynomial degree of the B-spline basis for each dimension of the continuous x (default degree=3, i.e. cubic spline)

**segments**  integer/vector specifying the number of segments of the B-spline basis for each dimension of the continuous x (i.e. number of knots minus one) (default segments=1, i.e. Bezier curve)

**include**  integer/vector specifying whether each of the nominal/ordinal (factor/ordered) predictors in x are included or omitted from the resulting estimate

**lambda**  a vector of bandwidths for each dimension of the categorical z

**lambda.discrete**  if lambda.discrete=TRUE, the bandwidth will be discretized into lambda.discrete.num+1 points and lambda will be chosen from these points

**lambda.discrete.num**  a positive integer indicating the number of discrete values that lambda can assume - this parameter will only be used when lambda.discrete=TRUE

**formula**  a symbolic description of the model to be fit

**data**  an optional data frame containing the variables in the model
cv a character string (default cv="nomad") indicating whether to use nonsmooth mesh adaptive direct search, exhaustive search, or no search (i.e. use user supplied values for degree, segments, and lambda)

cv.threshold an integer (default cv.threshold=1000) for simple problems with no categorical predictors (i.e. kernel=FALSE otherwise optim/snomadr search is necessary) such that, if the number of combinations of degree/segments is less than the threshold and cv="nomad", instead use exhaustive search (cv="exhaustive")

cv.func a character string (default cv.func="cv.ls") indicating which method to use to select smoothing parameters. cv.gcv specifies generalized cross-validation (Craven and Wahba (1979)), cv.aic specifies expected Kullback-Leibler cross-validation (Hurvich, Simonoff, and Tsai (1998)), and cv.ls specifies least-squares cross-validation

kernel a logical value (default kernel=TRUE) indicating whether to use kernel smoothing or not

degree.max the maximum degree of the B-spline basis for each of the continuous predictors (default degree.max=10)

segments.max the maximum segments of the B-spline basis for each of the continuous predictors (default segments.max=10)

degree.min the minimum degree of the B-spline basis for each of the continuous predictors (default degree.min=0)

segments.min the minimum segments of the B-spline basis for each of the continuous predictors (default segments.min=1)

cv.df.min the minimum degrees of freedom to allow when conducting NOMAD-based cross-validation (default cv.df.min=1)

complexity a character string (default complexity="degree-knots") indicating whether model 'complexity' is determined by the degree of the spline or by the number of segments (i.e. number of knots minus one). This option allows the user to use cross-validation to select either the spline degree (number of knots held fixed) or the number of knots (spline degree held fixed) or both the spline degree and number of knots

For the continuous predictors the regression spline model employs either the additive or tensor product B-spline basis matrix for a multivariate polynomial spline via the B-spline routines in the GNU Scientific Library (http://www.gnu.org/software/gsl/) and the tensor.prod.model.matrix function

knots a character string (default knots="quantiles") specifying where knots are to be placed. 'quantiles' specifies knots placed at equally spaced quantiles (equal number of observations lie in each segment) and 'uniform' specifies knots placed at equally spaced intervals. If knots="auto", the knot type will be automatically determined by cross-validation

basis a character string (default basis="auto") indicating whether the additive or tensor product B-spline basis matrix for a multivariate polynomial spline or generalized B-spline polynomial basis should be used. Note this can be automatically determined by cross-validation if cv="nomad" or cv="exhaustive" and basis="auto", and is an 'all or none' proposition (i.e. interaction terms for all predictors or for no predictors given the nature of 'tensor products'). Note also
that if there is only one predictor this defaults to `basis="additive"` to avoid unnecessary computation as the spline bases are equivalent in this case

`deriv` an integer (default `deriv=0`) specifying whether to compute the univariate 1th partial derivative for each continuous predictor (and difference in levels for each categorical predictor) or not and if so what order. Note that if `deriv` is higher than the spline degree of the associated continuous predictor then the derivative will be zero and a warning issued to this effect

`data.return` a logical value indicating whether to return `x`, `z`, `y` or not (default `data.return=FALSE`)

`prune` a logical value (default `prune=FALSE`) specifying whether the (final) model is to be ‘pruned’ using a stepwise cross-validation criterion based upon a modified version of `stepAIC` (see below for details)

`model.return` a logical value indicating whether to return the list of `lm` models or not when `kernel=TRUE` (default `model.return=FALSE`)

`restarts` integer specifying the number of times to restart the process of finding extrema of the cross-validation function (for the bandwidths only) from different (random) initial points

`random.seed` when it is not missing and not equal to 0, the initial points will be generated using this seed when using `frscvNOMAD` or `krscvNOMAD` and `nmulti > 0`

`max.bb.eval` argument passed to the NOMAD solver (see `snomadr` for further details)

`initial.mesh.size.real` argument passed to the NOMAD solver (see `snomadr` for further details)

`initial.mesh.size.integer` argument passed to the NOMAD solver (see `snomadr` for further details)

`min.mesh.size.real` argument passed to the NOMAD solver (see `snomadr` for further details)

`min.mesh.size.integer` arguments passed to the NOMAD solver (see `snomadr` for further details)

`min.poll.size.real` arguments passed to the NOMAD solver (see `snomadr` for further details)

`min.poll.size.integer` arguments passed to the NOMAD solver (see `snomadr` for further details)

`opts` list of optional arguments to be passed to `snomadr`

`nmulti` integer number of times to restart the process of finding extrema of the cross-validation function from different (random) initial points (default `nmulti=5`)

`tau` if non-null a number in (0,1) denoting the quantile for which a quantile regression spline is to be estimated rather than estimating the conditional mean (default `tau=NULL`). Criterion function set by `cv.func= are modified accordingly to admit quantile regression.

`weights` an optional vector of weights to be used in the fitting process. Should be ‘NULL’ or a numeric vector. If non-NULL, weighted least squares is used with weights ‘weights’ (that is, minimizing ‘sum(w*e^2)’); otherwise ordinary least squares is used.

`singular.ok` a logical value (default `singular.ok=FALSE`) that, when `FALSE`, discards singular bases during cross-validation (a check for ill-conditioned bases is performed).

`...` optional arguments
Details

Typical usages are (see below for a list of options and also the examples at the end of this help file):

```r
## Estimate the model and let the basis type be determined by
cross-validation (i.e. cross-validation will determine whether to
use the additive, generalized, or tensor product basis)
model <- crs(y~x1+x2)

## Estimate the model for a specified degree/segment/bandwidth
## combination and do not run cross-validation (will use the
## additive basis by default)
model <- crs(y~x1+factor(x2),cv="none",degree=3,segments=1,lambda=.1)

## Plot the mean and (asymptotic) error bounds
plot(model,mean=TRUE,ci=TRUE)

## Plot the first partial derivative and (asymptotic) error bounds
plot(model,deriv=1,ci=TRUE)
```

**crs** computes a regression spline estimate of a one (1) dimensional dependent variable on an \( r \)-dimensional vector of continuous and categorical (factor/ordered) predictors.


When `basis="additive"` the model becomes additive in nature (i.e. no interaction/tensor terms thus semiparametric not fully nonparametric).

When `basis="tensor"` the model uses the multivariate tensor product basis.

When `kernel=FALSE` the model uses indicator basis functions for the nominal/ordinal (factor/ordered) predictors rather than kernel weighting.

When `kernel=TRUE` the product kernel function for the discrete predictors is of the ‘Li-Racine’ type (see Li and Racine (2007) for details).

When `cv="nomad"`, numerical search is undertaken using Nonsmooth Optimization by Mesh Adaptive Direct Search (Abramson, Audet, Couture, Dennis, Jr., and Le Digabel (2011)).

When `kernel=TRUE` and `cv="exhaustive"`, numerical search is undertaken using `optim` and the box-constrained \( L-BFGS-B \) method (see `optim` for details). The user may restart the algorithm as many times as desired via the `restarts` argument (default `restarts=0`). The approach ascends from `degree=0` (or `segments=0`) through `degree.max` and for each value of `degree` (or `segments`) searches for the optimal bandwidths. After the most complex model has been searched then the optimal `degree/segments/lambda` combination is selected. If any element of the optimal `degree` (or `segments`) vector coincides with `degree.max` (or `segments.max`) a warning is produced and the user ought to restart their search with a larger value of `degree.max` (or `segments.max`).
Note that the default plot method for a crs object provides some diagnostic measures, in particular, a) residuals versus fitted values (useful for checking the assumption that \( \text{E}(u|x)=0 \)), b) a normal quantile-quantile plot which allows residuals to be assessed for normality (\texttt{qqnorm}), c) a scale-location plot that is useful for checking the assumption that the errors are iid and, in particular, that the variance is homogeneous, and d) ‘Cook’s distance’ which computes the single-case influence function. See below for other arguments for the plot function for a crs object.

Note that setting prune=TRUE produces a final ‘pruning’ of the model via a stepwise cross-validation criterion achieved by modifying \texttt{stepAIC} and replacing \texttt{extractAIC} with \texttt{extractCV} throughout the function. This option may be enabled to remove potentially superfluous bases thereby improving the finite-sample efficiency of the resulting model. Note that if the cross-validation score for the pruned model is no better than that for the original model then the original model is returned with a warning to this effect. Note also that this option can only be used when \texttt{kernel}=FALSE.

**Value**

\texttt{crs} returns a \texttt{crs} object. The generic functions \texttt{fitted} and \texttt{residuals} extract (or generate) estimated values and residuals. Furthermore, the functions \texttt{summary}, \texttt{predict}, and \texttt{plot} (options \texttt{mean}=FALSE, \texttt{deriv}=i where \( i \) is an integer, \texttt{ci}=FALSE, \texttt{persp.rgl}=FALSE, \texttt{plot.behavior}=c("plot","plot-data","data","persp-nrgl","plot-nbehavior") \texttt{xtrim}=0.0,\texttt{xq}=0.5) support objects of this type. The returned object has the following components:

- \texttt{fitted.values}: estimates of the regression function (conditional mean) at the sample points or evaluation points.
- \texttt{lwr}, \texttt{upr}: lower/upper bound for a 95% confidence interval for the \texttt{fitted.values} (conditional mean) obtained from \texttt{predict.lm} via the argument \texttt{interval}="confidence".
- \texttt{residuals}: residuals computed at the sample points or evaluation points.
- \texttt{degree}: integer/vector specifying the degree of the B-spline basis for each dimension of the continuous \( x \).
- \texttt{segments}: integer/vector specifying the number of segments of the B-spline basis for each dimension of the continuous \( x \).
- \texttt{include}: integer/vector specifying whether each of the nominal/ordinal (\texttt{factor/ordered}) predictors \( z \) are included or omitted from the resulting estimate if \texttt{kernel}=FALSE (see below).
- \texttt{kernel}: a logical value indicating whether kernel smoothing was used (\texttt{kernel}=TRUE) or not.
- \texttt{lambda}: vector of bandwidths used if \texttt{kernel}=TRUE.
- \texttt{call}: a symbolic description of the model.
- \texttt{r.squared}: coefficient of determination (Doksum and Samarov (1995)).
- \texttt{model.lm}: an object of ‘\texttt{class} ’‘\texttt{lm}’ if \texttt{kernel}=FALSE or a list of objects of ‘\texttt{class} ’‘\texttt{lm}’ if \texttt{kernel}=TRUE (accessed by \texttt{model.lm[[1]]}, \texttt{model.lm[[2]]},..., By way of example, if foo is a \texttt{crs} object and \texttt{kernel}=FALSE, then \texttt{foo$model.lm} is an object of ‘\texttt{class} ’‘\texttt{lm}’, while objects of ‘\texttt{class} ’‘\texttt{lm}’ return the \texttt{model.frame} in \texttt{model.lm$model} which can be accessed via \texttt{foo$model.lm$model} where \texttt{foo} is the \texttt{crs} object (the model frame \texttt{foo$model.lm$model} contains the B-spline bases underlying the estimate which might be of interest). Again by way of example, when \texttt{kernel}=TRUE then \texttt{foo$model.lm[[1]]$model} contains the model frame for the first unique combination of categorical predictors,
foo$model.lm[[2]]$model the second and so forth (the weights will potentially differ for each model depending on the value(s) of lambda)

deriv.mat a matrix of derivatives (or differences in levels for the categorical z) whose order is determined by deriv= in the crs call

deriv.mat.lwr a matrix of 95% coverage lower bounds for deriv.mat

deriv.mat.upr a matrix of 95% coverage upper bounds for deriv.mat

hatvalues the hatvalues for the estimated model

P.hat the kernel probability estimates corresponding to the categorical predictors in the estimated model

Usage Issues

Note that when kernel=FALSE summary supports the option sigtest=TRUE that conducts an F-test for significance for each predictor.

