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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:

\[ l(z_i, z, \lambda) = \begin{cases} 1 & \text{if } z_i = z, \\ \lambda & \text{if } z_i \neq z. \end{cases} \]

Note that \( \lambda \) must lie between 0 and 1.
(z is discrete/ordinal) \( l(z_i, z, \lambda) = 1 \) if \( |z_i - z| = 0 \), and \( \lambda |z_i - z| \) 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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References


clsd

Categorical Logspline Density

Description

clsd computes the logspline 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,
n.multi = 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 1st 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.

deriv.index: an integer 1 (default deriv.index=1) specifying the index (currently only supports 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 standard 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/log(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 log spline 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

## 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)

coeff(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.clsd <- mean((fitted(model)-f.dgp)^2)
model.logslpline <- logspline(x)

mse.logslpline <- mean((dlogspline(x,model.logslpline)-f.dgp)^2)

ylim <- c(0,max(fitted(model),dlogspline(x,model.logslpline),f.dgp))

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

dx <- model$x

lines(dx,dlogspline(dx,model.logslpline),col=2,lty=2)
lines(dx,dnorm(dx),col=1,lty=1)

rug(dx)

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

summary(model)

coe(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

## 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$cv.score, format = "f", digits = 3),
                "npreg-CV = ", formatC(model.np$bws$fval, 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")


**crs**

_Categorical Regression Splines_

**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 (2015)).

**Usage**

```r
## Default S3 method:
crs(...)
## 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 = c("nomad","exhaustive","none"), cv.threshold = 1000, cv.func = c("cv.ls","cv.gcv","cv.aic"), kernel = TRUE, lambda = NULL, data.return = FALSE, prune = FALSE, model.return = FALSE, tau = NULL, weights = NULL, ...)```

```r
## 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 = c("nomad","exhaustive","none"), cv.threshold = 1000, cv.func = c("cv.ls","cv.gcv","cv.aic"), kernel = TRUE, lambda = NULL, data.return = FALSE, prune = FALSE, model.return = FALSE, tau = NULL, weights = NULL, ...)```
lambda.discrete = FALSE,
lambda.discrete.num = 100,
complexity = c("degree-knots","degree","knots"),
knots = c("quantiles","uniform","auto"),
basis = c("auto","additive","tensor","grp"),
deriv = 0,
data.return = FALSE,
prune = FALSE,
model.return = FALSE,
restarts = 0,
random.seed = 42,
max.bb.eval = 100000,
initial.mesh.size.real = "1.0e-01",
initial.mesh.size.integer = "1",
min.mesh.size.real = paste(sqrt(Machine$double.eps)),
min.mesh.size.integer = 1,
min.poll.size.real = 1,
min.poll.size.integer = 1,
opts=list(),
nmulti = 5,
tau = NULL,
weights = NULL,
singular.ok = FALSE,
...

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 as-
sume - 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 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.

- **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.

The regression 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.

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 $E(u|x)=0$), b) a normal 
quantile-quantile plot which allows residuals to be assessed for normality (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 stepAIC and replacing extractAIC with 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 kernel=FALSE.

Value

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

```r
## 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*x2), 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,
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

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","Eeywz"), 
  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 α, the Tikhonov regularization parameter, when  
using method="Tikhonov"

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

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

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

iterate.diff.tol  
the search tolerance for the difference in the stopping rule from iteration to iter-  
ation 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 itera-  
tions or not (default TRUE)
smooth.residuals
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

start.from
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)

starting.values
a value indicating whether to commence Landweber-Fridman assuming \( \varphi^{-1} = starting.values \) (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 snomadr for further details)

deriv
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)

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 \( \|E(y|w) - E(\varphi_k(z,x)|w)\|^2 \) 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 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 \( \|E(y|w) - E(\varphi_k(z,x)|w)\|/E(y|w)\|^2 \) from iteration to iteration is less than iterate.diff.tol or we hit iterate.max or \( \|E(y|w) - E(\varphi_k(z,x)|w)\|E(y|w)\|^2 \) 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.
Value

crsiv returns a 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 mean=\texttt{FALSE}, deriv=i where i is an integer, ci=\texttt{FALSE}, plot.behavior=c("plot","plot-data","data")) support objects of this type.

See \texttt{crs} for details on the return object components.

In addition to the standard \texttt{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 $\phi(Z,X)$ and not that using \texttt{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

