Package 'qgam'

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Type Package

Title Smooth Additive Quantile Regression Models

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Description Smooth additive quantile regression models, fitted using

the methods of Fasiolo et al. (2020) <doi:10.1080/01621459.2020.1725521>. See Fasiolo at al. (2021) <doi:10.18637/jss.v100.i09> for an introduction to the package. Differently from

'quantreg', the smoothing parameters are estimated automatically by marginal loss minimization, while the regression coefficients are estimated using either PIRLS or Newton algorithm. The learning rate is determined so that the Bayesian credible intervals of the estimated effects have approximately the correct coverage. The main function is qgam() which is similar to gam() in 'mgcv', but fits non-parametric quantile regression models.

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Depends R (>= 3.5.0), mgcv (>= 1.8-28)

Imports shiny, plyr, doParallel, parallel, grDevices

Suggests knitr, rmarkdown, MASS, RhpcBLASctl, testthat

VignetteBuilder knitr

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AUDem

Australian electricity demand data

Description

Data set on electricity demand from Sidney, Australia. The data has been downloaded from https: //www.ausgrid.com.au, and it originally contained electricity demand from 300 customers, at 30min resolution. We discarded 53 customers because their demand was too irregular, and we integrated the demand data with temperature data from the National Climatic Data Center, covering the same period.

Usage

data(AUDem)

Format

AUDem is a list, where AUDem\$meanDem is a data.frame containing the following variables:

- doy the day of the year, from 1 to 365;
- tod the time of day, ranging from 18 to 22, where 18 indicates the period from 17:00 to 17:30, 18.5 the period from 17:30 to 18:00 and so on;
- dem the demand (in KW) during a 30min period, averaged over the 247 households;

dow factor variable indicating the day of the week;

check

temp the external temperature at Sidney airport, in degrees Celsius;

date local date and time;

dem48 the lagged mean demand, that is the average demand (dem) during the same 30min period of the previous day;

The second element is AUDem\$qDem48 which is a matrix with as many rows as AUDem\$meanDem. Each rows contains 20 equally spaced empirical quantiles of the lagged individual electricity demand of the 247 customers.

Value

A list where AUDem\$meanDem is a data.frame and AUDem\$qDem48 a matrix.

Examples

```
library(qgam)
data(AUDem)
# Mean demand over the period
plot(AUDem$meanDem$dem, type = 'l')
# 20 quantiles of individual demand over 5 days
matplot(seq(0.01, 0.99, length.out = 20),
        t(AUDem$qDem48[c(1, 50, 75, 100, 250), ]),
        type = 'l',
        ylab = "Electricity demand (KW)",
        xlab = expression("Probability level " * "(p)"),
        lty = 1)
```

check

Generic checking function

Description

Generic function for checking R objects which produces, for instance, convergence tests or diagnostic plots. For qgam objects check.qgam() will be used.

Usage

check(obj, ...)

Arguments

| obj | the object to be checked. |
|-----|----------------------------------------------------|
| | extra arguments, mainly used by graphic functions. |

Value

Reports the results of convergence tests and/or produces diagnostic plots.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

Examples

```
#######
# Using check.qgam
#######
library(qgam)
set.seed(0)
dat <- gamSim(1, n=200)
b<-qgam(y~s(x0)+s(x1)+s(x2)+s(x3), data=dat, qu = 0.5)
plot(b, pages=1)
check(b, pch=19, cex=.3)</pre>
```

check.learn

Visual checks for the output of tuneLearn()

Description

Provides some visual plots showing how the calibration criterion and the effective degrees of freedom of each smooth component vary with the learning rate.

Usage

S3 method for class 'learn'
check(obj, sel = 1:2, ...)

Arguments

| obj | the output of a call to tuneLearn. |
|-----|-------------------------------------------------------------------------------------------------------------------------------------------------|
| sel | this function produces two plots, set this parameter to 1 to plot only the first, to 2 to plot only the second or leave it to 1:2 to plot both. |
| | currently not used, here only for compatibility reasons. |

Details

The first plot shows how the calibrations loss, which we are trying to minimize, varies with the log learning rate. This function should look quite smooth, if it doesn't then try to increase err or control\$K (the number of bootstrap samples) in the original call to tuneLearn. The second plot shows how the effective degrees of freedom of each smooth term vary with log(sigma). Generally as log(sigma) increases the complexity of the fit decreases, hence the slope is negative.

Value

It produces several plots.

check.learnFast

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

References

Fasiolo, M., Wood, S.N., Zaffran, M., Nedellec, R. and Goude, Y., 2020. Fast calibrated additive quantile regression. Journal of the American Statistical Association (to appear). https://www.tandfonline.com/doi/full/10.1080/01621459.2020.1725521.

Examples

check.learnFast *Visual checks for the output of tuneLearnFast()*

Description

Provides some visual checks to verify whether the Brent optimizer used by tuneLearnFast() worked correctly.

Usage

```
## S3 method for class 'learnFast'
check(obj, sel = NULL, ...)
```

Arguments

| obj | the output of a call to tuneLearnFast. |
|-----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| sel | integer vector determining which of the plots will be produced. For instance if $sel = c(1,3)$ only the 1st and 3rd plots are showed. No entry of sel can be bigger than one plus the number of quantiles considered in the original tuneLearnFast() call. That is, if we estimated the learning rate for $qu = c(0.1, 0.4)$, then max(sel) must be <= 3. |
| | currently not used, here only for compatibility reasons. |

Details

The top plot in the first page shows the bracket used to estimate log(sigma) for each quantile. The brackets are delimited by the crosses and the red dots are the estimates. If a dot falls very close to one of the crosses, that might indicate problems. The bottom plot shows, for each quantile, the value of parameter err used. Sometimes the algorithm needs to increase err above its user-defined value to achieve convergence. Subsequent plots show, for each quantile, the value of the loss function corresponding to each value of log(sigma) explored by Brent algorithm.

