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. (2017) <arXiv:1707.03307>. 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.

License GPL (>= 2)
Depends R (>= 3.5.0), mgcv (>= 1.8-28)
Imports shiny, plyr, doParallel, parallel, grDevices
Suggests knitr, rmarkdown, MASS, RhpcBLASctl, testthat
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R topics documented:

AUDem ................................................................. 2
Description

Data set on electricity demand from Sidney, Australia. The data has been downloaded from [https://www.ausgrid.com.au](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;
- **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)

---

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.
Author(s)
Matteo Fasiolo <matteo.fasiolo@gmail.com>.

References

Examples
library(qgam)
set.seed(525)
dat <- gamSim(1, n=200)
b <- tuneLearn(lsig = seq(-0.5, 1, length.out = 10),
    y~s(x0)+s(x1)+s(x2)+s(x3),
    data=dat, qu = 0.5)
check(b)

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


Examples

```r
library(qgam)
set.seed(525)
dat <- gamSim(1, n=200)
b <- tuneLearnFast(y ~ s(x0)+s(x1)+s(x2)+s(x3),
                   data = dat, qu = c(0.4, 0.5),
                   control = list("tol" = 0.05)) # <- sloppy tolerance to speed-up calibration
check(b)
check(b, 3) # Produces only third plot
```

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

```r
## S3 method for class 'qgam'
check(obj, nbin = 10, lev = 0.05, ...)
```
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 $|F(\hat{\mu}) - F(\mu_0)|$, 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


Examples

```r
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)
```
cqcheck 

Visually checking a fitted quantile model

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.

y 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().
Having fitted an additive model for, say, quantile \( q_u = 0.4 \) one would expect that about 40 responses fall below the fitted quantile. This function allows to visually compare the empirical number of responses (\( qu_{hat}[i] \)) 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 \( i \)th 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 \( qu_{hat}[i] < qu \) and in green otherwise. If \( qu_{hat}[i] \) falls outside the confidence intervals we put an * next to the numeric \( qu_{hat}[i] \) and we use more intense colours.

**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)
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")

### Fit a constant model for median
qu <- 0.5
fit <- qgam(y~1, 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~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))

#### Let's add a linear effect for z
fit <- qgam(y~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~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)
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, cqcheck2D 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

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

y   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")
#### Fit a constant model for median

```r
qu <- 0.5
fit <- qgam(y~1, qu = qu, data = dataf)
```

# Look at what happens along x: clearly there is non linear pattern here
```r
cqcheckI(obj = fit, v = c("x"), X = dataf, y = y)
```

#### Add a smooth for x

```r
fit <- qgam(y~s(x), qu = qu, data = dataf)
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
```r
cqcheckI(obj = fit, v = c("x", "z"), X = dataf, y = y)
```

# The effect look pretty linear
```r
cqcheckI(obj = fit, v = c("z"), X = dataf, y = y)
```

#### Lets add a linear effect for z

```r
fit <- qgam(y~s(x)+z, qu = qu, data = dataf)
```

# Looks better!
```r
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.
```r
cqcheckI(obj = fit, v = c("x", "z"))
```

### Maybe adding an interaction would help?

```r
fit <- qgam(y~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)
```r
cqcheckI(obj = fit, v = c("x", "z"))
```

### 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 conjunction 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**

```r
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 \( \text{qu}=0.5 \).
- **co**: positive constant used to determine parameter lambda of the ELF density (\( \lambda = \text{co} / \sigma \)). 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**


**Examples**

```r
library(qgam)
set.seed(2)
dat <- gamSim(1,n=400,dist="normal",scale=2)

# Fit median using elf directly: FAST BUT NOT RECOMMENDED
fit <- gam(y~s(x0)+s(x1)+s(x2)+s(x3),
           family = elf(co = 0.1, qu = 0.5), data = dat)
plot(fit, scale = FALSE, pages = 1)

# Using qgam: RECOMMENDED
fit <- qgam(y~s(x0)+s(x1)+s(x2)+s(x3), data=dat, qu = 0.8)
plot(fit, scale = FALSE, pages = 1)
```
elflss

Extended log-F model with variable scale

Description

The elflss family implements the Extended log-F (ELF) density of Fasiolo et al. (2017) and it is supposed to work in conjunction 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 on 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.
- `co`: 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