```r
## 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 <- -.5*v + eps
w <- rnorm(n,mean=0,sd=1)

## In Darolles et al (2011) there exist two DGP. 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 <- .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)
```
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 \( \frac{1}{4} \) of one percent from each
## tail of \( y \) and \( z \))
trim <- 0.0025

curve(phi,min(z),max(z),
   xlab="z", ylab="y",
   xlim=quantile(z,c(trim,1-trim)),
   ylim=quantile(y,c(trim,1-trim)),
   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),"\(=\) E(y|z)")),
   expression(paste("Nonparametric \(\hat{\phi}(z)\)")),
   "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("Ey", "EYwz"), 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", 1, 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
weval
an \( q \)-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 \( x \)

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

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

constant
the constant to use when using Landweber-Fridman iteration

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

start.from
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)

starting.values
a value indicating whether to commence Landweber-Fridman assuming \( \varphi_{-1} = starting.values \) (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)

smooth.residuals
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

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

Details
For Landweber-Fridman iteration, an optimal stopping rule based upon \( \frac{||E(y|w) - E(\varphi_k(z,x)|w)||^2}{E(y|w)} \) 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 \( \text{nmulti} \) to a larger number than the default \( \text{nmulti}=5 \) for \texttt{crs} when using \texttt{cv="nomad"} or instead use \texttt{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 \( \frac{||E(y|w) - E(\varphi_k(z,x)|w)||^2}{E(y|w)} \) from iteration to iteration is less than \( \text{iterate.diff.tol} \) or we hit \texttt{iterate.max} or \( \frac{||E(y|w) - E(\varphi_k(z,x)|w)||^2}{E(y|w)} \) 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 \texttt{cv="nomad"} and instead use \texttt{cv="exhaustive"} since exhaustive search may be feasible (for \texttt{degree.max} and \texttt{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

crsvderiv 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 DGP's. 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$xz` for which the test of significance is to be conducted. Defaults to `(1,2,..,p)` where `p` is the number of columns in `model$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 replications. 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 \( F \)
- `P.asy`: the vector of asymptotic P-values for each statistic in `index`
- `F`: the vector of pseudo F-statistics \( F \)
- `F.boot`: the matrix of bootstrapped pseudo F-statistics generated under the null (one column for each statistic in \( F \))
- `df1`: the vector of numerator degrees of freedom for each statistic in \( F \) (based on the smoother matrix)
- `df2`: the vector of denominator degrees of freedom for each statistic in \( F \) (based on the smoother matrix)
- `rss`: the vector of restricted sums of squared residuals for each statistic in \( F \)
- `uss`: the vector of unrestricted sums of squared residuals for each statistic in \( F \)
- `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**

```r
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
## 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$logexp),]

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",
    pch=16,
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
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)

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).
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.\ degrees/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
- \( K.m\text{at} \): 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 \( K.m\text{at} \)

Author(s)

Jeffrey S. Racine <racinej@mcmaster.ca>

References


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 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(x, 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 = "1",
min.poll.size.integer = "1",
opts=list(),
nmulti = 0,
tau = NULL,
weights = NULL,
singular.ok = FALSE)

**Arguments**

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>y</code></td>
<td>continuous univariate vector</td>
</tr>
<tr>
<td><code>xz</code></td>
<td>continuous and/or nominal/ordinal <em>(factor/ordered)</em> predictors</td>
</tr>
<tr>
<td><code>degree.max</code></td>
<td>the maximum degree of the B-spline basis for each of the continuous predictors <em>(default degree.max=10)</em></td>
</tr>
<tr>
<td><code>segments.max</code></td>
<td>the maximum segments of the B-spline basis for each of the continuous predictors <em>(default segments.max=10)</em></td>
</tr>
<tr>
<td><code>degree.min</code></td>
<td>the minimum degree of the B-spline basis for each of the continuous predictors <em>(default degree.min=0)</em></td>
</tr>
<tr>
<td><code>segments.min</code></td>
<td>the minimum segments of the B-spline basis for each of the continuous predictors <em>(default segments.min=1)</em></td>
</tr>
<tr>
<td><code>cv.df.min</code></td>
<td>the minimum degrees of freedom to allow when conducting cross-validation <em>(default cv.df.min=1)</em></td>
</tr>
<tr>
<td><code>complexity</code></td>
<td>a character string <em>(default complexity=&quot;degree-knots&quot;)</em> 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</td>
</tr>
<tr>
<td><code>knots</code></td>
<td>a character string <em>(default knots=&quot;quantiles&quot;)</em> 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>a character string <em>(default basis=&quot;additive&quot;)</em> 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>
</tbody>
</table>
**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**