Value

It produces several plots.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

References

Fasiolo, M., Wood, S.N., Zaffran, M., Nedellec, R. and Goude, Y., 2020. Fast calibrated additive quantile regression. Journal of the American Statistical Association (to appear). https://www.tandfonline.com/doi/full/10.1080/01621459.2020.1725521.

Examples

check.qgam

Some diagnostics for a fitted qgam model

Description

Takes a fitted gam object produced by qgam() and produces some diagnostic information about the fitting procedure and results. It is partially based on mgcv::gam.check.

Usage

```
## S3 method for class 'qgam'
check(obj, nbin = 10, lev = 0.05, ...)
```

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check.qgam

Arguments

| obj | the output of a qgam() call. |
|------|----------------------------------------------------------------------------------------------------|
| nbin | number of bins used in the internal call to cqcheck(). |
| lev | the significance levels used by cqcheck(), which determines the width of the confidence intervals. |
| | extra arguments to be passed to plot() |

Details

This function provides two plots. The first shows how the number of responses falling below the fitted quantile (y-axis) changes with the fitted quantile (x-axis). To be clear: if the quantile is fixed to, say, 0.5 we expect 50% of the responses to fall below the fit. See ?cqcheck() for details. The second plot related to |F(hat(mu)) -F(mu0)|, which is the absolute bias attributable to the fact that qgam is using a smoothed version of the pinball-loss. The absolute bias is evaluated at each observation, and an histogram is produced. See Fasiolo et al. (2017) for details. The function also prints out the integrated absolute bias, and the proportion of observations lying below the regression line. It also provides some convergence diagnostics (regarding the optimization), which are the same as in mgcv::gam.check. It reports also the maximum (k') and the selected degrees of freedom of each smooth term.

Value

Simply produces some plots and prints out some diagnostics.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>, Simon N. Wood.

References

Fasiolo, M., Wood, S.N., Zaffran, M., Nedellec, R. and Goude, Y., 2020. Fast calibrated additive quantile regression. Journal of the American Statistical Association (to appear). https://www.tandfonline.com/doi/full/10.1080/01621459.2020.1725521.

Examples

```
library(qgam)
set.seed(0)
dat <- gamSim(1, n=200)
b<-qgam(y~s(x0)+s(x1)+s(x2)+s(x3), data=dat, qu = 0.5)
plot(b, pages=1)
check.qgam(b, pch=19, cex=.3)</pre>
```

cqcheck

Description

Given an additive quantile model, fitted using qgam, cqcheck provides some plots that allow to check what proportion of responses, y, falls below the fitted quantile.

Usage

```
cqcheck(
   obj,
   v,
   X = NULL,
   y = NULL,
   nbin = c(10, 10),
   bound = NULL,
   lev = 0.05,
   scatter = FALSE,
   ...
)
```

Arguments

| obj | the output of a qgam call. |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| v | if a 1D plot is required, v should be either a single character or a numeric vector. In the first case v should be the names of one of the variables in the dataframe X. In the second case, the length of v should be equal to the number of rows of X. If a 2D plot is required, v should be either a vector of two characters or a matrix with two columns. |
| X | a dataframe containing the data used to obtain the conditional quantiles. By default it is NULL, in which case predictions are made using the model matrix in obj\$model. |
| У | vector of responses. Its i-th entry corresponds to the i-th row of X. By default it is NULL, in which case it is internally set to obj\$y. |
| nbin | a vector of integers of length one (1D case) or two (2D case) indicating the number of bins to be used in each direction. Used only if bound==NULL. |
| bound | in the 1D case it is a numeric vector whose increasing entries represent the bounds of each bin. In the 2D case a list of two vectors should be provided. NULL by default. |
| lev | the significance levels used in the plots, this determines the width of the confidence intervals. Default is 0.05 . |
| scatter | if TRUE a scatterplot is added (using the points function). FALSE by default. |
| | extra graphical parameters to be passed to plot(). |

cqcheck

Details

Having fitted an additive model for, say, quantile qu=0.4 one would expect that about 40 responses fall below the fitted quantile. This function allows to visually compare the empirical number of responses (qu_hat) falling below the fit with its theoretical value (qu). In particular, the responses are binned, which the bins being constructed along one or two variables (given be arguments v). Let (qu_hat[i]) be the proportion of responses below the fitted quantile in the ith bin. This should be approximately equal to qu, for every i. In the 1D case, when v is a single character or a numeric vector, cqcheck provides a plot where: the horizontal line is qu, the dots correspond to qu_hat[i] and the grey lines are confidence intervals for qu. The confidence intervals are based on qbinom(lev/2,siz,qu), if the dots fall outside them, then qu_hat[i] might be deviating too much from qu. In the 2D case, when v is a vector of two characters or a matrix with two columns, we plot a grid of bins. The responses are divided between the bins as before, but now don't plot the confidence intervals. Instead we report the empirical proportions qu_hat[i] for the non-empty bin, and with colour the bins in red if qu_hat[i]

Value

Simply produces a plot.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

Examples

```
#######
# Bivariate additive model y~1+x+x^2+z+x*z/2+e, e~N(0, 1)
#######
## Not run:
library(qgam)
set.seed(15560)
n <- 500
x <- rnorm(n, 0, 1); z <- rnorm(n)</pre>
X <- cbind(1, x, x^2, z, x*z)
beta <- c(0, 1, 1, 1, 0.5)
y <- drop(X %*% beta) + rnorm(n)</pre>
dataf <- data.frame(cbind(y, x, z))</pre>
names(dataf) <- c("y", "x", "z")</pre>
#### Fit a constant model for median
qu <- 0.5
fit <- qgam(y\sim1, qu = qu, data = dataf)
# Look at what happens along x: clearly there is non linear pattern here
cqcheck(obj = fit, v = c("x"), X = dataf, y = y)
#### Add a smooth for x
fit <- qgam(y \sim s(x)), qu = qu, data = dataf)
cqcheck(obj = fit, v = c("x"), X = dataf, y = y) # Better!
```

```
# Lets look across x and z. As we move along z (x2 in the plot)
# the colour changes from green to red
cqcheck(obj = fit, v = c("x", "z"), X = dataf, y = y, nbin = c(5, 5))
# The effect look pretty linear
cqcheck(obj = fit, v = c("z"), X = dataf, y = y, nbin = c(10))
#### Lets add a linear effect for z
fit <- qgam(y \sim s(x)+z, qu = qu, data = dataf)
# Looks better!
cqcheck(obj = fit, v = c("z"))
# Lets look across x and y again: green prevails on the top-left to bottom-right
# diagonal, while the other diagonal is mainly red.
cqcheck(obj = fit, v = c("x", "z"), nbin = c(5, 5))
### Maybe adding an interaction would help?
fit <- qgam(y \sim s(x) + z + I(x \times z), qu = qu, data = dataf)
# It does! The real model is: y ~ 1 + x + x^2 + z + x*z/2 + e, e ~ N(0, 1)
cqcheck(obj = fit, v = c("x", "z"), nbin = c(5, 5))
## End(Not run)
```

