Package 'cgaim'

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Title Constrained Groupwise Additive Index Models

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Description Fits constrained groupwise additive index models and provides functions for inference and interpretation of these models. The method is described in Masselot, Chebana, Campagna, Lavigne, Ouarda, Gosselin (2022) `Constrained groupwise additive index models' doi:10.1093/biostatistics/kxac023 .
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Boostrap CGAIM

Description

Generates bootstrap replicates of a cgaim object.

Usage

```
boot.cgaim(object, boot.type = c("residuals", "wild", "pairs"),
  bsamples = NULL, B = 100, l = 1, nc = 1)
```

Arguments

object	A cgaim object.
boot.type	The type of bootstrap to perform. Currently available type are "residuals", "wild" and "pairs". See details
bsamples	A numerical matrix of observation indices specifying bootstrap samples. Rows indicate observations and columns bootstrap samples. If NULL (the default), samples are generated internally.
В	Number of bootstrap samples to generate when bsamples = NULL.
1	Block length for block-bootstrap. Samples are generated by resampling block of observation of length 1. The classical bootstrap corresponds to $1 = 1$ (the default).
nc	Positive integer. If nc > 1, the function is parallelized with nc indicating the number of cores to use.

Details

This function fits the cgaim on bootstrap samples. It is called internally by the confint.cgaim function, but can also be called directly to generate various statistics.

Three types of bootstrap are currently implemented. "residuals" (the default) resamples the residuals in object to then be added to fitted values, creating alternative response vectors. The cgaim is then fitted on these newly generated y values with the original x. "wild" is similar except that residuals are multiplied by random draws from a standard normal distribution before being added to fitted values. "pairs" resamples directly pairs of y and x to create bootstrap samples.

Bootstrap samples can either be prespecified by the user through bsamples or generated internally. In the former case, the columns of bsamples indicate the number of replications B and the rows should match the original number of observations. Internally generated bootstrap samples are controlled by the number of replications B and block length 1, implementing block bootstrap. The latter is particularly recommended for time series data.

As fitting a large number of cgaim models can be computationally intensive, the function can be run in parallel, using the doParallel package. This can be done by setting the argument nc to a value greater than 1, controlling the number of cores used in parallelization.

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Value

A boot.cgaim object with components

boot The bootstrap result. A list that includes all B replications of alpha, beta, gfit

and indexfit organized in arrays.

obs The original object passed to the function.

samples The bootstrap samples. A matrix with indices corresponding to original obser-

vations.

boot . type The type of bootstrap performed.

B The number of bootstrap replications.

1 The block length for block bootstrap.

Examples

```
# A simple CGAIM
n <- 200
x1 <- rnorm(n)</pre>
x2 <- x1 + rnorm(n)
z < -x1 + x2
y <- z + rnorm(n)
df1 <- data.frame(y, x1, x2)</pre>
ans <- cgaim(y \sim g(x1, x2, acons = list(monotone = 1)), data = df1)
# Use function to compute confidence intervals (B should be increased)
set.seed(1989)
boot1 <- boot.cgaim(ans, B = 10)</pre>
ci1 <- confint(boot1)</pre>
# Produces the same result as
set.seed(1989)
ci2 <- confint(ans, type = "boot", B = 10)</pre>
# Create sampling beforehand
bsamp <- matrix(sample(1:n, n * 10, replace = TRUE), n)</pre>
boot2 <- boot.cgaim(ans, bsamples = bsamp)</pre>
# Parallel computing (two cores)
boot3 <- boot.cgaim(ans, nc = 2)</pre>
```

build_constraints

Common constraints

Description

Build a constraint matrix from common simple constraints. Internally used by g to construct index-specific constraint matrices.

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Usage

```
build_constraints(p, first = 0, sign = 0, monotone = 0, convex = 0)
```

Arguments

р	The number of variables.
first	Indicates sign constraint for first coefficient. Recommended for identifiability if no other constraint is passed.
sign	Sign constraint applied to all coefficients. 0: no constraint,
monotone	Monotonicity constraint. 0: no constraint, -1: decreasing coefficients and 1: increasing coefficients.
convex	Convexity constraint. 0: no constraint, -1: convex coefficients and 1: concave coefficients.

Details

For monotonicity and convexity / concavity, the function assumes the coefficients are ordered. For instance, for increasing monotone coefficients, the first one will be lower than the second, which be lower than the third and so on.

The function automatically removes redundant constraints. For instance, if both sign = 1 and monotone = 1, then only the sign constraint on the first variable is kept as others are not needed.

Note that, for all arguments, any number can be passed to the function. In which case, the sign of the argument is used. Therefore passing monotone = 3.14 is the same as passing monotone = 1.