## 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

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

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 \( \text{max}(x) \)

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)

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

Value

\text{gsl.bs} returns a \text{gsl.bs} object. A matrix of dimension ‘c(length(x), degree+nbreak-1)’. The generic function \text{predict} extracts (or generates) predictions from the returned object.

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 <raccinej@mcmaster.ca>

References


See Also

\text{bs}

Examples

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

\[
\text{## Regression example}
\begin{align*}
n & \leftarrow 1000 \\
x & \leftarrow \text{sort}(\text{runif}(n)) \\
y & \leftarrow \cos(2\pi x) + \text{rnorm}(n, \text{sd}=.25)
\end{align*}
\]


```r
B <- gsl.bs(x, degree=5, intercept=FALSE)
plot(x,y,cex=.5,col="grey")
lines(x,fitted(lm(y~B)))
```

---

**krscv**

*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 degree.max/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 $K$ vector coincides with degree.max/segments.max a warning is produced and the user ought to restart their search with a larger value of degree.max/segments.max.

**Value**

`krscv` 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
- **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>

**References**


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 (1) dimensional dependent variable on an r-dimensional vector of continuous and nominal/ordinal (factor/ordered) predictors.
Usage

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 = "1",
  min.poll.size.real = "1",
  min.poll.size.integer = "1",
  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)
krscvNOMAD

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)

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

### Description

npglreg 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

npglreg(...)

## Default S3 method:
npglreg(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,
txdat = NULL,
eydat = NULL,
exdat = NULL,
bws = NULL,
degree = NULL,
leave.one.out = FALSE,
ckerertype = c("gaussian", "epanechnikov","uniform","truncated gaussian"),
ckerorder = 2,
ukertype = c("liracine", "aitchisonaitken"),
okertype = c("liracine", "wangvanryzin"),
bwtype = c("fixed", "generalized_nn", "adaptive_nn", "auto"),
cv = c("degree-bandwidth", "bandwidth", "none"),
cv.func = c("cv.ls", "cv.aic"),
nmulti = 5,
random.seed = 42,
degree.max = 10,
degree.min = 0,
bandwidth.max = .Machine$double.xmax,
bandwidth.min = sqrt(.Machine$double.eps),
bandwidth.min.numeric = 1.0e-02,
bandwidth.switch = 1.0e+06,
bandwidth.scale.categorical = 1.0e+04,
max.bb.eval = 100000,
min.epsilon = .Machine$double.eps,
initial.mesh.size.real = 1,
initial.mesh.size.integer = 1,
min.mesh.size.real = sqrt(.Machine$double.eps),
min.mesh.size.integer = 1,
min.poll.size.real = 1,
min.poll.size.integer = 1,
opts=list(),
restart.from.min = FALSE,
gradiant.vec = NULL,
gradiant.categorical = FALSE,
cv.shrink = TRUE,
cv.maxPenalty = sqrt(.Machine$double.xmax),
cv.warning = FALSE,
Bernstein = TRUE,
mpi = FALSE,
...)