cqcheckI

Interactive visual checks for additive quantile fits

Description

Given an additive quantile model, fitted using qgam, cqcheck2DI provides some interactive 2D plots that allow to check what proportion of responses, y, falls below the fitted quantile. This is an interactive version of the cqcheck function.

Usage

```
cqcheckI(
   obj,
   v,
   X = NULL,
   y = NULL,
   run = TRUE,
   width = "100%",
   height = "680px"
)
```

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cqcheckI

Arguments

| obj | the output of a qgam call. |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| v | if a 1D plot is required, v should be either a single character or a numeric vector. In the first case v should be the names of one of the variables in the dataframe X. In the second case, the length of v should be equal to the number of rows of X. If a 2D plot is required, v should be either a vector of two characters or a matrix with two columns. |
| X | a dataframe containing the data used to obtain the conditional quantiles. By default it is NULL, in which case predictions are made using the model matrix in obj\$model. |
| У | vector of responses. Its i-th entry corresponds to the i-th row of X. By default it is NULL, in which case it is internally set to obj\$y. |
| run | if TRUE (default) the function produces an interactive plot, otherwise it returns the corresponding shiny app. |
| width | the width of the main plot. Default is "100%". |
| height | width the width of the main plot. Default is "680px". |

Details

This is an interactive version of the cqcheck, see ?cqcheck for details. The main interactive feature is that one can select an area by brushing, and then double-click to zoom in. In the 1D case the vertical part of the selected area is not use: we zoom only along the x axis. Double-clicking without brushing zooms out.

Value

Simply produces an interactive plot.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

Examples

```
## Not run:
#######
# Example 1: Bivariate additive model y~1+x+x^2+z+x*z/2+e, e~N(0, 1)
#######
library(qgam)
set.seed(15560)
n <- 1000
x <- rnorm(n, 0, 1); z <- rnorm(n)
X <- cbind(1, x, x^2, z, x*z)
beta <- c(0, 1, 1, 1, 0.5)
y <- drop(X %*% beta) + rnorm(n)
dataf <- data.frame(cbind(y, x, z))
names(dataf) <- c("y", "x", "z")</pre>
```

```
#### Fit a constant model for median
qu <- 0.5
fit <- qgam(y~1, qu = qu, data = dataf)</pre>
# Look at what happens along x: clearly there is non linear pattern here
cqcheckI(obj = fit, v = c("x"), X = dataf, y = y)
#### Add a smooth for x
fit <- qgam(y~s(x), qu = qu, data = dataf)</pre>
cqcheckI(obj = fit, v = c("x"), X = dataf, y = y) # Better!
# Lets look across across x and z. As we move along z (x2 in the plot)
# the colour changes from green to red
cqcheckI(obj = fit, v = c("x", "z"), X = dataf, y = y)
# The effect look pretty linear
cqcheckI(obj = fit, v = c("z"), X = dataf, y = y)
#### Lets add a linear effect for z
fit <- qgam(y \sim s(x)+z, qu = qu, data = dataf)
# Looks better!
cqcheckI(obj = fit, v = c("z"))
# Lets look across x and y again: green prevails on the top-left to bottom-right
# diagonal, while the other diagonal is mainly red.
cqcheckI(obj = fit, v = c("x", "z"))
### Maybe adding an interaction would help?
fit <- qgam(y \sim s(x)+z+I(x*z), qu = qu, data = dataf)
# It does! The real model is: y ~ 1 + x + x^2 + z + x*z/2 + e, e ~ N(0, 1)
cqcheckI(obj = fit, v = c("x", "z"))
## End(Not run)
```

elf

Extended log-F model with fixed scale

Description

The elf family implements the Extended log-F density of Fasiolo et al. (2017) and it is supposed to work in conjuction with the extended GAM methods of Wood et al. (2017), implemented by mgcv. It differs from the elflss family, because here the scale of the density (sigma, aka the learning rate) is a single scalar, while in elflss it can depend on the covariates. At the moment the family is mainly intended for internal use, use the qgam function to fit quantile GAMs based on ELF.

Usage

```
elf(theta = NULL, link = "identity", qu, co)
```

Arguments

| theta | a scalar representing the log-scale log(sigma). |
|-------|----------------------------------------------------------------------------------------------------------------------|
| link | the link function between the linear predictor and the quantile location. |
| qu | parameter in $(0, 1)$ representing the chosen quantile. For instance, to fit the median choose qu=0.5. |
| со | positive constant used to determine parameter lambda of the ELF density (lambda = co / sigma). Can be vector valued. |

Details

This function is meant for internal use only.

Value

An object inheriting from mgcv's class extended.family.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com> and Simon N. Wood.

References

Fasiolo, M., Wood, S.N., Zaffran, M., Nedellec, R. and Goude, Y., 2020. Fast calibrated additive quantile regression. Journal of the American Statistical Association (to appear). https://www.tandfonline.com/doi/full/10.1080/01621459.2020.1725521.

Wood, Simon N., Pya, N. and Safken, B. (2017). Smoothing parameter and model selection for general smooth models. Journal of the American Statistical Association.