Value

A p-column constraint matrix.

```
# By default, produces only the identifiability constraint
build_constraints(4)

# Positive and increasing coefficients
build_constraints(4, sign = 1, monotone = 1)

# Concavity constraint
build_constraints(7, convex = -1)

# Any numeric can be passed to the function
build_constraints(5, monotone = pi)
```

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cgaim Constrained groupwise additive index models

Description

Fits constrained groupwise additive index models (CGAIM) to data. CGAIM fits indices subjected to constraints on their coefficients and shape of their association with the outcome. Such constraints can be specified in the formula through g for grouped terms and s for smooth covariates.

Usage

```
cgaim(formula, data, weights, subset, na.action, Cmat = NULL, bvec = NULL,
  control = list())
```

Arguments

formula	A CGAIM formula with index terms g, smooth terms s and linear terms. See details.
data	A data frame containing the variables of the model.
weights	An optional vector of observation weights.
subset	An optional vector specifying a subset of observations to be used in the fitting process.
na.action	A function indicating how to treat NAs. The default is set by the na.action setting of options. See na.fail.
Cmat	A constraint matrix for index coefficients alpha. Columns must match all variables entering any index through g. See details.
bvec	A vector of lower bounds for the constraints in Cmat. Potentially recycled to match the number of constraints.
control	A list of parameters controlling the fitting process. See cgaim.control.

Details

The CGAIM is expressed

$$y_i = \beta_0 + \sum_j \beta_j g_j(\alpha_j^T x_{ij}) + \sum_k \gamma_k f_k(w_{ik}) + \sum_l \theta_l u_{il} + e_i$$

where the x_{ij} are variables entering grouped indices, the w_{ik} are smooth covariates and the u_{il} are linear covariates.

The formula interface considers g to identify index terms, s for smooth functions and can also include linear terms as usual. All smooth terms can be shape constrained.

The CGAIM allows for linear constraints on the alpha coefficients. Such constraints can be specified through the g interface in the formula, or through alpha. control\$Cmat. The g interface is used for constraints meant for a specific index only. In this case, common constraints can easily be specified through the acons argument (see build_constraints). Alternatively, more general constraint can

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be specified by passing a matrix to the Cmat argument. Constraints encompassing several indices can be specified through an element Cmat in alpha.control. Its number of columns must match the total number of index coefficients alpha to estimate. In all cases, arguments byec are used to specify the bounds of constraints.

Both indices (g) and smooth covariate terms (s) allow shape constraints. See dedicated help for the list of constraints allowed.

The CGAIM is fitted through an iterative algorithm that alternates between estimating the ridge functions g_j (and other non-index terms) and updating the coefficients α_j . The smoothing of ridge functions currently supports three methods: scam (the default), cgam and scar. The list smooth.control controls the smoothing with allowed parameters defined in cgaim.control.

Value

A cgaim object, i.e. a list with components:

alpha A named list of index coefficients.

gfit A matrix containing the ridge and smooth functions evaluated at the observa-

tions. Note that column ordering puts indices first and covariates after.

indexfit A matrix containing the indices evaluated at the observations.

beta A vector containing the intercept and the scale coefficient of each ridge and

smooth function. Includes the γ_k of the CGAIM model above. Note that order-

ing puts indices first and covariates after.

index A vector identifying to which index the columns of the element x belong.

fitted A vector of fitted responses.

residuals A vector of residuals.

rss The residual sum of squares of the fit.

flag A flag indicating how the algorithm stopped. 1 for proper convergence, 2 when

the algorithm stopped for failing to decrease the RSS and 3 when the maximum

number of iterations has been reached.

niter Number of iterations performed.

edf Effective degrees of freedom of the estimator.

gcv Generalized cross validation score.

dg A matrix containing derivatives of ridge and smooth functions.

gse A matrix containing standard errors of ridge and smooth functions.

active A logical vector indicating which constraints are active at convergence.

Cmat The constraint matrix used to fit index coefficients alpha. Will include all con-

straints given through g and the Cmat parameter.

bvec The lower bound vector associated with Cmat.

A matrix containing the variables entering the indices. The variables are mapped

to each index through the element index.

y The response vector.

weights The weights used for estimation.

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A list of model elements for the smoothing step of the estimation. Notably includes the matrix Xcov that includes the covariates not entering any index. Other elements depend on the method chosen for smoothing.

Control

The control list used to fit the cgaim.

The model terms.

Note

A model without intercept can only be fitted when the smoothing step is performed with scam.