Author(s)

Jeffrey S. Racine <racinej@mcmaster.ca>

References


See Also

smooth.spline, loess, npreg
Examples

```r
set.seed(42)
## Example - simulated data
n <- 1000
num.eval <- 50
x1 <- runif(n)
x2 <- runif(n)
z <- rbinom(n,1,.5)
dgp <- cos(2*pi*x1)+sin(2*pi*x2)+z
z <- factor(z)
y <- dgp + rnorm(n,sd=.5)

## Estimate a model with specified degree, segments, and bandwidth
model <- crs(y~x1+x2+z,degree=c(5,5),
              segments=c(1,1),
              lambda=0.1,
              cv="none",
              kernel=TRUE)

summary(model)

## Perspective plot
x1.seq <- seq(min(x1),max(x1),length=num.eval)
x2.seq <- seq(min(x2),max(x2),length=num.eval)
x.grid <- expand.grid(x1.seq,x2.seq)
newdata <- data.frame(x1=x.grid[,1],x2=x.grid[,2],
                      z=factor(rep(0,num.eval*2),levels=c(0,1)))
z0 <- matrix(predict(model,newdata=newdata),num.eval,num.eval)
newdata <- data.frame(x1=x.grid[,1],x2=x.grid[,2],
                      z=factor(rep(1,num.eval),levels=c(0,1)))
z1 <- matrix(predict(model,newdata=newdata),num.eval,num.eval)
zlim=c(min(z0,z1),max(z0,z1))
persp(x=x1.seq,y=x2.seq,z=z0,
     xlab="x1",ylab="x2",zlab="y",zlim=zlim,
     ticktype="detailed",
     border="red",
     theta=45,phi=45)
par(new=TRUE)
persp(x=x1.seq,y=x2.seq,z=z1,
     xlab="x1",ylab="x2",zlab="y",zlim=zlim,
     theta=45,phi=45,
     ticktype="detailed",
     border="blue")

## Partial regression surface plot
plot(model,mean=TRUE,ci=TRUE)

## Not run:
## A plot example where we extract the partial surfaces, confidence
## intervals etc. automatically generated by plot(mean=TRUE,...) but do
## not plot, rather save for separate use.
pdat <- plot(model,mean=TRUE,ci=TRUE,plot.behavior="data")

## Column 1 is the (evaluation) predictor ([,1]), 2-4 ([,-1]) the mean,
```
## lwr, and upr (note the returned value is a 'list' hence pdat[[1]] is
## data for the first predictor, pdat[[2]] the second etc). Note that
## matplot() can plot this nicely.
matplot(pdat[[1]][,1],pdat[[1]][,-1],
xlab=names(pdat[[1]][1]),ylab=names(pdat[[1]][2]),
1ty=c(1,2,2),col=c(1,2,2),type="l")
```

---

## Nonparametric Instrumental Regression

**Description**

crsiv computes nonparametric estimation of an instrumental regression function \( \varphi \) defined by conditional moment restrictions stemming from a structural econometric model: \( E[Y - \varphi(Z, X)|W] = 0 \), and involving endogenous variables \( Y \) and \( Z \), exogenous variables \( X \), and instruments \( W \). The function \( \varphi \) is the solution of an ill-posed inverse problem.


**Usage**

```r
crsiv(y, z, w, x = NULL, zeval = NULL, weval = NULL, xeval = NULL, alpha = NULL, alpha.min = 1e-10, alpha.max = 1e-01, alpha.tol = .Machine$double.eps^0.25, deriv = 0, iterate.max = 1000, iterate.diff.tol = 1.0e-08, constant = 0.5, penalize.iteration = TRUE, smooth.residuals = TRUE, start.from = c("EyZ","EYwZ"), starting.values = NULL, stop.on.increase = TRUE, method = c("Landweber-Fridman","Tikhonov"), opts = list("MAX_BB_EVAL"=10000,
```
Arguments

y a one (1) dimensional numeric or integer vector of dependent data, each element 
i corresponding to each observation (row) i of z

z a p-variate data frame of endogenous predictors. The data types may be continuous, 
discrete (unordered and ordered factors), or some combination thereof

w a q-variate data frame of instruments. The data types may be continuous, discrete 
(unordered and ordered factors), or some combination thereof

x an r-variate data frame of exogenous predictors. The data types may be continuous, 
discrete (unordered and ordered factors), or some combination thereof

zeval a p-variate data frame of endogenous predictors on which the regression will 
be estimated (evaluation data). By default, evaluation takes place on the data 
provided by z

weval a q-variate data frame of instruments on which the regression will be estimated 
(evaluation data). By default, evaluation takes place on the data provided by w

xeval an r-variate data frame of exogenous predictors on which the regression will 
be estimated (evaluation data). By default, evaluation takes place on the data 
provided by x

alpha a numeric scalar that, if supplied, is used rather than numerically solving for 
alpha, when using method="Tikhonov"

alpha.min minimum of search range for \( \alpha \), the Tikhonov regularization parameter, when 
using method="Tikhonov"

alpha.max maximum of search range for \( \alpha \), the Tikhonov regularization parameter, when 
using method="Tikhonov"

alpha.tol the search tolerance for optimize when solving for \( \alpha \), the Tikhonov regularization 
parameter, when using method="Tikhonov"

iterate.max an integer indicating the maximum number of iterations permitted before termination 
occurs when using method="Landweber-Fridman"

iterate.diff.tol the search tolerance for the difference in the stopping rule from iteration to iteration 
when using method="Landweber-Fridman" (disable by setting to zero)

constant the constant to use when using method="Landweber-Fridman"

method the regularization method employed (default "Landweber-Fridman", see Horowitz 
(2011); see Darolles, Fan, Florens and Renault (2011) for details for "Tikhonov")

penalize.iteration a logical value indicating whether to penalize the norm by the number of iterations or not (default TRUE)
smooth.residuals

a logical value (defaults to TRUE) indicating whether to optimize bandwidths for the regression of \( y - \phi(z) \) on \( w \) or for the regression of \( \phi(z) \) on \( w \) during iteration.

start.from

a character string indicating whether to start from \( E(Y|z) \) (default, "E(yz)") or from \( E(E(Y|z)|z) \) (this can be overridden by providing starting.values below).

starting.values

a value indicating whether to commence Landweber-Fridman assuming \( \varphi_1 = \text{starting.values} \) (proper Landweber-Fridman) or instead begin from \( E(y|z) \) (defaults to NULL, see details below).

stop.on.increase

a logical value (defaults to TRUE) indicating whether to halt iteration if the stopping criterion (see below) increases over the course of one iteration (i.e. it may be above the iteration tolerance but increased).

opts

arguments passed to the NOMAD solver (see \texttt{snomadr} for further details).

derv

an integer 1 (default deriv=0) specifying whether to compute the univariate 1th partial derivative for each continuous predictor (and difference in levels for each categorical predictor) or not and if so what order. Note that if deriv is higher than the spline degree of the associated continuous predictor then the derivative will be zero and a warning issued to this effect (see important note below).

... additional arguments supplied to \texttt{crs}.

\section*{Details}

Tikhonov regularization requires computation of weight matrices of dimension \( n \times n \) which can be computationally costly in terms of memory requirements and may be unsuitable (i.e. unfeasible) for large datasets. Landweber-Fridman will be preferred in such settings as it does not require construction and storage of these weight matrices while it also avoids the need for numerical optimization methods to determine \( \alpha \), though it does require iteration that may be equally or even more computationally demanding in terms of total computation time.

When using method="Landweber-Fridman", an optimal stopping rule based upon \( ||E(y|w) - E(\phi_k(z, x)|w)||^2 \) is used to terminate iteration. However, if local rather than global optima are encountered the resulting estimates can be overly noisy. To best guard against this eventuality set nmulti to a larger number than the default nmulti=5 for \texttt{crs} when using cv="nomad" or instead use cv="exhaustive" if possible (this may not be feasible for non-trivial problems).

When using method="Landweber-Fridman", iteration will terminate when either the change in the value of \( ||(E(y|w) - E(\phi_k(z, x)|w))/E(y|w)||^2 \) from iteration to iteration is less than iterate.diff.tol or we hit iterate.max or \( ||(E(y|w) - E(\phi_k(z, x)|w))/E(y|w)||^2 \) stops falling in value and starts rising.

When your problem is a simple one (e.g. univariate \( Z, W, \) and \( X \)) you might want to avoid cv="nomad" and instead use cv="exhaustive" since exhaustive search may be feasible (for degree.max and segments.max not overly large). This will guarantee an exact solution for each iteration (i.e. there will be no errors arising due to numerical search).

demo(crsiv), demo(crsiv_exog), and demo(crsiv_exog_persp) provide flexible interactive demonstrations similar to the example below that allow you to modify and experiment with parameters such as the sample size, method, and so forth in an interactive session.
crsiv

Value

crsiv returns a crs object. The generic functions fitted and residuals extract (or generate) estimated values and residuals. Furthermore, the functions summary, predict, and plot (options mean=FALSE, deriv=i where i is an integer, ci=FALSE, plot.behavior=c("plot","plot-data","data")) support objects of this type.

See crs for details on the return object components.

In addition to the standard crs components, crsiv returns components phi and either alpha when method="Tikhonov" or phi, phi.mat, num.iterations, norm.stop, norm.value and convergence when method="Landweber-Fridman".

Note

Using the option deriv= computes (effectively) the analytical derivative of the estimated ϕ(Z,X) and not that using crsivderiv, which instead uses the method of Florens and Racine (2012). Though both are statistically consistent, practitioners may desire one over the other hence we provide both.

Note

This function should be considered to be in ‘beta test’ status until further notice.

Author(s)

Jeffrey S. Racine <racinej@mcmaster.ca>, Samuele Centorrino <samuele.centorrino@univ-tlse1.fr>

References


See Also

npreg.crs

Examples

## Not run:
## This illustration was made possible by Samuele Centorrino
## <samuele.centorrino@univ-tlse1.fr>

set.seed(42)
n <- 1500

## The DGP is as follows:

## 1) y = phi(z) + u

## 2) E(u|z) != 0 (endogeneity present)

## 3) Suppose there exists an instrument w such that z = f(w) + v and
## E(u|w) = 0

## 4) We generate v, w, and generate u such that u and z are
## correlated. To achieve this we express u as a function of v (i.e. u =
## gamma v + eps)

v <- rnorm(n,mean=0,sd=0.27)
eps <- rnorm(n,mean=0,sd=0.05)
u <- -0.5*v + eps
w <- rnorm(n,mean=0,sd=1)

## In Darolles et al (2011) there exist two DGPs. The first is
## phi(z)=z^2 and the second is phi(z)=exp(-abs(z)) (which is
## discontinuous and has a kink at zero).

fun1 <- function(z) { z^2 }
fun2 <- function(z) { exp(-abs(z)) }

z <- 0.2*w + v

## Generate two y vectors for each function.
y1 <- fun1(z) + u
y2 <- fun2(z) + u

## You set y to be either y1 or y2 (ditto for phi) depending on which
## DGP you are considering:
y <- y1
phi <- fun1

## Create an evaluation dataset sorting on z (for plotting)
```
crsivderiv <- 

evaldata <- data.frame(y,z,w)
evaldata <- evaldata[order(evaldata$z),]

## Compute the non-IV regression spline estimator of E(y|z)
model.noniv <- crs(y~z,opts=opts)
mean.noniv <- predict(model.noniv,newdata=evaldata)

## Compute the IV-regression spline estimator of phi(z)
model.iv <- crsiv(y=y,z=z,w=w)
phi.iv <- predict(model.iv,newdata=evaldata)