Examples

elflss

Description

The elflss family implements the Extended log-F (ELF) density of Fasiolo et al. (2017) and it is supposed to work in conjuction with the general GAM fitting methods of Wood et al. (2017), implemented by mgcv. It differs from the elf family, because here the scale of the density (sigma, aka the learning rate) can depend of the covariates, while in while in elf it is a single scalar. NB this function was use within the qgam function, but since qgam version 1.3 quantile models with varying learning rate are fitted using different methods (a parametric location-scale model, see Fasiolo et al. (2017) for details.).

Usage

```
elflss(link = list("identity", "log"), qu, co, theta, remInter = TRUE)
```

Arguments

| link | vector of two characters indicating the link function for the quantile location and for the log-scale. |
|----------|-----------------------------------------------------------------------------------------------------------|
| qu | parameter in $(0, 1)$ representing the chosen quantile. For instance, to fit the median choose qu=0.5. |
| со | positive vector of constants used to determine parameter lambda of the ELF density (lambda = co / sigma). |
| theta | a scalar representing the intercept of the model for the log-scale log(sigma). |
| remInter | if TRUE the intercept of the log-scale model is removed. |

Details

This function is meant for internal use only.

Value

An object inheriting from mgcv's class general.family.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com> and Simon N. Wood.

References

Fasiolo, M., Wood, S.N., Zaffran, M., Nedellec, R. and Goude, Y., 2020. Fast calibrated additive quantile regression. Journal of the American Statistical Association (to appear). https://www.tandfonline.com/doi/full/10.1080/01621459.2020.1725521.

Wood, Simon N., Pya, N. and Safken, B. (2017). Smoothing parameter and model selection for general smooth models. Journal of the American Statistical Association.

log1pexp

Examples

```
## Not run:
set.seed(651)
n <- 1000
x \le seq(-4, 3, length.out = n)
X <- cbind(1, x, x^2)
beta <- c(0, 1, 1)
sigma = 1.2 + sin(2*x)
f <- drop(X %*% beta)</pre>
dat <- f + rnorm(n, 0, sigma)</pre>
dataf <- data.frame(cbind(dat, x))</pre>
names(dataf) <- c("y", "x")</pre>
# Fit median using elflss directly: NOT RECOMMENDED
fit <- gam(list(y~s(x, bs = "cr"), ~ s(x, bs = "cr")),</pre>
            family = elflss(theta = 0, co = rep(0.2, n), qu = 0.5),
           data = dataf)
plot(x, dat, col = "grey", ylab = "y")
tmp <- predict(fit, se = TRUE)</pre>
lines(x, tmp$fit[ , 1])
lines(x, tmp$fit[ , 1] + 3 * tmp$se.fit[ , 1], col = 2)
lines(x, tmp$fit[, 1] - 3 * tmp$se.fit[, 1], col = 2)
## End(Not run)
```

log1pexp

Calculating log(1+exp(x)) accurately

Description

Calculates log(1+exp(x)) in a numerically stable fashion.

Usage

log1pexp(x)

Arguments

x a numeric vector.

Details

We follow the recipe of Machler (2012), that is formula (10) page 7.

Value

A numeric vector where the i-th entry is equal to log(1+exp(x[i])), but computed more stably.

mqgam

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

References

Machler, M. (2012). Accurately computing log(1-exp(-lal)). URL: https://cran.r-project. org/package=Rmpfr/vignettes/log1mexp-note.pdf.

Examples

```
set.seed(141)
library(qgam);
x <- rnorm(100, 0, 100)
log1pexp(x) - log1p(exp(x))</pre>
```

```
mqgam
```

Fit multiple smooth additive quantile regression models

Description

This function fits a smooth additive regression model to several quantiles.

Usage

```
mqgam(
  form,
  data,
  qu,
  lsig = NULL,
  err = NULL,
  multicore = !is.null(cluster),
  cluster = NULL,
  ncores = detectCores() - 1,
  paropts = list(),
  control = list(),
  argGam = NULL
)
```

Arguments

| form | A GAM formula, or a list of formulae. See ?mgcv::gam details. |
|------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| data | A data frame or list containing the model response variable and covariates re- quired by the formula. By default the variables are taken from environment(formula): typically the environment from which gam is called. |
| qu | A vectors of quantiles of interest. Each entry should be in $(0, 1)$. |

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| lsig | The value of the log learning rate used to create the Gibbs posterior. By defauls lsig=NULL and this parameter is estimated by posterior calibration described in Fasiolo et al. (2017). Obviously, the function is much faster if the user provides a value. |
|-----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| err | An upper bound on the error of the estimated quantile curve. Should be in $(0, 1)$. If it is a vector, it should be of the same length of qu. Since qgam v1.3 it is selected automatically, using the methods of Fasiolo et al. (2017). The old default was err=0.05. |
| multicore | If TRUE the calibration will happen in parallel. |
| cluster | An object of class c("SOCKcluster", "cluster"). This allowes the user to pass her own cluster, which will be used if multicore == TRUE. The user has to remember to stop the cluster. |
| ncores | Number of cores used. Relevant if multicore == TRUE. |
| paropts | a list of additional options passed into the foreach function when parallel compu- tation is enabled. This is important if (for example) your code relies on external data or packages: use the .export and .packages arguments to supply them so that all cluster nodes have the correct environment set up for computing. |
| control | A list of control parameters. The only one relevant here is link, which is the link function used (see ?elf and ?elflss for defaults). All other control parameters are used by tuneLearnFast. See ?tuneLearnFast for details. |
| argGam | A list of parameters to be passed to $mgcv::gam$. This list can potentially include all the arguments listed in ?gam, with the exception of formula, family and data. |

Value

A list with entries:

- fit = a gamObject, one for each entry of qu. Notice that the slots model and smooth of each object has been removed to save memory. See ?gamObject.
- model = the model slot of the gamObjects in the fit slot. This is the same for every fit, hence only one copy is stored.
- smooth = the smooth slot of the gamObjects in the fit slot. This is the same for every fit, hence only one copy is stored.
- calibr = a list which is the output of an internal call to tuneLearnFast, which is used for calibrating the learning rate. See ?tuneLearnFast for details.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

References

Fasiolo, M., Wood, S.N., Zaffran, M., Nedellec, R. and Goude, Y., 2020. Fast calibrated additive quantile regression. Journal of the American Statistical Association (to appear). https://www.tandfonline.com/doi/full/10.1080/01621459.2020.1725521.