Examples

```r
## Not run:
set.seed(651)
n <- 1000
x <- 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)
dat <- f + rnorm(n, 0, sigma)
dataf <- data.frame(cbind(dat, x))
names(dataf) <- c("y", "x")

# Fit median using elflss directly: NOT RECOMMENDED
fit <- gam(list(y~s(x, bs = "cr"), ~ s(x, bs = "cr")),
           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)
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)
```

log1pexp

Calculating \( \log(1+\exp(x)) \) accurately

Description

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

Usage

```r
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

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).

Examples

set.seed(141)
library(qgam);
x <- rnorm(100, 0, 100)
log1pexp(x) - log1p(exp(x))
**mqgam**

lsig  
The value of the log learning rate used to create the Gibbs posterior. By defaults \( \text{lsig} = \text{NULL} \) 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 \( \text{qu} \). Since qgam v1.3 it is selected automatically, using the methods of Fasiolo et al. (2017). The old default was \( \text{err} = 0.05 \).

multicore  
If \text{TRUE} the calibration will happen in parallel.

cluster  
An object of class \text{c("SOCKcluster","cluster")}. This allows the user to pass her own cluster, which will be used if \text{multicore} == \text{TRUE}. The user has to remember to stop the cluster.

ncores  
Number of cores used. Relevant if \text{multicore} == \text{TRUE}.

paropts  
a list of additional options passed into the foreach function when parallel computation 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 \text{link}, which is the link function used (see ?elf and ?elflss for defaults). All other control parameters are used by \text{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:

- \text{fit} = a \text{gamObject}, one for each entry of \text{qu}. Notice that the slots model and smooth of each object has been removed to save memory. See ?gamObject.

- \text{model} = the \text{model} slot of the \text{gamObjects} in the \text{fit} slot. This is the same for every fit, hence only one copy is stored.

- \text{smooth} = the \text{smooth} slot of the \text{gamObjects} in the \text{fit} slot. This is the same for every fit, hence only one copy is stored.

- \text{calibr} = a list which is the output of an internal call to \text{tuneLearnFast}, which is used for calibrating the learning rate. See ?tuneLearnFast for details.

**Author(s)**

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

**References**

Examples

#####
# Multivariate Gaussian example
#####
library(qgam)
set.seed(2)
dat <- gamSim(1, n=300, dist="normal", scale=2)

fit <- mqgam(y~s(x0)+s(x1)+s(x2)+s(x3), data=dat, qu = c(0.2, 0.8))
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)

# Plot the fit
xSeq <- data.frame(cbind("accel" = rep(0, 1e3), "times" = seq(2, 58, length.out = 1e3)))
plot(mcycle$times, mcycle$accel, xlab = "Times", ylab = "Acceleration", ylim = c(-150, 80))
for(iq in quSeq){
  pred <- qdo(fit, iq, predict, newdata = xSeq)
  lines(xSeq$times, pred, col = 2)
}

---

pinLoss

Pinball loss function

Description

Evaluates the pinball loss.

Usage

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

Arguments

y 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.
qdo

Value

A numeric vector or matrix of evaluate losses.

Author(s)

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

Examples

```r
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")
```

---

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

```r
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

```r
library(qgam); library(MASS)

quSeq <- c(0.4, 0.6)
set.seed(737)
fit <- mqgam(accels~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)
```

---

**qgam**  
*Fit a smooth additive quantile regression model*

---

**Description**

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

**Usage**

```r
qgam(
  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 required 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).
The value of the log learning rate used to create the Gibbs posterior. By default
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.

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.

If TRUE the calibration will happen in parallel.

An object of class c("SOCKcluster","cluster"). This allows the user to pass her own cluster, which will be used if multicore == TRUE. The user has to remember to stop the cluster.

Number of cores used. Relevant if multicore == TRUE.

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.

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.

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.

A gamObject. See ?gamObject.

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


# Univariate "car" example
library(qgam); library(MASS)

# Fit for quantile 0.5 using the best sigma
set.seed(6436)
fit <- qgam(accl~s(times, k=20, bs="ad"), data = mcycle, qu = 0.5)
# Plot the fit
xSeq <- data.frame(cbind("accel" = rep(0, 1e3), "times" = seq(2, 58, length.out = 1e3)))
pred <- predict(fit, newdata = xSeq, se=TRUE)
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)), data = mcycle, qu = 0.8)
pred <- predict(fit, newdata = xSeq, se=TRUE)
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)

## End(Not run)

#####
# Multivariate Gaussian example
#####
library(qgam)
set.seed(2)
dat <- gamSim(1,n=400,dist="normal",scale=2)
fit <- qgam(y~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 <- 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)
dat <- f + rnorm(n, 0, sigma)
dataf <- data.frame(cbind(dat, x))
names(dataf) <- c("y", "x")
fit <- qgam(list(y~s(x, k = 30, bs="cr"), ~ s(x, k = 30, bs = "cr")),
            data = dataf, qu = 0.95)
plot(x, dat, col = "grey", ylab = "y")
tmp <- predict(fit, se = TRUE)
lines(x, tmp$fit)
sigmoid

Sigmoid function and its derivatives

Description

Calculates the sigmoid function and its derivatives.

Usage

sigmoid(y, deriv = FALSE)

Arguments

y

a numeric vector.

deriv

if TRUE also 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 bootstrapping or by k-fold cross-validation. Here the calibration loss function is evaluated on a grid of values provided by the user.

**Usage**