## For the plots, restrict focal attention to the bulk of the data
## (i.e. for the plotting area trim out 1/4 of one percent from each tail of y and z)
trim <- 0.0025

curve(phi,min(z),max(z),
      xlab="z",
      ylab="y",
      main="Nonparametric Instrumental Spline Regression",
      sub=paste("Landweber-Fridman: iterations = ", model.iv$num.iterations, sep=""),
      lwd=1,lty=1)

points(z,y,type="p",cex=.25,col="grey")

lines(evaldata$z,evaldata$z^2-0.325*evaldata$z,lwd=1,lty=1)

lines(evaldata$z,phi.iv,col="blue",lwd=2,lty=2)

lines(evaldata$z,mean.noniv,col="red",lwd=2,lty=4)

legend(quantile(z,trim),quantile(y,1-trim),
       c(expression(paste(varphi(z),"\hat\), E(y|z)")),
       expression(paste("Nonparametric ",hat(varphi)(z))),
       "Nonparametric E(y|z)",
       lty=c(1,2,4),
       col=c("black","blue","red"),
       lwd=c(1,2,2))

## End(Not run)
```
Description

crsivderiv uses the approach of Florens and Racine (2012) to compute the partial derivative of a nonparametric estimation of an instrumental regression function $\varphi$ defined by conditional moment restrictions stemming from a structural econometric model: $E[Y - \varphi(Z, X)|W] = 0$, and involving endogenous variables $Y$ and $Z$ and exogenous variables $X$ and instruments $W$. The derivative function $\varphi'$ is the solution of an ill-posed inverse problem, and is computed using Landweber-Fridman regularization.

Usage

```r
crsivderiv(y, z, w, x = NULL, zeval = NULL, weval = NULL, xeval = NULL, 
iterate.max = 1000, iterate.diff.tol = 1.0e-08, constant = 0.5, 
penalize.iteration = TRUE, 
start.from = c("Eyz","Eeywz"), 
starting.values = NULL, 
stop.on.increase = TRUE, 
smooth.residuals = TRUE, 
opts = list("MAX_BB_EVAL"=10000, 
"EPSILON"=.Machine$double.eps, 
"INITIAL_MESH_SIZE"="r1.0e-01", 
"MIN_MESH_SIZE"=paste("r",sqrt(.Machine$double.eps),sep=""), 
"MIN_POLL_SIZE"=paste("r",sqrt(.Machine$double.eps),sep=""), 
"DISPLAY_DEGREE"=0), 
...)
```

Arguments

- **y**: a one (1) dimensional numeric or integer vector of dependent data, each element $i$ corresponding to each observation (row) $i$ of $z$
- **z**: a $p$-variate data frame of endogenous predictors. The data types may be continuous, discrete (unordered and ordered factors), or some combination thereof
- **w**: a $q$-variate data frame of instruments. The data types may be continuous, discrete (unordered and ordered factors), or some combination thereof
- **x**: an $r$-variate data frame of exogenous predictors. The data types may be continuous, discrete (unordered and ordered factors), or some combination thereof
- **zeval**: a $p$-variate data frame of endogenous predictors on which the regression will be estimated (evaluation data). By default, evaluation takes place on the data provided by $z$
a $q$-variate data frame of instruments on which the regression will be estimated (evaluation data). By default, evaluation takes place on the data provided by $w$.

an $r$-variate data frame of exogenous predictors on which the regression will be estimated (evaluation data). By default, evaluation takes place on the data provided by $x$.

an integer indicating the maximum number of iterations permitted before termination occurs when using Landweber-Fridman iteration.

the search tolerance for the difference in the stopping rule from iteration to iteration when using Landweber-Fridman (disable by setting to zero).

the constant to use when using Landweber-Fridman iteration.

a logical value indicating whether to penalize the norm by the number of iterations or not (default TRUE).

a character string indicating whether to start from $E(Y|z)$ (default, "EyZ") or from $E(E(Y|z)|z)$ (this can be overridden by providing starting.values below).

a value indicating whether to commence Landweber-Fridman assuming $\varphi_{k-1} = starting.values$ (proper Landweber-Fridman) or instead begin from $E(y|z)$ (defaults to NULL, see details below).

a logical value (defaults to TRUE) indicating whether to halt iteration if the stopping criterion (see below) increases over the course of one iteration (i.e. it may be above the iteration tolerance but increased).

a logical value (defaults to TRUE) indicating whether to optimize bandwidths for the regression of $y - \varphi(z)$ on $w$ or for the regression of $\varphi(z)$ on $w$ during iteration.

arguments passed to the NOMAD solver (see snomadr for further details).

additional arguments supplied to crs.

For Landweber-Fridman iteration, an optimal stopping rule based upon $\left|\frac{E(y|w) - E(\varphi_k(z,x)\mid w)}{E(y|w)}\right|^2$ is used to terminate iteration. However, if local rather than global optima are encountered the resulting estimates can be overly noisy. To best guard against this eventuality set `nmulti` to a larger number than the default `nmulti=5` for crs when using cv="nomad" or instead use cv="exhaustive" if possible (this may not be feasible for non-trivial problems).

When using Landweber-Fridman iteration, iteration will terminate when either the change in the value of $\left|\frac{E(y|w) - E(\varphi_k(z,x)\mid w)}{E(y|w)}\right|^2$ from iteration to iteration is less than `iterate.diff.tol` or we hit `iterate.max` or $\left|\frac{E(y|w) - E(\varphi_k(z,x)\mid w)}{E(y|w)}\right|^2$ stops falling in value and starts rising.

When your problem is a simple one (e.g. univariate $Z$, $W$, and $X$) you might want to avoid cv="nomad" and instead use cv="exhaustive" since exhaustive search may be feasible (for `degree.max` and `segments.max` not overly large). This will guarantee an exact solution for each iteration (i.e. there will be no errors arising due to numerical search).
Value

crsivderiv returns components phi.prime, phi, phi.prime.mat, num.iterations, norm.stop, norm.value and convergence.

Note

This function currently supports univariate z only. This function should be considered to be in ‘beta test’ status until further notice.

Author(s)

Jeffrey S. Racine <racinej@mcmaster.ca>

References


See Also

npreg, crsiv, crs

Examples

## Not run:
## This illustration was made possible by Samuele Centorrino
## <samuele.centorrino@univ-tlse1.fr>

set.seed(42)
n <- 1000

## For trimming the plot (trim .5% from each tail)
trim <- 0.005

## The DGP is as follows:

## 1) y = phi(z) + u

## 2) E(u|z) != 0 (endogeneity present)

## 3) Suppose there exists an instrument w such that z = f(w) + v and
## E(u|w) = 0

## 4) We generate v, w, and generate u such that u and z are
## correlated. To achieve this we express u as a function of v (i.e. u =
## gamma v + eps)

v <- rnorm(n,mean=0,sd=0.27)
eps <- rnorm(n,mean=0,sd=0.05)
u <- -0.5*v + eps
w <- rnorm(n,mean=0,sd=1)

## In Darolles et al (2011) there exist two DGPs. The first is
## phi(z)=z^2 and the second is phi(z)=exp(-abs(z)) (which is
## discontinuous and has a kink at zero).

fun1 <- function(z) { z^2 }
fun2 <- function(z) { exp(-abs(z)) }

z <- 0.2*w + v

## Generate two y vectors for each function.

y1 <- fun1(z) + u
y2 <- fun2(z) + u

## You set y to be either y1 or y2 (ditto for phi) depending on which
## DGP you are considering:

y <- y1
phi <- fun1

## Sort on z (for plotting)

ivdata <- data.frame(y,z,w,u,v)
ivdata <- ivdata[order(ivdata$z),]
rm(y,z,w,u,v)
attach(ivdata)

model.ivderiv <- crsivderiv(y=y,z=z,w=w)
ylim <- c(quantile(model.ivderiv$phi.prime,trim),
         quantile(model.ivderiv$phi.prime,1-trim))
crssigtest

Regression Spline Significance Test with Mixed Data Types

Description

crssigtest implements a consistent test of significance of an explanatory variable in a nonparametric regression setting that is analogous to a simple t-test in a parametric regression setting. The test is based on Ma and Racine (2011).

Usage

```r
crssigtest(model = NULL, 
    index = NULL, 
    boot.num = 399, 
    boot.type = c("residual","reorder"), 
    random.seed = 42, 
    boot = TRUE)
```

Arguments

- **model**: a crs model object.
- **index**: a vector of indices for the columns of `model$xz` for which the test of significance is to be conducted. Defaults to \((1,2,\ldots,p)\) where \(p\) is the number of columns in `model$xz`.
- **boot.num**: an integer value specifying the number of bootstrap replications to use. Defaults to 399.
- **boot.type**: whether to conduct ‘residual’ bootstrapping (iid) or permute (reorder) in place the predictor being tested when imposing the null.
- **random.seed**: an integer used to seed R’s random number generator. This is to ensure replicability. Defaults to 42.
- **boot**: a logical value (default TRUE) indicating whether to compute the bootstrap P-value or simply return the asymptotic P-value.
Value

`crssigtest` returns an object of type `sigtest`. `summary` supports `sigtest` objects. It has the following components:

- **index**: the vector of indices input
- **P**: the vector of bootstrap P-values for each statistic in \( \mathbf{F} \)
- **P.asy**: the vector of asymptotic P-values for each statistic in `index`
- **F**: the vector of pseudo F-statistics \( \mathbf{F} \)
- **F.boot**: the matrix of bootstrapped pseudo F-statistics generated under the null (one column for each statistic in \( \mathbf{F} \))
- **df1**: the vector of numerator degrees of freedom for each statistic in \( \mathbf{F} \) (based on the smoother matrix)
- **df2**: the vector of denominator degrees of freedom for each statistic in \( \mathbf{F} \) (based on the smoother matrix)
- **rss**: the vector of restricted sums of squared residuals for each statistic in \( \mathbf{F} \)
- **uss**: the vector of unrestricted sums of squared residuals for each statistic in \( \mathbf{F} \)
- **boot.num**: the number of bootstrap replications
- **boot.type**: the `boot.type`
- **xnames**: the names of the variables in `model$z`

Usage Issues

This function should be considered to be in 'beta status' until further notice.

Caution: bootstrap methods are, by their nature, *computationally intensive*. This can be frustrating for users possessing large datasets. For exploratory purposes, you may wish to override the default number of bootstrap replications, say, setting them to `boot.num=99`.

Author(s)

Jeffrey S. Racine <racinej@mcmaster.ca>

References


Examples

```r
## Not run:
options(crs.messages=FALSE)
set.seed(42)

n <- 1000
```
Engel95

1995 British Family Expenditure Survey

Description

British cross-section data consisting of a random sample taken from the British Family Expenditure Survey for 1995. The households consist of married couples with an employed head-of-household between the ages of 25 and 55 years. There are 1655 household-level observations in total.

Usage

data("Engel95")

Format

A data frame with 10 columns, and 1655 rows.

- **food**: expenditure share on food, of type numeric
- **catering**: expenditure share on catering, of type numeric
- **alcohol**: expenditure share on alcohol, of type numeric
- **fuel**: expenditure share on fuel, of type numeric
- **motor**: expenditure share on motor, of type numeric
- **fares**: expenditure share on fares, of type numeric
- **leisure**: expenditure share on leisure, of type numeric
- **logexp**: logarithm of total expenditure, of type numeric
- **logwages**: logarithm of total earnings, of type numeric
- **nkids**: number of children, of type numeric

Source

Richard Blundell and Dennis Kristensen
References


Examples

```r
# Not run:
# Example - we compute nonparametric instrumental regression of an
# Engel curve for food expenditure shares using Landweber-Fridman
# iteration of Fredholm integral equations of the first kind.