Fasiolo, M., Wood, S.N., Zaffran, M., Nedellec, R. and Goude, Y., 2021. qgam: Bayesian Nonparametric Quantile Regression Modeling in R. Journal of Statistical Software, 100(9), 1-31, doi: 10.18637/ jss.v100.i09.

Examples

```
#####
# Multivariate Gaussian example
####
library(qgam)
set.seed(2)
dat <- gamSim(1, n=300, dist="normal", scale=2)</pre>
fit <- mqgam(y~s(x0)+s(x1)+s(x2)+s(x3), data=dat, qu = c(0.2, 0.8))</pre>
invisible( qdo(fit, 0.2, plot, pages = 1) )
#####
# Univariate "car" example
####
library(qgam); library(MASS)
# Fit for quantile 0.8 using the best sigma
quSeq <- c(0.2, 0.4, 0.6, 0.8)
set.seed(6436)
fit <- mqgam(accel~s(times, k=20, bs="ad"), data = mcycle, qu = quSeq)</pre>
# Plot the fit
xSeq <- data.frame(cbind("accel" = rep(0, 1e3), "times" = seq(2, 58, length.out = 1e3)))</pre>
plot(mcycle$times, mcycle$accel, xlab = "Times", ylab = "Acceleration", ylim = c(-150, 80))
for(iq in quSeq){
  pred <- qdo(fit, iq, predict, newdata = xSeq)</pre>
  lines(xSeq$times, pred, col = 2)
}
```

pinLoss

Pinball loss function

Description

Evaluates the pinball loss.

Usage

pinLoss(y, mu, qu, add = TRUE)

Arguments

| У | points at which the loss is evaluated. |
|-----|--------------------------------------------------------------|
| mu | location parameter of the pinball loss. |
| qu | quantile level of the loss. |
| add | if TRUE the losses at which quantile level will be added up. |

Value

A numeric vector or matrix of evaluate losses.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

Examples

```
n <- 1000
x <- seq(0, 4, length.out = n)
plot(x, pinLoss(x, rep(2, n), qu = 0.9, add = FALSE), type = 'l', ylab = "loss")</pre>
```

qdo

Manipulating the output of mqgam

Description

Contrary to qgam, mqgam does not output a standard gamObject, hence methods such as predict.gam or plot.gam cannot be used directly. qdo provides a simple wrapper for such methods.

Usage

qdo(obj, qu = NULL, fun = I, ...)

Arguments

| obj | the output of a mqgam call. |
|-----|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| qu | A vector whose elements must be in (0, 1). Each element indicates a quantile of interest, which should be an element of names(obj\$fit). If left to NULL the function fun will be applied to each of the quantile fits in obj. |
| fun | The method or function that we want to use on the gamObject corresponding to quantile qu. For instance predict, plot or summary. By default this is the identity function (I), which means that the fitted model for quantile qu is returned. |
| | Additional arguments to be passed to fun. |

Value

A list where the i-th entry is the output of fun (whatever that is) corresponding to quantile qu[i].

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

Examples

```
library(qgam); library(MASS)
quSeq <- c(0.4, 0.6)
set.seed(737)
fit <- mqgam(accel~s(times, k=20, bs="ad"), data = mcycle, qu = quSeq)
qdo(fit, 0.4, summary)
invisible(qdo(fit, 0.4, plot, pages = 1))
# Return the object for qu = 0.6 and then plot it
tmp <- qdo(fit, 0.6)
plot(tmp)</pre>
```

| q | ga | m |
|---|----|---|

Fit a smooth additive quantile regression model

Description

This function fits a smooth additive regression model for a single quantile.

Usage

```
qgam(
  form,
  data,
  qu,
  lsig = NULL,
  err = NULL,
  multicore = !is.null(cluster),
  cluster = NULL,
  ncores = detectCores() - 1,
  paropts = list(),
  control = list(),
  argGam = NULL
)
```

qgam

Arguments

| form | A GAM formula, or a list of formulae. See ?mgcv::gam details. |
|-----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| data | A data frame or list containing the model response variable and covariates re- quired by the formula. By default the variables are taken from environment(formula): typically the environment from which gam is called. |
| qu | The quantile of interest. Should be in $(0, 1)$. |
| lsig | The value of the log learning rate used to create the Gibbs posterior. By defauls lsig=NULL and this parameter is estimated by posterior calibration described in Fasiolo et al. (2017). Obviously, the function is much faster if the user provides a value. |
| err | An upper bound on the error of the estimated quantile curve. Should be in $(0, 1)$. Since qgam v1.3 it is selected automatically, using the methods of Fasiolo et al. (2017). The old default was err=0.05. |
| multicore | If TRUE the calibration will happen in parallel. |
| cluster | An object of class c("SOCKcluster", "cluster"). This allowes the user to pass her own cluster, which will be used if multicore == TRUE. The user has to remember to stop the cluster. |
| ncores | Number of cores used. Relevant if multicore == TRUE. |
| paropts | a list of additional options passed into the foreach function when parallel compu- tation is enabled. This is important if (for example) your code relies on external data or packages: use the .export and .packages arguments to supply them so that all cluster nodes have the correct environment set up for computing. |
| control | A list of control parameters. The only one relevant here is link, which is the link function used (see ?elf and ?elflss for defaults). All other control parameters are used by tuneLearnFast. See ?tuneLearnFast for details. |
| argGam | A list of parameters to be passed to mgcv::gam. This list can potentially include all the arguments listed in ?gam, with the exception of formula, family and data. |

Value

A gamObject. See ?gamObject.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

References

Fasiolo, M., Wood, S.N., Zaffran, M., Nedellec, R. and Goude, Y., 2020. Fast calibrated additive quantile regression. Journal of the American Statistical Association (to appear). https://www.tandfonline.com/doi/full/10.1080/01621459.2020.1725521.