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 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 aitchisonaitken 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$double.xmax)
bandwidth.min the minimum bandwidth scale for each of the categorical predictors (default sqrt(.Machine$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 re-
sponse 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 polyno-
mials (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 pack-
age, 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)

## 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

plot(model, deriv=1, ci=TRUE)

## Plot the first second partial derivatives and bootstrap
## confidence intervals

plot(model, deriv=2, ci=TRUE)

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(.025,.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

```r
x <- runif(100, 10000, 11000)
y <- x + rnorm(100, sd=1000)
```

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

```r
X <- poly(x, degree=5, raw=TRUE)
solve(t(X)%*%X)
```

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

```r
X <- poly(x, degree=5, raw=TRUE)
lm(y~X)
```

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:
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

mpreg

Examples

```r
x <- as.numeric(scale(x))
X <- poly(x, degree=5, raw=TRUE)
solve(t(X) %*% X)
lm(y~X)
```

```
x <- as.numeric(scale(x))
X <- poly(x, degree=5, raw=TRUE)
solve(t(X) %*% X)
lm(y~X)
```

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

mpreg

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]][,2],type="l")
matplot(myplot.dat[[2]][,1],myplot.dat[[2]][,2],type="l")
```

```
x <- as.numeric(scale(x))
X <- poly(x, degree=5, raw=TRUE)
solve(t(X) %*% X)
lm(y~X)
```

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

mpreg

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]][,2],type="l")
matplot(myplot.dat[[2]][,1],myplot.dat[[2]][,2],type="l")
```
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

\[
\begin{align*}
\text{min} & \quad f(x) \\
\text{x in } \mathbb{R}^n & \\
\text{s.t.} & \quad g(x) \leq 0 \\
& \quad x_L \leq x \leq x_U
\end{align*}
\]

where \( f(x): \mathbb{R}^n \rightarrow \mathbb{R}^k \) is the objective function, and \( g(x): \mathbb{R}^n \rightarrow \mathbb{R}^m \) 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 http://www.gerad.ca/nomad/Project/Home.html and the references below for details.

Usage

```r
snomadr(eval.f, 
  n, 
  bbin = NULL, 
  bbout = 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)
- **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 [https://www.gerad.ca/nomad/Downloads/user_guide.pdf](https://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" = 1
  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

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 func-
tions. 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 frscvNOMAD and krscvNOMAD for the functions called
when cv="nomad" while using 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 crs.

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

NOMAD project”. Software available at http://www.gerad.ca/nomad.


See Also

optim, nlm, nlminb
Examples

## 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
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(0.0, 5 )

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

## Bounds
lb <- rep(-6.0,5 )
ub <- c(5.0, 6.0, 7.0, 1000000, 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"=1)

snomadr(eval.f=eval.f,n=5, x0=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

## Solve using snomadr
snomadr(n = 1, 
  x0 = x0, 
  eval.f = eval.f.ex1, 
  params = params)

## Second example: define an environment that contains extra parameters

## Objective function and gradient in terms of parameters
## 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
x0 <- 0

## Define a new environment that contains params
auxdata <- new.env()
auxdata$params <- c(1, 2, 3)

## Pass the environment that should be used to evaluate functions to snomadr
snomadr(n = 1, 
  x0 = x0, 
  eval.f = eval.f.ex2, 
  snomadr.environment = auxdata)

## Solve using algebra

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 multinomadRsolve to resolve the problem.
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]

epi <- 6
for(i in 5:NBC){
  x1[i]<-x[epi]
  epi <- epi+1
  y1[i]<-x[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) > 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()
tensor.prod.model.matrix

Utility functions for constructing tensor product smooths
 tensor.prod.model.matrix

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]], ... X[[m]] are the model matrices of the marginal bases of a tensor product smooth then the ith row of the model matrix for the whole tensor product smooth is given by 
X[[1]][i,] %x% X[[2]][i,] %x% ... X[[m]][i,], where %x% 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

tensor.construct.tensor.smooth.spec

Examples

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

uniquecombs(x)

Arguments

x is an \( \mathbb{R} \) 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

\[
\begin{align*}
X & \leftarrow \text{matrix}(c(1,2,3,1,2,3,4,5,6,1,3,2,4,5,6,1,1,1),6,3,\text{byrow}\leftarrow\text{TRUE}) \\
\text{print}(X) \\
Xu & \leftarrow \text{uniquecombs}(X); Xu \\
\text{ind} & \leftarrow \text{attr}(Xu, "index") \\
\text{## find the value for row 3 of the original from Xu} \\
Xu[\text{ind}[3], ]; Xu[3, ]
\end{align*}
\]
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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