# We consider an equation with an endogenous predictor ('z') and an
# instrument ('w'). Let y = phi(z) + u where phi(z) is the function of
# interest. Here E(u|z) is not zero hence the conditional mean E(y|z)
# does not coincide with the function of interest, but if there exists
# an instrument w such that E(u|w) = 0, then we can recover the
# function of interest by solving an ill-posed inverse problem.

data(Engel95)

# Sort on logexp (the endogenous predictor) for plotting purposes
# (i.e. so we can plot a curve for the fitted values versus logexp)
Engel95 <- Engel95[order(Engel95$food),]

attach(Engel95)

model.iv <- crsiv(y=food,z=logexp,w=logwages,method="Landweber-Fridman")
phihat <- model.iv$phi

# Compute the non-IV regression (i.e. regress y on z)
ghat <- crs(food~logexp)

# For the plots, we restrict focal attention to the bulk of the data
# (i.e. for the plotting area trim out 1/4 of one percent from each
# tail of y and z). This is often helpful as estimates in the tails of
# the support are less reliable (i.e. more variable) so we are
# interested in examining the relationship 'where the action is'.

trim <- 0.0025

plot(logexp,food,
    ylab="Food Budget Share",
    xlab="log(Total Expenditure)",
    xlim=quantile(logexp,c(trim,1-trim)),
    ylim=quantile(food,c(trim,1-trim)),
    main="Nonparametric Instrumental Regression Splines",
    type="p",
```
Description

frscv computes exhaustive cross-validation directed search for a regression spline estimate of a one (1) dimensional dependent variable on an r-dimensional vector of continuous predictors and nominal/ordinal (factor/ordered) predictors.

Usage

frscv(xz, y,
  degree.max = 10,
  segments.max = 10,
  degree.min = 0,
  segments.min = 1,
  complexity = c("degree-knots","degree","knots"),
  knots = c("quantiles","uniform","auto"),
  basis = c("additive","tensor","glp","auto"),
  cv.func = c("cv.ls","cv.gcv","cv.aic"),
  degree = degree,
  segments = segments,
  tau = NULL,
  weights = NULL,
  singular.ok = FALSE)

Arguments

y  continuous univariate vector

xz  continuous and/or nominal/ordinal (factor/ordered) predictors
### Model Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Default Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>degree.max</code></td>
<td>(default: 10)</td>
<td>the maximum degree of the B-spline basis for each of the continuous predictors</td>
</tr>
<tr>
<td><code>segments.max</code></td>
<td>(default: 10)</td>
<td>the maximum segments of the B-spline basis for each of the continuous predictors</td>
</tr>
<tr>
<td><code>degree.min</code></td>
<td>(default: 0)</td>
<td>the minimum degree of the B-spline basis for each of the continuous predictors</td>
</tr>
<tr>
<td><code>segments.min</code></td>
<td>(default: 1)</td>
<td>the minimum segments of the B-spline basis for each of the continuous predictors</td>
</tr>
<tr>
<td><code>complexity</code></td>
<td>(default: &quot;degree=knots&quot;)</td>
<td>a character string indicating whether model 'complexity' is determined by the degree of the spline or by the number of segments (&quot;knots&quot;). This option allows the user to use cross-validation to select either the spline degree (number of knots held fixed) or the number of knots (spline degree held fixed) or both the spline degree and number of knots</td>
</tr>
<tr>
<td><code>knots</code></td>
<td>(default: &quot;quantiles&quot;)</td>
<td>a character string specifying where knots are to be placed. 'quantiles' specifies knots placed at equally spaced quantiles (equal number of observations lie in each segment) and 'uniform' specifies knots placed at equally spaced intervals. If knots=&quot;auto&quot;, the knot type will be automatically determined by cross-validation</td>
</tr>
<tr>
<td><code>basis</code></td>
<td>(default: &quot;additive&quot;)</td>
<td>a character string indicating whether the additive or tensor product B-spline basis matrix for a multivariate polynomial spline or generalized B-spline polynomial basis should be used. Note this can be automatically determined by cross-validation if cv=TRUE and basis=&quot;auto&quot;, and is an 'all or none' proposition (i.e. interaction terms for all predictors or for no predictors given the nature of 'tensor products'). Note also that if there is only one predictor this defaults to basis=&quot;additive&quot; to avoid unnecessary computation as the spline bases are equivalent in this case</td>
</tr>
<tr>
<td><code>cv.func</code></td>
<td>(default: &quot;cv.ls&quot;)</td>
<td>a character string indicating which method to use to select smoothing parameters. <code>cv.gcv</code> specifies generalized cross-validation (Craven and Wahba (1979)), <code>cv.aic</code> specifies expected Kullback-Leibler cross-validation (Hurvich, Simonoff, and Tsai (1998)), and <code>cv.ls</code> specifies least-squares cross-validation</td>
</tr>
<tr>
<td><code>degree</code></td>
<td>integer/vector</td>
<td>integer/vector specifying the degree of the B-spline basis for each dimension of the continuous x</td>
</tr>
<tr>
<td><code>segments</code></td>
<td>integer/vector</td>
<td>integer/vector specifying the number of segments of the B-spline basis for each dimension of the continuous x (i.e. number of knots minus one)</td>
</tr>
<tr>
<td><code>tau</code></td>
<td>(default: NULL)</td>
<td>if non-null a number in (0,1) denoting the quantile for which a quantile regression spline is to be estimated rather than estimating the conditional mean (default tau=NULL)</td>
</tr>
<tr>
<td><code>weights</code></td>
<td>(default: NULL)</td>
<td>an optional vector of weights to be used in the fitting process. Should be 'NULL' or a numeric vector. If non-NULL, weighted least squares is used with weights 'weights' (that is, minimizing 'sum(w*e^2)'); otherwise ordinary least squares is used.</td>
</tr>
<tr>
<td><code>singular.ok</code></td>
<td>(default: FALSE)</td>
<td>a logical value (default singular.ok=FALSE) that, when FALSE, discards singular bases during cross-validation (a check for ill-conditioned bases is performed).</td>
</tr>
</tbody>
</table>
Details

frscv computes exhaustive cross-validation for a regression spline estimate of a one (1) dimensional dependent variable on an \( r \)-dimensional vector of continuous and nominal/ordinal (factor/ordered) predictors. The optimal \( K/I \) combination (i.e., degree/segments/I) is returned along with other results (see below for return values).

For the continuous predictors the regression spline model employs either the additive or tensor product B-spline basis matrix for a multivariate polynomial spline via the B-spline routines in the GNU Scientific Library (http://www.gnu.org/software/gsl/) and the tensor.prod.model.matrix function.

For the nominal/ordinal (factor/ordered) predictors the regression spline model uses indicator basis functions.

Value

frscv returns a crscv object. Furthermore, the function summary supports objects of this type. The returned objects have the following components:

- **K**: scalar/vector containing optimal degree(s) of spline or number of segments
- **I**: scalar/vector containing an indicator of whether the predictor is included or not for each dimension of the nominal/ordinal (factor/ordered) predictors
- **K.mat**: vector/matrix of values of \( K \) evaluated during search
- **cv.func**: objective function value at optimum
- **cv.func.vec**: vector of objective function values at each degree of spline or number of segments in K.mat

Author(s)

Jeffrey S. Racine <racinej@mcmaster.ca>

References


See Also

loess, npregbw,
frscvNOMAD

Examples

```r
set.seed(42)
# Simulated data
n <- 1000

x <- runif(n)
z <- round(runif(n, min=0.5, max=1.5))
z.unique <- uniquecombs(as.matrix(z))
ind <- attr(z.unique, "index")
ind.vals <- sort(unique(ind))
dgp <- numeric(length=n)
for(i in 1:nrow(z.unique)) {
  zz <- ind == ind.vals[i]
  dgp[zz] <- z[zz] * cos(2*pi*x[zz])
}

y <- dgp + rnorm(n, sd=.1)

xdata <- data.frame(x, z=factor(z))
# Compute the optimal K and I, determine optimal number of knots, set
# spline degree for x to 3

cv <- frscv(x=xdata, y=y, complexity="knots", degree=c(3))
summary(cv)
```

---

frscvNOMAD  

**Categorical Factor Regression Spline Cross-Validation**

Description

frscvNOMAD computes NOMAD-based (Nonsmooth Optimization by Mesh Adaptive Direct Search, Abramson, Audet, Couture and Le Digabel (2011)) cross-validation directed search for a regression spline estimate of a one (1) dimensional dependent variable on an r-dimensional vector of continuous predictors and nominal/ordinal (factor/ordered) predictors.

Usage

```r
frscvNOMAD(xz,
  y,
  degree.max = 10,
  segments.max = 10,
  degree.min = 0,
  segments.min = 1,
  cv.df.min = 1,
  complexity = c("degree-knots","degree","knots"),
  knots = c("quantiles","uniform","auto"),
  basis = c("additive","tensor","glp","auto"),
```
cv.func = c("cv.ls","cv.gcv","cv.aic"),
degree = degree,
segments = segments,
include = include,
random.seed = 42,
max.bb.eval = 10000,
initial.mesh.size.integer = "1",
min.mesh.size.integer = paste("r",sqrt(.Machine$double.eps),sep=""),
min.poll.size.integer = paste("r",sqrt(.Machine$double.eps),sep=""),
opts=list(),
nmulti = 0,
tau = NULL,
weights = NULL,
singular.ok = FALSE)

Arguments

y    continuous univariate vector
xz   continuous and/or nominal/ordinal (factor/ordered) predictors
degree.max  the maximum degree of the B-spline basis for each of the continuous predictors
            (default degree.max=10)
segments.max  the maximum segments of the B-spline basis for each of the continuous predictors
               (default segments.max=10)
degree.min  the minimum degree of the B-spline basis for each of the continuous predictors
            (default degree.min=0)
segments.min  the minimum segments of the B-spline basis for each of the continuous predictors
              (default segments.min=1)
cv.df.min  the minimum degrees of freedom to allow when conducting cross-validation
            (default cv.df.min=1)
complexity  a character string (default complexity="degree-knots") indicating whether
            model 'complexity' is determined by the degree of the spline or by the number
            of segments ('knots'). This option allows the user to use cross-validation to
            select either the spline degree (number of knots held fixed) or the number of
            knots (spline degree held fixed) or both the spline degree and number of knots
knots  a character string (default knots="quantiles") specifying where knots are
            to be placed. 'quantiles' specifies knots placed at equally spaced quantiles
            (equal number of observations lie in each segment) and 'uniform' specifies knots
            placed at equally spaced intervals. If knots="auto", the knot type will be
            automatically determined by cross-validation
basis  a character string (default basis="additive") indicating whether the additive
            or tensor product B-spline basis matrix for a multivariate polynomial spline or
            generalized B-spline polynomial basis should be used. Note this can be
            automatically determined by cross-validation if cv=TRUE and basis="auto", and is
            an 'all or none' proposition (i.e. interaction terms for all predictors or for no
            predictors given the nature of 'tensor products'). Note also that if there is only one
            predictor this defaults to basis="additive" to avoid unnecessary computation
            as the spline bases are equivalent in this case
cv.func  a character string (default cv.func="cv.ls") indicating which method to use to select smoothing parameters. cv.gcv specifies generalized cross-validation (Craven and Wahba (1979)), cv.aic specifies expected Kullback-Leibler cross-validation (Hurvich, Simonoff, and Tsai (1998)), and cv.ls specifies least-squares cross-validation

degree  integer/vector specifying the degree of the B-spline basis for each dimension of the continuous x

segments  integer/vector specifying the number of segments of the B-spline basis for each dimension of the continuous x (i.e. number of knots minus one)

include  integer/vector for the categorical predictors. If it is not NULL, it will be the initial value for the fitting

random.seed  when it is not missing and not equal to 0, the initial points will be generated using this seed when nmulti > 0

max.bb.eval  argument passed to the NOMAD solver (see snomadr for further details)

initial.mesh.size.integer  argument passed to the NOMAD solver (see snomadr for further details)

min.mesh.size.integer  arguments passed to the NOMAD solver (see snomadr for further details)

min.poll.size.integer  arguments passed to the NOMAD solver (see snomadr for further details)

opts  list of optional arguments to be passed to snomadr

nmulti  integer number of times to restart the process of finding extrema of the cross-validation function from different (random) initial points (default nmulti=0)

tau  if non-null a number in (0,1) denoting the quantile for which a quantile regression spline is to be estimated rather than estimating the conditional mean (default tau=NULL)

weights  an optional vector of weights to be used in the fitting process. Should be 'NULL' or a numeric vector. If non-NULL, weighted least squares is used with weights 'weights' (that is, minimizing 'sum(w*e^2)'); otherwise ordinary least squares is used.

singular.ok  a logical value (default singular.ok=FALSE) that, when FALSE, discards singular bases during cross-validation (a check for ill-conditioned bases is performed).

Details

frscvNOMAD computes NOMAD-based cross-validation for a regression spline estimate of a one-dimensional dependent variable on an r-dimensional vector of continuous and nominal/ordinal (factor/ordered) predictors. Numerical search for the optimal degree/segments/I is undertaken using snomadr.

The optimal K/I combination is returned along with other results (see below for return values).

For the continuous predictors the regression spline model employs either the additive or tensor product B-spline basis matrix for a multivariate polynomial spline via the B-spline routines in the GNU Scientific Library (http://www.gnu.org/software/gsl/) and the tensor.prod.model.matrix function.
For the nominal/ordinal (factor/ordered) predictors the regression spline model uses indicator basis functions.

Value

`frscvNOMAD` returns a `crscv` object. Furthermore, the function `summary` supports objects of this type. The returned objects have the following components:

- **K**: scalar/vector containing optimal degree(s) of spline or number of segments
- **I**: scalar/vector containing an indicator of whether the predictor is included or not for each dimension of the nominal/ordinal (factor/ordered) predictors
- **K.mat**: vector(matrix of values of K evaluated during search
- **degree.max**: the maximum degree of the B-spline basis for each of the continuous predictors (default `degree.max=10`)
- **segments.max**: the maximum segments of the B-spline basis for each of the continuous predictors (default `segments.max=10`)
- **degree.min**: the minimum degree of the B-spline basis for each of the continuous predictors (default `degree.min=0`)
- **segments.min**: the minimum segments of the B-spline basis for each of the continuous predictors (default `segments.min=1`)
- **cv.func**: objective function value at optimum
- **cv.func.vec**: vector of objective function values at each degree of spline or number of segments in `K.mat`

Author(s)

Jeffrey S. Racine <racinej@mcmaster.ca> and Zhenghua Nie <niez@mcmaster.ca>

References


g lp. model. matrix

See Also

loess, npregbw.

Examples

set.seed(42)
## Simulated data
n <- 1000

x <- runif(n)
z <- round(runif(n, min=-0.5, max=1.5))
z.unique <- uniquecombs(as.matrix(z))
ind <- attr(z.unique, "index")
ind.vals <- sort(unique(ind))
dgp <- numeric(length=n)
for(i in 1:nrow(z.unique)) {
  zz <- ind == ind.vals[i]
  dgp[zz] <- z[zz] + cos(2*pi*x[zz])
}

y <- dgp + rnorm(n, sd=.1)

xdata <- data.frame(x, z = factor(z))

## Compute the optimal K and I, determine optimal number of knots, set
## spline degree for x to 3

cv <- frscvNOMAD(x=xdata, y=y, complexity="knots", degree=c(3), segments=c(5))
summary(cv)

---

**glp.model.matrix**

*Utility function for constructing generalized polynomial smooths*

**Description**

Produce model matrices for a generalized polynomial smooth from the model matrices for the marginal bases of the smooth.

**Usage**