Fasiolo, M., Wood, S.N., Zaffran, M., Nedellec, R. and Goude, Y., 2021. qgam: Bayesian Nonparametric Quantile Regression Modeling in R. Journal of Statistical Software, 100(9), 1-31, doi: 10.18637/ jss.v100.i09.

Examples

```
#####
# Univariate "car" example
####
library(qgam); library(MASS)
# Fit for quantile 0.5 using the best sigma
set.seed(6436)
fit <- qgam(accel~s(times, k=20, bs="ad"), data = mcycle, qu = 0.5)</pre>
# Plot the fit
xSeq <- data.frame(cbind("accel" = rep(0, 1e3), "times" = seq(2, 58, length.out = 1e3)))</pre>
pred <- predict(fit, newdata = xSeq, se=TRUE)</pre>
plot(mcycle$times, mcycle$accel, xlab = "Times", ylab = "Acceleration", ylim = c(-150, 80))
lines(xSeq$times, pred$fit, lwd = 1)
lines(xSeq$times, pred$fit + 2*pred$se.fit, lwd = 1, col = 2)
lines(xSeq$times, pred$fit - 2*pred$se.fit, lwd = 1, col = 2)
## Not run:
# You can get a better fit by letting the learning rate change with "accel"
# For instance
fit <- qgam(list(accel ~ s(times, k=20, bs="ad"), ~ s(times)),</pre>
           data = mcycle, qu = 0.8)
pred <- predict(fit, newdata = xSeq, se=TRUE)</pre>
plot(mcycle$times, mcycle$accel, xlab = "Times", ylab = "Acceleration", ylim = c(-150, 80))
lines(xSeg$times, pred$fit, lwd = 1)
lines(xSeq$times, pred$fit + 2*pred$se.fit, lwd = 1, col = 2)
lines(xSeq$times, pred$fit - 2*pred$se.fit, lwd = 1, col = 2)
## End(Not run)
#####
# Multivariate Gaussian example
####
library(qgam)
set.seed(2)
dat <- gamSim(1,n=400,dist="normal",scale=2)</pre>
fit <- ggam(y \sim s(x0) + s(x1) + s(x2) + s(x3)), data=dat, qu = 0.5)
plot(fit, scale = FALSE, pages = 1)
######
# Heteroscedastic example
######
## Not run:
set.seed(651)
n <- 2000
x \le seq(-4, 3, length.out = n)
X <- cbind(1, x, x^2)
beta <- c(0, 1, 1)
sigma = 1.2 + sin(2*x)
```

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sigmoid

sigmoid

Sigmoid function and its derivatives

Description

Calculates the sigmoid function and its derivatives.

Usage

sigmoid(y, deriv = FALSE)

Arguments

| У | a numeric vector. |
|-------|------------------------------------------------------------------------------------|
| deriv | if TRUE alse the first three derivatives of the sigmoid function will be computed. |

Value

If deriv==FALSE, it returns a numeric vector equal to 1/(1+exp(-x)). If deriv==TRUE it returns a list where the slot \$D0 contains 1/(1+exp(-x)), while \$D1, \$D2 and \$D3 contain its first three derivatives.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

Examples

```
library(qgam)
set.seed(90)
h <- 1e-6
p <- rnorm(1e4, 0, 1e6)
sigmoid(p[1:50]) - 1/(1+exp(-p[1:50]))
###### Testing sigmoid derivatives
e1 <- abs((sigmoid(p+h) - sigmoid(p-h)) / (2*h) - sigmoid(p, TRUE)[["D1"]]) / (2*h)
e2 <- abs((sigmoid(p+h, TRUE)$D1 - sigmoid(p-h, TRUE)$D1) /
        (2*h) - sigmoid(p, TRUE)[["D2"]]) / (2*h)
e3 <- abs((sigmoid(p+h, TRUE)$D2 - sigmoid(p-h, TRUE)$D2) /
        (2*h) - sigmoid(p, TRUE)[["D3"]]) / (2*h)
if( any(c(e1, e2, e3) > 1) ) stop("Sigmoid derivatives are not estimated accurately")
```

tuneLearn

Tuning the learning rate for Gibbs posterior

Description

The learning rate (sigma) of the Gibbs posterior is tuned either by calibrating the credible intervals for the fitted curve, or by minimizing the pinball loss on out-of-sample data. This is done by bootrapping or by k-fold cross-validation. Here the calibration loss function is evaluated on a grid of values provided by the user.

Usage

```
tuneLearn(
  form,
  data,
  lsig,
  qu,
  err = NULL,
  multicore = !is.null(cluster),
  cluster = NULL,
  ncores = detectCores() - 1,
  paropts = list(),
  control = list(),
  argGam = NULL
}
```

)

Arguments

form

A GAM formula, or a list of formulae. See ?mgcv::gam details.