```r
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.
- **data** A data frame or list containing the model response variable and covariates required 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 allows 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 computation 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 bootstrap datasets, while if `sam="kfold"` this is the number of folds. By default `K=50`.
- **b** = offset parameter used by the mgcv::gamlss. 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 regression coefficients on bootstrap data. In particular, if `|dev-dev_0ld|/(|dev|+0.1)<epsB` then convergence is achieved. Default is `epsB=1e-5`.
- **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 columns 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


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"),
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)]
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)
summary(fit)

pred <- predict(fit, se=TRUE)
plot(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)

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 bootstrapping or by k-fold cross-validation. Here the loss function is minimized, for each quantile, using a Brent search.

Usage

tuneLearnFast(form,
tuneLearnFast

```
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 required 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 allows 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 computation 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.
• \( K = \text{if } \text{sam}=="\text{boot}" \) this is the number of bootstrap datasets, while if \( \text{sam}=="\text{kfold}" \) this is the number of folds. By default \( K=50 \).

• \( \text{init} \) = an initial value for the log learning rate (\( \log(\sigma) \)). By default \( \text{init}=\text{NULL} \) and the optimization is initialized by other means.

• \( \text{brac} \) = initial bracket for Brent method. By default \( \text{brac}=\text{log}(c(0.5,2)) \), so the initial search range is \( (\text{init} + \text{log}(0.5),\text{init} + \text{log}(2)) \).

• \( \text{tol} \) = tolerance used in the Brent search. By default \( \text{tol}=.\text{Machine}\$\text{double.e}\text{ps}^0.25 \). See ?optimize for details.

• \( a\text{To}1 \) = Brent search parameter. If the solution to a Brent get closer than \( a\text{To}1 \times \text{abs}(\text{diff}(\text{brac})) \) to one of the extremes of the bracket, the optimization is stop and restarted with an enlarged and shifted bracket. \( a\text{To}1=0.05 \) should be \( >0 \) and values \( >0.1 \) don’t quite make sense. By default \( a\text{To}1=0.05 \).

• \( \text{redWd} \) = parameter which determines when the bracket will be reduced. If \( \text{redWd}=10 \) then the bracket is halved if the nearest solution falls within the central 10% of the bracket’s width. By default \( \text{redWd}=10 \).

• \( b \) = offset parameter used by the mgcv::gausslss, which we estimate to initialize the quantile fit (when a variance model is used). By default \( b=0 \).

• \( \text{link} \) = Link function to be used. See ?elf and ?elflss for defaults.

• \( \text{verbose} = \text{if } \text{TRUE } \) some more details are given. By default \( \text{verbose}=\text{FALSE} \).

• \( \text{progress} = \text{if } \text{TRUE } \) progress in learning rate estimation is reported via printed text. \( \text{TRUE} \) by default.

\texttt{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 \texttt{formula}, \texttt{family} and \texttt{data}.

\textbf{Value}

A list with entries:

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

• \( \text{err} \) = the error bound used for each quantile. Generally each entry is identical to the argument \texttt{err}, but in some cases the function increases it to enhance stably.

• \( \text{ranges} \) = the search ranges by the Brent algorithm to find \( \log-\sigma \), for each quantile.

• \( \text{store} \) = 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.

\textbf{Author(s)}

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

\textbf{References}

### Examples

```r
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"),
                      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$lsig)
pred <- predict(fit, se=TRUE)
plot(mcycle$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"),
                      data = mcycle,
                      qu = quSeq)

# Fit using estimated sigmas
fit <- mqgam(accel~s(times, k=20, bs="ad"), 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)
  lines(mcycle$times, pred, col = 2)
  }

## Not run:
# You can get a better fit by letting the learning rate change with "accel"
# For instance

# Calibrate learning rate on a grid
fit <- tuneLearnFast(form = list(accel ~ s(times, k=20, bs="ad"), ~ s(times)),
                      data = mcycle,
                      qu = quSeq)

# Fit using estimated sigmas
fit <- mqgam(list(accel ~ s(times, k=20, bs="ad"), ~ s(times)),
              data = mcycle, qu = quSeq, lsig = tun$lsig)
```
```r
# Plot fitted quantiles
plot(mcycle$times, mcycle$accel, xlab = "Times", ylab = "Acceleration",
ylim = c(-150, 80))
for(iq in quSeq){
  pred <- qdo(fit, iq, predict)
  lines(mcycle$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/](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 $w_{M_{s95}[i]} = a \cdot w_{M_{s95}[i-1]} + (1-a) \cdot w_{M[i]}$ with $a=0.95$.
- **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


Examples

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