```r
glp.model.matrix(X)
```

**Arguments**

- `X` a list of model matrices for the marginal bases of a smooth

**Details**

This function computes a generalized polynomial where the orders of each term entering the polynomial may vary.
Value

A model matrix for a generalized polynomial smooth.

Author(s)

Jeffrey S. Racine <racinej@mcmaster.ca>

References


Examples

```r
X <- list(matrix(1:4,2,2),matrix(5:10,2,3))
glp.model.matrix(X)
```

Description

gsl.bs generates the B-spline basis matrix for a polynomial spline and (optionally) the B-spline basis matrix derivative of a specified order with respect to each predictor

Usage

```r
gsl.bs(...)  
## Default S3 method:  
gsl.bs(x,  
  degree = 3,  
  nbreak = 2,  
  deriv = 0,  
  x.min = NULL,  
  x.max = NULL,  
  intercept = FALSE,  
  knots = NULL,  
  ...)```

Arguments

- `x`: the predictor variable. Missing values are not allowed
- `degree`: degree of the piecewise polynomial - default is '3' (cubic spline)
- `nbreak`: number of breaks in each interval - default is '2'
- `deriv`: the order of the derivative to be computed-default if 0
- `x.min`: the lower bound on which to construct the spline - defaults to min(x)
x.max the upper bound on which to construct the spline - defaults to \( \max(x) \)
intercept if ‘TRUE’, an intercept is included in the basis; default is ‘FALSE’
knots a vector (default knots="NULL") specifying knots for the spline basis (default enables uniform knots, otherwise those provided are used)
... optional arguments

Details

Typical usages are (see below for a list of options and also the examples at the end of this help file)

\[
B \leftarrow \text{gsl}().bs(x, \text{degree}=10)
\]

Value

gsl().bs returns a gsl().bs object. A matrix of dimension \(c(\text{length}(x), \text{degree}+\text{nbreak}-1)\).
A primary use is in modelling formulas to directly specify a piecewise polynomial term in a model.
See \url{http://www.gnu.org/software/gsl/} for further details.

Author(s)

Jeffrey S. Racine <raceijn@mcmaster.ca>

References


See Also

bs

Examples

\#
\#
\#
\#
\#

\#
## Plot the spline bases and their first order derivatives
x \leftarrow \text{seq}(0,1,\text{length}=100)
\text{matplot}(x,\text{gsl}().bs(x, \text{degree}=5), \text{type}="1")
\text{matplot}(x,\text{gsl}().bs(x, \text{degree}=5, \text{deriv}=1), \text{type}="1")

\#
## Regression example
n \leftarrow 1000
x \leftarrow \text{sort(runif(n))}
y \leftarrow \text{cos}(2*\pi*x) + \text{rnorm(n, sd=.25)}
B \leftarrow \text{gsl}().bs(x, \text{degree}=5, \text{intercept}=\text{FALSE})
\text{plot}(x,y, \text{cex}=.5, \text{col}="grey")
\text{lines}(x,\text{fitted(1m(y-B))})
krscv is a function for Categorical Kernel Regression Spline Cross-Validation.

### Description

krscv computes exhaustive cross-validation directed search for a regression spline estimate of a one-dimensional dependent variable on an r-dimensional vector of continuous and nominal/ordinal (factor/ordered) predictors.

### Usage

```r
krscv(xz, y,
     degree.max = 10,
     segments.max = 10,
     degree.min = 0,
     segments.min = 1,
     restarts = 0,
     complexity = c("degree-knots","degree","knots"),
     knots = c("quantiles","uniform","auto"),
     basis = c("additive","tensor","glp","auto"),
     cv.func = c("cv.ls","cv.gcv","cv.aic"),
     degree = degree,
     segments = segments,
     tau = NULL,
     weights = NULL,
     singular.ok = FALSE)
```

### Arguments

- `y`: continuous univariate vector
- `xz`: continuous and/or nominal/ordinal (factor/ordered) predictors
- `degree.max`: the maximum degree of the B-spline basis for each of the continuous predictors (default `degree.max=10`)
- `segments.max`: the maximum segments of the B-spline basis for each of the continuous predictors (default `segments.max=10`)
- `degree.min`: the minimum degree of the B-spline basis for each of the continuous predictors (default `degree.min=0`)
- `segments.min`: the minimum segments of the B-spline basis for each of the continuous predictors (default `segments.min=1`)
- `restarts`: number of times to restart `optim` from different initial random values (default `restarts=0`) when searching for optimal bandwidths for the categorical predictors for each unique K combination (i.e.\ `degree.segments`)
complexity: a character string (default complexity="degree-knots") indicating whether model 'complexity' is determined by the degree of the spline or by the number of segments ('knots'). This option allows the user to use cross-validation to select either the spline degree (number of knots held fixed) or the number of knots (spline degree held fixed) or both the spline degree and number of knots.

knots: a character string (default knots="quantiles") specifying where knots are to be placed. ‘quantiles’ specifies knots placed at equally spaced quantiles (equal number of observations lie in each segment) and ‘uniform’ specifies knots placed at equally spaced intervals. If knots="auto", the knot type will be automatically determined by cross-validation.

basis: a character string (default basis="additive") indicating whether the additive or tensor product B-spline basis matrix for a multivariate polynomial spline or generalized B-spline polynomial basis should be used. Note this can be automatically determined by cross-validation if cv=TRUE and basis="auto", and is an ‘all or none’ proposition (i.e. interaction terms for all predictors or for no predictors given the nature of ‘tensor products’). Note also that if there is only one predictor this defaults to basis="additive" to avoid unnecessary computation as the spline bases are equivalent in this case.

cv.func: a character string (default cv.func="cv.ls") indicating which method to use to select smoothing parameters. cv.gcv specifies generalized cross-validation (Craven and Wahba (1979)), cv.aic specifies expected Kullback-Leibler cross-validation (Hurvich, Simonoff, and Tsai (1998)), and cv.ls specifies least-squares cross-validation.

degree: integer/vector specifying the degree of the B-spline basis for each dimension of the continuous x.

segments: integer/vector specifying the number of segments of the B-spline basis for each dimension of the continuous x (i.e. number of knots minus one).

tau: if non-null a number in (0,1) denoting the quantile for which a quantile regression spline is to be estimated rather than estimating the conditional mean (default tau=NULL).

weights: an optional vector of weights to be used in the fitting process. Should be ‘NULL’ or a numeric vector. If non-NULL, weighted least squares is used with weights ‘weights’ (that is, minimizing ‘sum(w*e^2)’); otherwise ordinary least squares is used.

singular.ok: a logical value (default singular.ok=FALSE) that, when FALSE, discards singular bases during cross-validation (a check for ill-conditioned bases is performed).

Details

krscv computes exhaustive cross-validation for a regression spline estimate of a one (1) dimensional dependent variable on an r-dimensional vector of continuous and nominal/ordinal (factor/ordered) predictors. The optimal K/lambda combination is returned along with other results (see below for return values). The method uses kernel functions appropriate for categorical (ordinal/nominal) predictors which avoids the loss in efficiency associated with sample-splitting procedures that are typically used when faced with a mix of continuous and nominal/ordinal (factor/ordered) predictors.
For the continuous predictors the regression spline model employs either the additive or tensor product B-spline basis matrix for a multivariate polynomial spline via the B-spline routines in the GNU Scientific Library (http://www.gnu.org/software/gsl/) and the tensor.prod.model.matrix function.

For the discrete predictors the product kernel function is of the ‘Li-Racine’ type (see Li and Racine (2007) for details).

For each unique combination of degree and segment, numerical search for the bandwidth vector lambda is undertaken using optim and the box-constrained L-BFGS-B method (see optim for details). The user may restart the optim algorithm as many times as desired via the restarts argument. The approach ascends from $K=0$ through $\text{degree}.\max / \text{segments}.\max$ and for each value of $K$ searches for the optimal bandwidths for this value of $K$. After the most complex model has been searched then the optimal $K/\lambda$ combination is selected. If any element of the optimal $\lambda$ vector coincides with $\text{degree}.\max / \text{segments}.\max$ a warning is produced and the user ought to restart their search with a larger value of $\text{degree}.\max / \text{segments}.\max$.

Value

$\text{krscv}$ returns a $\text{crscv}$ object. Furthermore, the function $\text{summary}$ supports objects of this type. The returned objects have the following components:

- $K$ scalar/vector containing optimal degree(s) of spline or number of segments
- $K.\text{mat}$ vector/matrix of values of $K$ evaluated during search
- $\text{restarts}$ number of restarts during search, if any
- $\lambda$ optimal bandwidths for categorical predictors
- $\lambda.\text{mat}$ vector/matrix of optimal bandwidths for each degree of spline
- $\text{cv}.\text{func}$ objective function value at optimum
- $\text{cv}.\text{func}.\text{vec}$ vector of objective function values at each degree of spline or number of segments in $K.\text{mat}$

Author(s)

Jeffrey S. Racine <racenej@mcmaster.ca>

References


krscvNOMAD

See Also

loess, npregbw.

Examples

```r
set.seed(42)
## Simulated data
n <- 1000

x <- runif(n)
z <- round(runif(n,min=-0.5,max=1.5))
z.unique <- uniquecombs(as.matrix(z))
ind <- attr(z.unique,"index")
ind.vals <- sort(unique(ind))
dgp <- numeric(length=n)
for(i in 1:nrow(z.unique)) {
  zz <- ind == ind.vals[i]
  dgp[zz] <- z[zz]*cos(2*pi*x[zz])
}
y <- dgp + rnorm(n,sd=.1)

xdata <- data.frame(x,z=factor(z))

## Compute the optimal K and lambda, determine optimal number of knots, set
## spline degree for x to 3

cv <- krscv(x=xdata,y=y,complexity="knots",degree=c(3))
summary(cv)
```

krscvNOMAD  

**Categorical Kernel Regression Spline Cross-Validation**

Description

krscvNOMAD computes NOMAD-based (Nonsmooth Optimization by Mesh Adaptive Direct Search, Abramson, Audet, Couture and Le Digabel (2011)) cross-validation directed search for a regression spline estimate of a one-dimensional dependent variable on an r-dimensional vector of continuous and nominal/ordinal (factor/ordered) predictors.