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| data | A data frame or list containing the model response variable and covariates re- quired by the formula. By default the variables are taken from environment(formula): typically the environment from which gam is called. |
|-----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| lsig | A vector of value of the log learning rate (log(sigma)) over which the calibration loss function is evaluated. |
| qu | The quantile of interest. Should be in $(0, 1)$. |
| err | An upper bound on the error of the estimated quantile curve. Should be in $(0, 1)$. Since qgam v1.3 it is selected automatically, using the methods of Fasiolo et al. (2017). The old default was err=0.05. |
| multicore | If TRUE the calibration will happen in parallel. |
| cluster | An object of class c("SOCKcluster", "cluster"). This allowes the user to pass her own cluster, which will be used if multicore == TRUE. The user has to remember to stop the cluster. |
| ncores | Number of cores used. Relevant if multicore == TRUE. |
| paropts | a list of additional options passed into the foreach function when parallel compu- tation is enabled. This is important if (for example) your code relies on external data or packages: use the .export and .packages arguments to supply them so that all cluster nodes have the correct environment set up for computing. |
| control | A list of control parameters for tuneLearn with entries: |
| | • loss = loss function use to tune log(sigma). If loss=="cal" is chosen, then log(sigma) is chosen so that credible intervals for the fitted curve are calibrated. See Fasiolo et al. (2017) for details. If loss=="pin" then log(sigma) approximately minimizes the pinball loss on the out-of-sample data. |
| | sam = sampling scheme use: sam=="boot" corresponds to bootstrapping and sam=="kfold" to k-fold cross-validation. The second option can be used only if ctrl\$loss=="pin". |
| | K = if sam=="boot" this is the number of boostrap datasets, while if sam=="kfold" this is the number of folds. By default K=50. |
| | • b = offset parameter used by the mgcv::gauslss. By default b=0. |
| | vtype = type of variance estimator used to standardize the deviation from the main fit in the calibration. If set to "m" the variance estimate obtained by the full data fit is used, if set to "b" than the variance estimated produced by the bootstrap fits are used. By default vtype="m". |
| | epsB = positive tolerance used to assess convergence when fitting the re- gression coefficients on bootstrap data. In particular, if dev-dev_old /(dev +0.1)<epsb then convergence is achieved. Default is epsB=1e-5.</epsb |
| | • verbose = if TRUE some more details are given. By default verbose=FALSE. |
| | • link = link function to be used. See ?elf and ?elflss for defaults. |
| | progress = argument passed to plyr::llply. By default progress="text" so that progress is reported. Set it to "none" to avoid it. |
| argGam | A list of parameters to be passed to $mgcv::gam$. This list can potentially include all the arguments listed in ?gam, with the exception of formula, family and data. |

Value

A list with entries:

- lsig = the value of log(sigma) resulting in the lowest loss.
- loss = vector containing the value of the calibration loss function corresponding to each value of log(sigma).
- edf = a matrix where the first colums contain the log(sigma) sequence, and the remaining columns contain the corresponding effective degrees of freedom of each smooth.
- convProb = a logical vector indicating, for each value of log(sigma), whether the outer optimization which estimates the smoothing parameters has encountered convergence issues.
 FALSE means no problem.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

References

Fasiolo, M., Wood, S.N., Zaffran, M., Nedellec, R. and Goude, Y., 2020. Fast calibrated additive quantile regression. Journal of the American Statistical Association (to appear). https://www.tandfonline.com/doi/full/10.1080/01621459.2020.1725521.

Examples

```
library(qgam); library(MASS)
# Calibrate learning rate on a grid
set.seed(41444)
sigSeq <- seq(1.5, 5, length.out = 10)
closs <- tuneLearn(form = accel~s(times,k=20,bs="ad"),</pre>
                    data = mcycle,
                    lsig = sigSeq,
                    qu = 0.5)
plot(sigSeq, closs$loss, type = "b", ylab = "Calibration Loss", xlab = "log(sigma)")
# Pick best log-sigma
best <- sigSeq[ which.min(closs$loss) ]</pre>
abline(v = best, lty = 2)
# Fit using the best sigma
fit <- qgam(accel~s(times,k=20,bs="ad"), data = mcycle, qu = 0.5, lsig = best)</pre>
summary(fit)
pred <- predict(fit, se=TRUE)</pre>
plot(mcycle$times, mcycle$accel, xlab = "Times", ylab = "Acceleration",
     ylim = c(-150, 80))
lines(mcycle$times, pred$fit, lwd = 1)
lines(mcycle$times, pred$fit + 2*pred$se.fit, lwd = 1, col = 2)
lines(mcycle$times, pred$fit - 2*pred$se.fit, lwd = 1, col = 2)
```

tuneLearnFast

Description

The learning rate (sigma) of the Gibbs posterior is tuned either by calibrating the credible intervals for the fitted curve, or by minimizing the pinball loss on out-of-sample data. This is done by bootrapping or by k-fold cross-validation. Here the loss function is minimized, for each quantile, using a Brent search.

Usage

```
tuneLearnFast(
  form,
  data,
  qu,
  err = NULL,
  multicore = !is.null(cluster),
  cluster = NULL,
  ncores = detectCores() - 1,
  paropts = list(),
  control = list(),
  argGam = NULL
)
```

Arguments

| form | A GAM formula, or a list of formulae. See ?mgcv::gam details. |
|-----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| data | A data frame or list containing the model response variable and covariates re- quired by the formula. By default the variables are taken from environment(formula): typically the environment from which gam is called. |
| qu | The quantile of interest. Should be in $(0, 1)$. |
| err | An upper bound on the error of the estimated quantile curve. Should be in $(0, 1)$. Since qgam v1.3 it is selected automatically, using the methods of Fasiolo et al. (2017). The old default was err=0.05. |
| multicore | If TRUE the calibration will happen in parallel. |
| cluster | An object of class c("SOCKcluster", "cluster"). This allowes the user to pass her own cluster, which will be used if multicore == TRUE. The user has to remember to stop the cluster. |
| ncores | Number of cores used. Relevant if multicore == TRUE. |
| paropts | a list of additional options passed into the foreach function when parallel compu- tation is enabled. This is important if (for example) your code relies on external data or packages: use the .export and .packages arguments to supply them so that all cluster nodes have the correct environment set up for computing. |
| control | A list of control parameters for tuneLearn with entries: |