Usage

```r
krscvNOMAD(xz, y, 
  degree.max = 10, 
  segments.max = 10, 
  degree.min = 0, 
  segments.min = 1, 
  cv.df.min = 1, 
  complexity = c("degree-knots","degree","knots"),
```
knots = c("quantiles", "uniform", "auto"),
basis = c("additive", "tensor", "glp", "auto"),
cv.func = c("cv.ls", "cv.gcv", "cv.aic"),
degree = degree,
segments = segments,
lambda = lambda,
lambda.discrete = FALSE,
lambda.discrete.num = 100,
random.seed = 42,
max.bb.eval = 10000,
initial.mesh.size.real = "r0.1",
initial.mesh.size.integer = "1",
min.mesh.size.real = paste("r", sqrt(.Machine$double.eps), sep=""),
min.mesh.size.integer = paste("r", sqrt(.Machine$double.eps), sep=""),
min.poll.size.real = paste("r", sqrt(.Machine$double.eps), sep=""),
min.poll.size.integer = paste("r", sqrt(.Machine$double.eps), sep=""),
opts=list(),
nmulti = 0,
tau = NULL,
weights = NULL,
singular.ok = FALSE)

Arguments

y  continuous univariate vector
xz  continuous and/or nominal/ordinal (factor/ordered) predictors
degree.max  the maximum degree of the B-spline basis for each of the continuous predictors (default degree.max=10)
segments.max  the maximum segments of the B-spline basis for each of the continuous predictors (default segments.max=10)
degree.min  the minimum degree of the B-spline basis for each of the continuous predictors (default degree.min=0)
segments.min  the minimum segments of the B-spline basis for each of the continuous predictors (default segments.min=1)
cv.df.min  the minimum degrees of freedom to allow when conducting cross-validation (default cv.df.min=1)
complexity  a character string (default complexity="degree-knots") indicating whether model 'complexity' is determined by the degree of the spline or by the number of segments ('knots'). This option allows the user to use cross-validation to select either the spline degree (number of knots held fixed) or the number of knots (spline degree held fixed) or both the spline degree and number of knots
knots  a character string (default knots="quantiles") specifying where knots are to be placed. 'quantiles' specifies knots placed at equally spaced quantiles (equal number of observations lie in each segment) and 'uniform' specifies knots placed at equally spaced intervals. If knots="auto", the knot type will be automatically determined by cross-validation
basis

A character string (default basis = "additive") indicating whether the additive or tensor product B-spline basis matrix for a multivariate polynomial spline or generalized B-spline polynomial basis should be used. Note this can be automatically determined by cross-validation if cv = TRUE and basis = "auto", and is an "all or none" proposition (i.e. interaction terms for all predictors or for no predictors given the nature of 'tensor products'). Note also that if there is only one predictor this defaults to basis = "additive" to avoid unnecessary computation as the spline bases are equivalent in this case.

cv.func

A character string (default cv.func = "cv.ls") indicating which method to use to select smoothing parameters. cv.gcv specifies generalized cross-validation (Craven and Wahba (1979)), cv.aic specifies expected Kullback-Leibler cross-validation (Hurvich, Simonoff, and Tsai (1998)), and cv.ls specifies least-squares cross-validation.

degree

Integer/vector specifying the degree of the B-spline basis for each dimension of the continuous x.

segments

Integer/vector specifying the number of segments of the B-spline basis for each dimension of the continuous x (i.e. number of knots minus one).

lambda

Real/vector for the categorical predictors. If it is not NULL, it will be the starting value(s) for lambda.

lambda.discrete

If lambda.discrete = TRUE, the bandwidth will be discretized into lambda.discrete.num + 1 points and lambda will be chosen from these points.

lambda.discrete.num

A positive integer indicating the number of discrete values that lambda can assume - this parameter will only be used when lambda.discrete = TRUE.

random.seed

When it is not missing and not equal to 0, the initial points will be generated using this seed when nmulti > 0.

max.bb.eval

Argument passed to the NOMAD solver (see snomadr for further details).

initial.mesh.size.real

Argument passed to the NOMAD solver (see snomadr for further details).

initial.mesh.size.integer

Argument passed to the NOMAD solver (see snomadr for further details).

min.mesh.size.real

Argument passed to the NOMAD solver (see snomadr for further details).

min.mesh.size.integer

Arguments passed to the NOMAD solver (see snomadr for further details).

min.poll.size.real

Arguments passed to the NOMAD solver (see snomadr for further details).

min.poll.size.integer

Arguments passed to the NOMAD solver (see snomadr for further details).

opts

List of optional arguments to be passed to snomadr.

nmulti

Integer number of times to restart the process of finding extrema of the cross-validation function from different (random) initial points (default nmulti = 0).
tau if non-null a number in (0,1) denoting the quantile for which a quantile regression spline is to be estimated rather than estimating the conditional mean (default tau=NULL)

weights an optional vector of weights to be used in the fitting process. Should be ‘NULL’ or a numeric vector. If non-NULL, weighted least squares is used with weights ‘weights’ (that is, minimizing ‘sum(w*e^2)’); otherwise ordinary least squares is used.

singular.ok a logical value (default singular.ok=FALSE) that, when FALSE, discards singular bases during cross-validation (a check for ill-conditioned bases is performed).

Details

krscvNOMAD computes NOMAD-based cross-validation for a regression spline estimate of a one-dimensional dependent variable on an r-dimensional vector of continuous and nominal/ordinal (factor/ordered) predictors. Numerical search for the optimal degree/segments/lambda is undertaken using snomadr.

The optimal K/lambda combination is returned along with other results (see below for return values). The method uses kernel functions appropriate for categorical (ordinal/nominal) predictors which avoids the loss in efficiency associated with sample-splitting procedures that are typically used when faced with a mix of continuous and nominal/ordinal (factor/ordered) predictors.

For the continuous predictors the regression spline model employs either the additive or tensor product B-spline basis matrix for a multivariate polynomial spline via the B-spline routines in the GNU Scientific Library (http://www.gnu.org/software/gsl/) and the tensor.prod.model.matrix function.

For the discrete predictors the product kernel function is of the ‘Li-Racine’ type (see Li and Racine (2007) for details).

Value

krscvNOMAD returns a crscv object. Furthermore, the function summary supports objects of this type. The returned objects have the following components:

K scalar/vector containing optimal degree(s) of spline or number of segments
K.mat vector/matrix of values of K evaluated during search
degree.max the maximum degree of the B-spline basis for each of the continuous predictors (default degree.max=10)
segments.max the maximum segments of the B-spline basis for each of the continuous predictors (default segments.max=10)
degree.min the minimum degree of the B-spline basis for each of the continuous predictors (default degree.min=0)
segments.min the minimum segments of the B-spline basis for each of the continuous predictors (default segments.min=1)
restarts number of restarts during search, if any
lambda optimal bandwidths for categorical predictors
lambda.mat vector/matrix of optimal bandwidths for each degree of spline
cv.func objective function value at optimum
cv.func.vec vector of objective function values at each degree of spline or number of segments in K.mat

Author(s)

Jeffrey S. Racine <racej@mcmaster.ca> and Zhenghua Nie <niez@mcmaster.ca>

References


See Also

loess, npregbw,

Examples

set.seed(42)
## Simulated data
n <- 1000

x <- runif(n)
z <- round(runif(n, min=0.5, max=1.5))
z.unique <- uniquecombs(as.matrix(z))
ind <- attr(z.unique, "index")
ind.vals <- sort(unique(ind))
dgp <- numeric(length=n)
for(i in 1:nrow(z.unique)) {
  zz <- ind == ind.vals[i]
  dgp[zz] <- z[zz]+cos(2*pi*x[zz])
}
y <- dgp + rnorm(n, sd=1)
xdata <- data.frame(x,z=factor(z))

## Compute the optimal K and lambda, determine optimal number of knots, set
## spline degree for x to 3

cv <- krscvNOMAD(x=xdata,y=y,complexity="knots",degree=c(3),segments=c(5))
summary(cv)

**Description**

`npglpreg` computes a generalized local polynomial kernel regression estimate (Hall and Racine (forthcoming)) of a one (1) dimensional dependent variable on an \( r \)-dimensional vector of continuous and categorical (factor/ordered) predictors.

**Usage**

npglpreg(...) 

## Default S3 method:
npglpreg(tydat = NULL, 
    txdat = NULL, 
    eydat = NULL, 
    exdat = NULL, 
    bws = NULL, 
    degree = NULL, 
    leave_one_out = FALSE, 
    ckertype = c("gaussian", "epanechnikov", "uniform", "truncated gaussian"), 
    ckerorder = 2, 
    ukertype = c("liracine", "aitchisonaitken"), 
    okertype = c("liracine", "wangvanryzin"), 
    bwtype = c("fixed", "generalized_nn", "adaptive_nn", "auto"), 
    gradient.vec = NULL, 
    gradient.categorical = FALSE, 
    cv.shrink = TRUE, 
    cv.maxPenalty = sqrt(.Machine$double.xmax), 
    cv.warning = FALSE, 
    Bernstein = TRUE, 
    mpi = FALSE, 
    ...) 

## S3 method for class 'formula'
npglpreg(formula, 
    data = list(), 
    tydat = NULL,
Arguments

formula a symbolic description of the model to be fit

data an optional data frame containing the variables in the model

tydat a one (1) dimensional numeric or integer vector of dependent data, each element
    corresponding to each observation (row) of txdat. Defaults to the training
data used to compute the bandwidth object
txdat a \( p \)-variate data frame of explanatory data (training data) used to calculate the regression estimators. Defaults to the training data used to compute the bandwidth object.

eydat a one (1) dimensional numeric or integer vector of the true values of the dependent variable. Optional, and used only to calculate the true errors.

exdat a \( p \)-variate data frame of points on which the regression will be estimated (evaluation data). By default, evaluation takes place on the data provided by txdat.

bws a vector of bandwidths, with each element \( i \) corresponding to the bandwidth for column \( i \) in txdat.

degree integer/vector specifying the polynomial degree of the for each dimension of the continuous \( x \) in txdat.

leave.one.out a logical value to specify whether or not to compute the leave one out sums. Will not work if exdat is specified. Defaults to FALSE.

ckertype character string used to specify the continuous kernel type. Can be set as gaussian, epanechnikov, or uniform. Defaults to gaussian.

ckerorder numeric value specifying kernel order (one of \( (2, 4, 6, 8) \)). Kernel order specified along with a uniform continuous kernel type will be ignored. Defaults to 2.

ukertype character string used to specify the unordered categorical kernel type. Can be set as aitchisonaikten or liracine. Defaults to liracine.

okertype character string used to specify the ordered categorical kernel type. Can be set as wangvanryzin or liracine. Defaults to liracine.

bwtype character string used for the continuous variable bandwidth type, specifying the type of bandwidth to compute and return in the bandwidth object. If bwtype=“auto”, the bandwidth type type will be automatically determined by cross-validation. Defaults to fixed. Option summary:

fixed: compute fixed bandwidths

generalized\_nn: compute generalized nearest neighbor bandwidths

adaptive\_nn: compute adaptive nearest neighbor bandwidths

cv a character string (default cv=“nomad”) indicating whether to use nonsmooth mesh adaptive direct search, or no search (i.e. use supplied values for degree and bws).

cv.func a character string (default cv.func=“cv.ls”) indicating which method to use to select smoothing parameters. cv.aic specifies expected Kullback-Leibler cross-validation (Hurvich, Simonoff, and Tsai (1998)), and cv.ls specifies least-squares cross-validation.

max.bb.eval argument passed to the NOMAD solver (see snomadr for further details)

min.epsilon argument passed to the NOMAD solver (see snomadr for further details)

initial.mesh.size.real argument passed to the NOMAD solver (see snomadr for further details)

initial.mesh.size.integer argument passed to the NOMAD solver (see snomadr for further details)

min.mesh.size.real argument passed to the NOMAD solver (see snomadr for further details)
min.mesh.size.integer
  arguments passed to the NOMAD solver (see snomadr for further details)

min.poll.size.real
  arguments passed to the NOMAD solver (see snomadr for further details)

min.poll.size.integer
  arguments passed to the NOMAD solver (see snomadr for further details)

opts
  list of optional arguments passed to the NOMAD solver (see snomadr for further details)

nmulti
  integer number of times to restart the process of finding extrema of the cross-validation function from different (random) initial points (default nmulti=5)

random.seed
  when it is not missing and not equal to 0, the initial points will be generated using this seed when using snomadr

degree.max
  the maximum degree of the polynomial for each of the continuous predictors (default degree.max=10)

degree.min
  the minimum degree of the polynomial for each of the continuous predictors (default degree.min=0)

bandwidth.max
  the maximum bandwidth scale (i.e. number of scaled standard deviations) for each of the continuous predictors (default bandwidth.max=Machine$double.xmax)

bandwidth.min
  the minimum bandwidth scale for each of the categorical predictors (default bandwidth.min=sqrt(Machine$double.eps))

bandwidth.min.numeric
  the minimum bandwidth scale (i.e. number of scaled standard deviations) for each of the continuous predictors (default bandwidth.min=1.0e-02)

bandwidth.switch
  the minimum bandwidth scale (i.e. number of scaled standard deviations) for each of the continuous predictors (default bandwidth.switch=1.0e+06) before the local polynomial is treated as global during cross-validation at which point a global categorical kernel weighted least squares fit is used for computational efficiency

bandwidth.scale.categorical
  the upper end for the rescaled bandwidths for the categorical predictors (default bandwidth.scale.categorical=1.0e+04) - the aim is to ‘even up’ the scale of the search parameters as much as possible, so when very large scale factors are selected for the continuous predictors, a larger value may improve search

restart.from.min
  a logical value indicating to recommence snomadr with the optimal values found from its first invocation (typically quick but sometimes recommended in the field of optimization)

gradient.vec
  a vector corresponding to the order of the partial (or cross-partial) and which variable the partial (or cross-partial) derivative(s) are required

gradient.categorical
  a logical value indicating whether discrete gradients (i.e. differences in the response from the base value for each categorical predictor) are to be computed
cv.shrink  a logical value indicating whether to use ridging (Seifert and Gasser (2000)) for ill-conditioned inversion during cross-validation (default cv.shrink=TRUE) or to instead test for ill-conditioned matrices and penalize heavily when this is the case (much stronger condition imposed on cross-validation)

cv.maxPenalty  a penalty applied during cross-validation when a delete-one estimate is not finite or the polynomial basis is not of full column rank

cv.warning  a logical value indicating whether to issue an immediate warning message when ill conditioned bases are encountered during cross-validation (default cv.warning=FALSE)

Bernstein  a logical value indicating whether to use raw polynomials or Bernstein polynomials (default) (note that a Bernstein polynomial is also know as a Bezier curve which is also a B-spline with no interior knots)

mpi  a logical value (default mpi=FALSE) that, when mpi=TRUE, can call the nprmpi rather than the np package (note - code needs to mirror examples in the demo directory of the nprmpi package, you need to broadcast loading of the crs package, and need .Rprofile in your current directory)

...  additional arguments supplied to specify the regression type, bandwidth type, kernel types, training data, and so on, detailed below

Details

Typical usages are (see below for a list of options and also the examples at the end of this help file)

```r
## Conduct generalized local polynomial estimation
model <- npglpreg(y~x1+x2)

## Conduct degree 0 local polynomial estimation
## (i.e. Nadaraya-Watson)
model <- npglpreg(y~x1+x2,cv="bandwidth",degree=c(0,0))

## Conduct degree 1 local polynomial estimation (i.e. local linear)
model <- npglpreg(y~x1+x2,cv="bandwidth",degree=c(1,1))

## Conduct degree 2 local polynomial estimation (i.e. local quadratic)
model <- npglpreg(y~x1+x2,cv="bandwidth",degree=c(2,2))

## Plot the mean and bootstrap confidence intervals
plot(model,ci=TRUE)

## Plot the first partial derivatives and bootstrap confidence intervals
```
This function is in beta status until further notice (eventually it will be rolled into the np/npRmpi packages after the final status of snomadr/NOMAD gets sorted out).

Optimizing the cross-validation function jointly for bandwidths (vectors of continuous parameters) and polynomial degrees (vectors of integer parameters) constitutes a mixed-integer optimization problem. These problems are not only 'hard' from the numerical optimization perspective, but are also computationally intensive (contrast this to where we conduct, say, local linear regression which sets the degree of the polynomial vector to a global value degree=1 hence we only need to optimize with respect to the continuous bandwidths). Because of this we must be mindful of the presence of local optima (the objective function is non-convex and non-differentiable). Restarting search from different initial starting points is recommended (see nmulti) and by default this is done more than once. We encourage users to adopt 'multistarting' and to investigate the impact of changing default search parameters such as initial.mesh.size.real, initial.mesh.size.integer, min.mesh.size.real, min.mesh.size.integer, min.poll.size.real, and min.poll.size.integer. The default values were chosen based on extensive simulation experiments and were chosen so as to yield robust performance while being mindful of excessive computation - of course, no one setting can be globally optimal.

**Value**

`npglpreg` returns a `npglpreg` object. The generic functions `fitted` and `residuals` extract (or generate) estimated values and residuals. Furthermore, the functions `summary`, `predict`, and `plot` (options `deriv=0, ci=FALSE` [ci=TRUE produces pointwise bootstrap error bounds], `persp.rgl=FALSE`, `plot.behavior=c("plot","plot-data","data"), plot.errors.boot.num=99, plot.errors.type=c("quantiles","standard" ["quantiles" produces percentiles determined by plot.errors.quantiles below, "standard" produces error bounds given by +/- 1.96 bootstrap standard deviations], `plot.errors.quantiles=c(0.025,0.975), xtrim=0.0, xq=0.5) support objects of this type. The returned object has the following components:

- `fitted.values` estimates of the regression function (conditional mean) at the sample points or evaluation points
- `residuals` residuals computed at the sample points or evaluation points
- `degree` integer/vector specifying the degree of the polynomial for each dimension of the continuous x
- `gradient` the estimated gradient (vector) corresponding to the vector `gradient.vec`
- `gradient.categorical.mat` the estimated gradient (matrix) for the categorical predictors
- `gradient.vec` the supplied `gradient.vec`
- `bws` vector of bandwidths
bwtype the supplied bwtype
call a symbolic description of the model
r.squared coefficient of determination (Doksum and Samarov (1995))

**Note**

Note that the use of raw polynomials (Bernstein=FALSE) for approximation is appealing as they can be computed and differentiated easily, however, they can be unstable (their inversion can be ill conditioned) which can cause problems in some instances as the order of the polynomial increases. This can hamper search when excessive reliance on ridging to overcome ill conditioned inversion becomes computationally burdensome.

npglpreg tries to detect whether this is an issue or not when Bernstein=FALSE for each numeric predictor and will adjust the search range for snomadr and the degree fed to npglpreg if appropriate. However, if you suspect that this might be an issue for your specific problem and you are using raw polynomials (Bernstein=FALSE), you are encouraged to investigate this by limiting degree.max to value less than the default value (say 3). Alternatively, you might consider re-scaling your numeric predictors to lie in \([0, 1]\) using scale.

For a given predictor \(x\) you can readily determine if this is an issue by considering the following:

Suppose \(x\) is given by

\[
\begin{align*}
x & \leftarrow \text{runif}(100, 10000, 11000) \\
y & \leftarrow x + \text{rnorm}(100, \text{sd}=1000)
\end{align*}
\]

so that a polynomial of order, say, 5 would be ill conditioned. This would be apparent if you considered

\[
\begin{align*}
X & \leftarrow \text{poly}(x, \text{degree}=5, \text{raw}=\text{TRUE}) \\
\text{solve}(t(X)^{\text{**X}})
\end{align*}
\]

which will throw an error when the polynomial is ill conditioned, or

\[
\begin{align*}
X & \leftarrow \text{poly}(x, \text{degree}=5, \text{raw}=\text{TRUE}) \\
\text{lm}(y \sim X)
\end{align*}
\]

which will return NA for one or more coefficients when this is an issue.

In such cases you might consider transforming your numeric predictors along the lines of the following:

\[
\begin{align*}
x & \leftarrow \text{as.numeric} \left( \text{scale}(x) \right) \\
X & \leftarrow \text{poly}(x, \text{degree}=5, \text{raw}=\text{TRUE}) \\
\text{solve}(t(X)^{\text{**X}}) \\
\text{lm}(y \sim X)
\end{align*}
\]

Note that now your least squares coefficients (i.e. first derivative of \(y\) with respect to \(x\)) represent the effect of a one standard deviation change in \(x\) and not a one unit change. Alternatively, you can use Bernstein polynomials by not setting Bernstein=FALSE.
Author(s)

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References


See Also

npreg

Examples

```r
## Not run:
set.seed(42)
n <- 100
x1 <- runif(n,-2,2)
x2 <- runif(n,-2,2)
y <- x1^3 + rnorm(n,sd=1)

## Ideally the method should choose large bandwidths for x1 and x2 and a
generalized polynomial that is a cubic for x1 and degree 0 for x2.
model <- npglpreg(y=x1+x2,nmulti=1)
summary(model)

## Plot the partial means and percentile confidence intervals
plot(model,ci=T)

## Extract the data from the plot object and plot it separately
myplot.dat <- plot(model,plot.behavior="data",ci=T)
matplot(myplot.dat[[1]][,1],myplot.dat[[1]][,-1],type="1")
matplot(myplot.dat[[2]][,1],myplot.dat[[2]][,-1],type="1")

## End(Not run)
```
Description

snomadr is an R interface to NOMAD (Nonsmooth Optimization by Mesh Adaptive Direct Search, Abramson, Audet, Couture and Le Digabel (2011)), an open source software C++ implementation of the Mesh Adaptive Direct Search (MADS, Le Digabel (2011)) algorithm designed for constrained optimization of blackbox functions.

NOMAD is designed to find (local) solutions of mathematical optimization problems of the form

\[
\begin{align*}
\min & \quad f(x) \\
\text{subject to} & \quad g(x) \leq 0 \\
& \quad x_L \leq x \leq x_U
\end{align*}
\]

where \( f(x) : \mathbb{R}^n \to \mathbb{R}^k \) is the objective function, and \( g(x) : \mathbb{R}^n \to \mathbb{R}^m \) are the constraint functions. The vectors \( x_L \) and \( x_U \) are the bounds on the variables \( x \). The functions \( f(x) \) and \( g(x) \) can be nonlinear and nonconvex. The variables can be integer, continuous real number, binary, and categorical.

Kindly see \url{http://www.gerad.ca/nomad/Project/Home.html} and the references below for details.

Usage

```r
snomadr(eval.f, 
    n, 
    bbin = NULL, 
    bout = NULL, 
    x0 = NULL, 
    lb = NULL, 
    ub = NULL, 
    nmulti = 0, 
    random.seed = 0, 
    opts = list(), 
    print.output = TRUE, 
    information = list(), 
    snomadr.environment = new.env(), 
    ...) 
```

Arguments

- `eval.f` function that returns the value of the objective function
- `n` the number of variables
- `bbin` types of variables. Variable types are 0 (CONTINUOUS), 1 (INTEGER), 2 (CATEGORICAL), 3 (BINARY)
- `bout` types of output of `eval.f`. See the NOMAD User Guide \url{http://www.gerad.ca/NOMAD/Downloads/user_guide.pdf}
- `x0` vector with starting values for the optimization. If it is provided and `nmulti` is bigger than 1, `x0` will be the first initial point for multiple initial points
lb vector with lower bounds of the controls (use -1.0e19 for controls without lower bound)

ub vector with upper bounds of the controls (use 1.0e19 for controls without upper bound)

nmulti when it is missing, or it is equal to 0 and x0 is provided, snomadRSolve will be called to solve the problem. Otherwise, smultinomadRSolve will be called

random.seed when it is not missing and not equal to 0, the initial points will be generated using this seed when nmulti > 0

opts list of options for NOMAD, see the NOMAD user guide http://www.gerad.ca/NOMAD/Downloads/user_guide.pdf. Options can also be set by nomad.opt which should be in the folder where R (snomadr) is executed. Options that affect the solution and their defaults and some potential values are

"MAX_BB_EVAL"=10000
"INITIAL_MESH_SIZE"=1
"MIN_MESH_SIZE"="r1.0e-10"
"MIN_POLL_SIZE"="r1.0e-10"

Note that the "r..." denotes relative measurement (relative to lb and ub)

Note that decreasing the maximum number of black box evaluations ("MAX_BB_EVAL") will terminate search sooner and may result in a less accurate solution. For complicated problems you may want to increase this value. When experimenting it is desirable to set "DISPLAY_DEGREE"=1 (or a larger integer) to get some sense for how the algorithm is progressing

print.output when FALSE, no output from snomadr is displayed on the screen. If the NOMAD option "DISPLAY_DEGREE"=0, is set, there will also be no output from NOMAD. Higher integer values for "DISPLAY_DEGREE"= provide successively more detail

information is a list. snomadr will call snomadRInfo to return the information about NOMAD according to the values of "info", "version" and "help".