- loss = loss function use to tune log(sigma). If loss=="cal" is chosen, then log(sigma) is chosen so that credible intervals for the fitted curve are calibrated. See Fasiolo et al. (2017) for details. If loss=="pin" then log(sigma) approximately minimizes the pinball loss on the out-of-sample data.
- sam = sampling scheme use: sam=="boot" corresponds to bootstrapping and sam=="kfold" to k-fold cross-validation. The second option can be used only if ctrl\$loss=="pin".
- vtype = type of variance estimator used to standardize the deviation from the main fit in the calibration. If set to "m" the variance estimate obtained by the full data fit is used, if set to "b" than the variance estimated produced by the bootstrap fits are used. By default vtype="m".
- epsB = positive tolerance used to assess convergence when fitting the regression coefficients on bootstrap data. In particular, if |dev-dev_old|/(|dev|+0.1)<epsB then convergence is achieved. Default is epsB=1e-5.
- K = if sam=="boot" this is the number of boostrap datasets, while if sam=="kfold" this is the number of folds. By default K=50.
- init = an initial value for the log learning rate (log(sigma)). By default init=NULL and the optimization is initialized by other means.
- brac = initial bracket for Brent method. By default brac=log(c(0.5,2)), so the initial search range is (init + log(0.5), init + log(2)).
- tol = tolerance used in the Brent search. By default tol=.Machine\$double.eps^0.25.
 See ?optimize for details.
- aTol = Brent search parameter. If the solution to a Brent get closer than aTol * abs(diff(brac)) to one of the extremes of the bracket, the optimization is stop and restarted with an enlarged and shifted bracket. aTol=0.05 should be > 0 and values > 0.1 don't quite make sense. By default aTol=0.05.
- redWd = parameter which determines when the bracket will be reduced. If redWd==10 then the bracket is halved if the nearest solution falls within the central 10% of the bracket's width. By default redWd = 10.
- b = offset parameter used by the mgcv::gauslss, which we estimate to initialize the quantile fit (when a variance model is used). By default b=0.
- link = Link function to be used. See ?elf and ?elflss for defaults.
- verbose = if TRUE some more details are given. By default verbose=FALSE.
- progress = if TRUE progress in learning rate estimation is reported via printed text. TRUE by default.

A list of parameters to be passed to mgcv::gam. This list can potentially include all the arguments listed in ?gam, with the exception of formula, family and data.

Value

A list with entries:

• lsig = a vector containing the values of log(sigma) that minimize the loss function, for each quantile.

tuneLearnFast

- err = the error bound used for each quantile. Generally each entry is identical to the argument err, but in some cases the function increases it to enhance stabily.
- ranges = the search ranges by the Brent algorithm to find log-sigma, for each quantile.
- store = a list, where the i-th entry is a matrix containing all the locations (1st row) at which the loss function has been evaluated and its value (2nd row), for the i-th quantile.

Author(s)

Matteo Fasiolo <matteo.fasiolo@gmail.com>.

References

Fasiolo, M., Wood, S.N., Zaffran, M., Nedellec, R. and Goude, Y., 2020. Fast calibrated additive quantile regression. Journal of the American Statistical Association (to appear). https://www.tandfonline.com/doi/full/10.1080/01621459.2020.1725521.

Examples

```
library(qgam); library(MASS)
###
# Single quantile fit
###
# Calibrate learning rate on a grid
set.seed(5235)
tun <- tuneLearnFast(form = accel~s(times,k=20,bs="ad"),</pre>
                     data = mcycle,
                      qu = 0.2)
# Fit for quantile 0.2 using the best sigma
fit <- qgam(accel~s(times, k=20, bs="ad"), data = mcycle, qu = 0.2, lsig = tun$lsig)
pred <- predict(fit, se=TRUE)</pre>
plot(mcycle$times, mcycle$accel, xlab = "Times", ylab = "Acceleration",
     ylim = c(-150, 80))
lines(mcycle$times, pred$fit, lwd = 1)
lines(mcycle$times, pred$fit + 2*pred$se.fit, lwd = 1, col = 2)
lines(mcycle$times, pred$fit - 2*pred$se.fit, lwd = 1, col = 2)
###
# Multiple quantile fits
###
# Calibrate learning rate on a grid
quSeq <- c(0.25, 0.5, 0.75)
set.seed(5235)
tun <- tuneLearnFast(form = accel~s(times, k=20, bs="ad"),</pre>
                     data = mcycle,
                      qu = quSeq)
# Fit using estimated sigmas
fit <- mqgam(accel~s(times, k=20, bs="ad"), data = mcycle, qu = quSeq, lsig = tun$lsig)</pre>
```

```
# Plot fitted quantiles
plot(mcycle$times, mcycle$accel, xlab = "Times", ylab = "Acceleration",
     ylim = c(-150, 80))
for(iq in quSeq){
  pred <- qdo(fit, iq, predict)</pre>
  lines(mcycle$times, pred, col = 2)
}
## Not run:
# You can get a better fit by letting the learning rate change with "accel"
# For instance
tun <- tuneLearnFast(form = list(accel ~ s(times, k=20, bs="ad"), ~ s(times)),</pre>
                       data = mcycle,
                       qu = quSeq)
fit <- mqgam(list(accel ~ s(times, k=20, bs="ad"), ~ s(times)),</pre>
             data = mcycle, qu = quSeq, lsig = tun$lsig)
# Plot fitted quantiles
plot(mcycle$times, mcycle$accel, xlab = "Times", ylab = "Acceleration",
     ylim = c(-150, 80))
for(iq in quSeq){
  pred <- qdo(fit, iq, predict)</pre>
  lines(mcycle$times, pred, col = 2)
}
## End(Not run)
```

UKload

UK electricity load data

Description

Dataset on UK electricity demand, taken from the national grid (https://www.nationalgrid.com/).

Usage

data(UKload)

Format

UKload contains the following variables:

NetDemand net electricity demand between 11:30am and 12am.

wM instantaneous temperature, averaged over several English cities.

 wM_s95 exponential smooth of wM, that is $wM_s95[i] = a*wM_s95[i-1] + (1-a)*wM[i]$ with a=0.95.

UKload

Posan periodic index in [0,1] indicating the position along the year.
Dow factor variable indicating the day of the week.
Trend progressive counter, useful for defining the long term trend.
NetDemand.48 lagged version of NetDemand, that is NetDemand.48[i] = NetDemand[i-2].
Holy binary variable indicating holidays.
Year should be obvious.
Date should be obvious.

Details

See Fasiolo et al. (2017) for details.

Value

matrix of replicate data series

References

Fasiolo, M., Goude, Y., Nedellec, R. and Wood, S. N. (2017). Fast calibrated additive quantile regression. Available at https://arxiv.org/abs/1707.03307.

Examples

library(qgam)
data(UKload)
plot(UKload\$NetDemand, type = 'l')

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