"info"="-i": display the usage and copyright of NOMAD
"version"="-v": display the version of NOMAD you are using
"help"="-h": display all options

You also can display a specific option, for example, "help"="-h x0", this will tell you how to set x0

snomadr.environment environment that is used to evaluate the functions. Use this to pass additional data or parameters to a function

... arguments that will be passed to the user-defined objective and constraints functions. See the examples below

Details

snomadr is used in the crs package to numerically minimize an objective function with respect to the spline degree, number of knots, and optionally the kernel bandwidths when using crs with the option cv="nomad" (default). This is a constrained mixed integer combinatoric problem and
is known to be computationally ‘hard’. See \texttt{frscvNOMAD} and \texttt{krscvNOMAD} for the functions called when cv="nomad" while using \texttt{crs}.

However, the user should note that for simple problems involving one predictor exhaustive search may be faster and potentially more accurate, so please bear in mind that cv="exhaustive" can be useful when using \texttt{crs}.

Naturally, exhaustive search is also useful for verifying solutions returned by \texttt{snomadr}. See \texttt{frscv} and \texttt{krscv} for the functions called when cv="exhaustive" while using \texttt{crs}.

### Value

The return value contains a list with the inputs, and additional elements

- **call**: the call that was made to solve
- **status**: integer value with the status of the optimization
- **message**: more informative message with the status of the optimization
- **iterations**: number of iterations that were executed, if multiple initial points are set, this number will be the sum for each initial point.
- **objective**: value if the objective function in the solution
- **solution**: optimal value of the controls

### Author(s)

Zhenghua Nie <niez@mcmaster.ca>

### References


### See Also

\texttt{optim}, \texttt{nlm}, \texttt{nlminb}

### Examples

```r
## Not run:
## List all options
snomadr(information=list("help"="-h"))

## Print given option, for example, MESH_SIZE
snomadr(information=list("help"="-h MESH_SIZE"))

## Print the version of NOMAD
snomadr(information=list("version"="-v"))

## Print usage and copyright
```
## Example in NOMAD/Examples/Basic/library/single_obj/basic_lib.cpp

```r
snomadr(information=list("info"="-i"))

# This is the example found in
# NOMAD/examples/basic/library/single_obj/basic_lib.cpp

eval.f <- function( x ) {
    f <- c(Inf, Inf, Inf);
    n <- length(x);
    if ( n == 5 && ( is.double(x) || is.integer(x) ) ) {
        f[1] <- x[5];
        f[2] <- sum ( (x-1)^2 ) - 25;
        f[3] <- 25 - sum ( (x+1)^2 );
    }
    return ( as.double(f) );
}

# Initial values
x0 <- rep(0, 5)

bbin <- c(1, 1, 1, 1)

# Bounds
lb <- rep(-6, 5)
ub <- c(5, 6.0, 7.0, 100000, 100000)

bbout <- c(0, 2, 1)

# Options
opts <- list("MAX_BB_EVAL"=500,
             "MIN_MESH_SIZE"=0.001,
             "INITIAL_MESH_SIZE"=0.1,
             "MIN_POLL_SIZE"=0.0001)

snomadr(eval.f=eval.f, n=5, x=x0, bbin=bbin, bbout=bbout, lb=lb, ub=ub, opts=opts)

# How to transfer other parameters into eval.f
#
# First example: supply additional arguments in user-defined functions
#
# objective function and gradient in terms of parameters
eval.f.ex1 <- function(x, params) {
    return( params[1]*x^2 + params[2]*x + params[3] )
}

# Define parameters that we want to use
params <- c(1, 2, 3)

# Define initial value of the optimization problem
x0 <- 0
```
## Second example: define an environment that contains extra parameters

### Objective function and gradient in terms of parameters

```r
# without supplying params as an argument
eval.f.ex2 <- function(x) {
  return( params[1]*x^2 + params[2]*x + params[3] )
}
```

### Define initial value of the optimization problem

```r
x0 <- 0
```

### Define a new environment that contains params

```r
auxdata <- new.env()
auxdata$params <- c(1, 2, 3)
```

### pass The environment that should be used to evaluate functions to snomadr

```r
snomadr(n = 1,
  x0 = x0,
  eval.f = eval.f.ex2,
  params = params )
```

## Solve using algebra

```r
cat( paste( "Minimizing f(x) = ax^2 + bx + c\n" ) )
cat( paste( "Optimal value of control is b/(2a) = ", -params[2]/(2*params[1]), "\n" ) )
cat( paste( "With value of the objective function f(-b/(2a)) = ", eval.f.ex1( -params[2]/(2*params[1]), params ), "\n" ) )
```

## The following example is NOMAD/examples/advanced/multi_start/multi.cpp

### This will call smultinomadRSolve to resolve the problem.

```r
eval.f.ex1 <- function(x, params) {
  M<as.numeric(params$M)
  NBC<as.numeric(params$NBC)

  f<-rep(0, M+1)
  x<-as.numeric(x)

  x1 <- rep(0.0, NBC)
  y1 <- rep(0.0, NBC)

  x1[1]<-x[1]
```r
epi <- 6
for(i in 5:NBC){
  x1[i] <- x[epi]
  y1[i] <- y[epi]
  epi <- epi + 1
}
constraint <- 0.0
ic <- 1
f[ic] <- constraint
ic <- ic + 1

constraint <- as.numeric(1.0)
distmax <- as.numeric(0.0)
avg_dist <- as.numeric(0.0)
dist1 <- as.numeric(0.0)

for(i in 1:(NBC-1)){
  for (j in (i+1):NBC){
    dist1 <- as.numeric((x1[i]-x1[j])*(x1[i]-x1[j]) + (y1[i]-y1[j])*(y1[i]-y1[j]))
    if(dist1 > distmax) {distmax <- as.numeric(dist1)}
    if(dist1[i] < 1) {constraint <- constraint + sqrt(dist1)}
    else if(dist1[i] > 14) {avg_dist <- avg_dist + sqrt(dist1)}
  }
}

if(constraint < 0.9999) constraint <- 1001.0 - constraint
else constraint = sqrt(distmax) + avg_dist/(10.0*NBC)

f[2] <- 0.0
f[M+1] <- constraint

return(as.numeric(f))
}

## Define parameters that we want to use
params <- list()
NBC <- 5
M <- 2
n <- 2*NBC - 3

params$NBC <- NBC
params$M <- M
x0 <- rep(0.1, n)
lb <- rep(0, n)
ub <- rep(4.5, n)

eval.f.ex1(x0, params)
bbout <- c(2, 2, 0)
```
tensor.prod.model.matrix

Utility functions for constructing tensor product smooths

Description

Produce model matrices or penalty matrices for a tensor product smooth from the model matrices or penalty matrices for the marginal bases of the smooth.

Usage

tensor.prod.model.matrix(X)

Arguments

X a list of model matrices for the marginal bases of a smooth
Details

If $X[[1]], X[[2]] \ldots X[[m]]$ are the model matrices of the marginal bases of a tensor product smooth then the $i$th row of the model matrix for the whole tensor product smooth is given by $X[[1]][i,] \otimes x X[[2]][i,] \otimes \ldots \otimes X[[m]][i,]$, where $\otimes$ is the Kronecker product. Of course the routine operates column-wise, not row-wise!

Value

Either a single model matrix for a tensor product smooth, or a list of penalty terms for a tensor product smooth.

Author(s)

Simon N. Wood <simon.wood@r-project.org>

References


See Also

t, smooth.construct.tensor.smooth.spec

Examples

```r
X <- list(matrix(1:4,2,2), matrix(5:10,2,3))
tensor.prod.model.matrix(X)
```

---

**uniquecombs**  
Find the unique rows in a matrix

Description

This routine returns a matrix containing all the unique rows of the matrix supplied as its argument. That is, all the duplicate rows are stripped out. Note that the ordering of the rows on exit is not the same as on entry. It also returns an index attribute for relating the result back to the original matrix.

Usage

```r
uniquecombs(x)
```

Arguments

- `x` is an R matrix (numeric)
Details

Models with more parameters than unique combinations of covariates are not identifiable. This routine provides a means of evaluating the number of unique combinations of covariates in a model. The routine calls compiled C code.

Value

A matrix consisting of the unique rows of x (in arbitrary order).

The matrix has an "index" attribute. index[i] gives the row of the returned matrix that contains row i of the original matrix.

Author(s)

Simon N. Wood <simon.wood@r-project.org>

See Also

unique can do the same thing, including for non-numeric matrices, but more slowly and without returning the index.

Examples

```r
X <- matrix(c(1,2,3,1,2,3,4,5,6,1,3,2,4,5,6,1,1,1,6,3), byrow=TRUE)
print(X)
Xu <- uniquecombs(X);Xu
ind <- attr(Xu,"index")
## find the value for row 3 of the original from Xu
Xu[ind[3],];X[3,]
```

---

wage1

Cross-Sectional Data on Wages

Description

Cross-section wage data consisting of a random sample taken from the U.S. Current Population Survey for the year 1976. There are 526 observations in total.

Usage

data("wage1")
Format

A data frame with 24 columns, and 526 rows.

- **wage**: column 1, of type numeric, average hourly earnings
- **educ**: column 2, of type numeric, years of education
- **exper**: column 3, of type numeric, years potential experience
- **tenure**: column 4, of type numeric, years with current employer
- **nonwhite**: column 5, of type factor, =“Nonwhite” if nonwhite, “White” otherwise
- **female**: column 6, of type factor, =“Female” if female, “Male” otherwise
- **married**: column 7, of type factor, =“Married” if Married, “Nonmarried” otherwise
- **numdep**: column 8, of type numeric, number of dependents
- **smsa**: column 9, of type numeric, =1 if live in SMSA
- **northcen**: column 10, of type numeric, =1 if live in north central U.S
- **south**: column 11, of type numeric, =1 if live in southern region
- **west**: column 12, of type numeric, =1 if live in western region
- **construc**: column 13, of type numeric, =1 if work in construc. indus.
- **ndurman**: column 14, of type numeric, =1 if in nondur. manuf. indus.
- **trcommpu**: column 15, of type numeric, =1 if in trans, commun, pub ut
- **trade**: column 16, of type numeric, =1 if in wholesale or retail
- **services**: column 17, of type numeric, =1 if in services indus.
- **profserv**: column 18, of type numeric, =1 if in prof. serv. indus.
- **profocc**: column 19, of type numeric, =1 if in profess. occupation
- **clerocc**: column 20, of type numeric, =1 if in clerical occupation
- **servocc**: column 21, of type numeric, =1 if in service occupation
- **lwage**: column 22, of type numeric, log(wage)
- **expersq**: column 23, of type numeric, exper^2
- **tenursq**: column 24, of type numeric, tenure^2

Source

Jeffrey M. Wooldridge

References

Examples

```r
## Not run:
data(wage1)

## Cross-validated model selection for spline degree and bandwidths Note
## - we override the default nmulti here to get a quick illustration
## (we don't advice doing this, in fact advise using more restarts in
## serious applications)

model <- crs(lwage~married+
    female+
    nonwhite+
    educ+
    exper+
    tenure,
    basis="additive",
    complexity="degree",
    data=wage1,
    segments=c(1,1,1),
    nmulti=1)

summary(model)

## Residual plots
plot(model)
## Partial mean plots (control for non axis predictors)
plot(model,mean=TRUE)
## Partial first derivative plots (control for non axis predictors)
plot(model,deriv=1)
## Partial second derivative plots (control for non axis predictors)
plot(model,deriv=2)
## Compare with local linear kernel regression
require(np)
model <- npreg(lwage~married+
    female+
    nonwhite+
    educ+
    exper+
    tenure,
    regtype="ll",
    bwmethod="cv.aic",
    data=wage1)

summary(model)

## Partial mean plots (control for non axis predictors)
plot(model,common.scale=FALSE)
## Partial first derivative plots (control for non axis predictors)
plot(model,gradients=TRUE,common.scale=FALSE)
detach("package:np")

## End(Not run)
```
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