See Also

confint.cgaim for confidence intervals, predict.cgaim to predict on new data, plot.cgaim to plot ridge functions.

```
## Simulate some data
n <- 200
x1 <- rnorm(n)
x2 <- rnorm(n)
x3 <- rnorm(n)
x4 <- rnorm(n)
mu \leftarrow 4 * exp(8 * x1) / (1 + exp(8 * x1)) + exp(x3)
y <- mu + rnorm(n)
df1 \leftarrow data.frame(y, x1, x2, x3, x4)
## Fit an unconstrained the model
ans <- cgaim(y \sim g(x1, x2) + g(x3, x4), data = df1)
# Compute confidence intervals
# In practice, higher B values are warranted
cia \leftarrow confint(ans, B = 100)
cia$alpha
cia$beta
# Display ridge functions
plot(ans, ci = cia)
# Predict
newdf <- as.data.frame(matrix(rnorm(100), 25, 4))</pre>
names(newdf) <- sprintf("x%i", 1:4)</pre>
yhat <- predict(ans, newdf)</pre>
## Fit constrained model
ans2 <- cgaim(y \sim g(x1, x2, acons = list(monotone = -1)) +
  g(x3, x4, fcons = "cvx"), data = df1)
# Check results
ans2
plot(ans2)
```

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```
# Same result
Cmat <- as.matrix(Matrix::bdiag(list(build_constraints(2, monotone = -1),
    build_constraints(2, first = 1))))
ans3 <- cgaim(y ~ g(x1, x2) + g(x3, x4, fcons = "cvx"), data = df1,
    Cmat = Cmat)

## A mis-specified model
ans4 <- cgaim(y ~ g(x1, x2, acons = list(monotone = 1)) +
    g(x3, x4, fcons = "dec"), data = df1)</pre>
```

cgaim.control

Parameters controlling the CGAIM fit

Description

Internal function setting the parameters to control the CGAIM fit. Sets default values and check parameters passed by the user. It is called internally by cgaim and should not be called directly by the user.

Usage

```
cgaim.control(max.iter = 50, tol = 0.001, halving = TRUE,
  min.step.len = 0.1, convergence_criterion = "rss", trace = FALSE,
  alpha.start = NULL, init.type = "regression", norm.type = "1",
  check.Cmat = TRUE, solver = "osqp", ctol = 0.001, qp_pars = list(),
  sample_pars = list(), sm_method = "scam", sm_pars = list())
```

Arguments

max.iter	The maximum number of iteration allowed.
tol	The tolerance for convergence. The algorithm stops when the convergence criterion falls below tol.
halving	Logical turning on and off halving for bad steps. See details.
min.step.len	Numeric between 0 and 1 giving the minimum descent step length to be considered in case of bad step. See details.
convergence_criterion	
	Character indicating the convergence criterion for the algorithm. See details.
trace	If TRUE, prints the convergence criterion and alpha coefficients at each step.
alpha.start	An optional vector or list of starting alpha values. If NULL, starting values are generated internally. See the init.type argument.
init.type	The type of initialization to perform if no initial value is provided. If init.type = "regression" (the default), starting values are generated by regressing the index design matrix on the response. If init.type = "random", feasible starting values are generated randomly.

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norm.type The type of norm used to normalize index coefficients vectors. See norm for available norms. Default to L1 norm meaning that, for each index, absolute values of coefficients sum to 1. check.Cmat Logical indicating whether to check for redundant constraints and remove them from Cmat. solver The quadratic programming solver to use. One of "osqp" (the default), "quadprog" or "coneproj". Tolerance value on constraints. See details. ctol A named list of parameters to be passed to the solver function. qp_pars A named list of parameters to be passed to xsample when randomly generating sample_pars initial alpha coefficients. sm_method Character specifying which method to use for constrained smoothing. Either scam (the default), cgam or scar. Named list to pass specific parameters to the smoothing function of sm_method. sm_pars

Details

The model is fitted by an iterative sequential quadratic programming algorithm. The algorithm iterates between updating the index alpha coefficients and updating the smoothing of indices and covariates. It stops when the criterion given in convergence_criterion is below tol, or when max.iter is reached. Convergence criteria include rss for which the algorithm stops when the relative decrease in residual sum of squares, (rss_new - rss_old) / rss_old is below tol, alpha for which the algorithm stops when the largest update max(abs(alpha_new - alpha_old) / abs(alpha_old)) is below tol, and offset when the scalar product between the RSS and current direction (measuring orthogonality) is below tol (EXPERIMENTAL, use at your own risk).

See help pages of corresponding functions.

By default, when the RSS fails to decrease during a step (a "bad" step), the step length is iteratively halved until the RSS decreases. The minimum step length allowed is controlled by min.step.len as the proportion of the original step length. This is a common behaviour in non-linear least squares and is implement in nls for instance, but can be turned off by setting halving = FALSE, in which case the algorithm stops for any bad step.

The alpha updating step consists in estimating an update vector in a descent direction by a constrained regression of index derivatives on the current residuals of the model. This is fitted through a quadratic program, ensuring the updated coefficients respect the constraints at each step of the algorithm. Initial values can either be provided by the user through the argument alpha.start or be internally generated. The latter is controlled by the argument init.type allowing to initialize the weights either by regressing the index variables on the response (init.type = "regression") ensuring feasible starting values (the default), or by randomly generating feasible values (init.type = "random"). In the latter case, random generation is performed by the function xsample which can be controlled by the parameter sample_pars. When random initial values are chosen, it is recommended to fit the algorithm several time and keep the best fit, to avoid falling into a local minimum.

At the moment, three solvers are available to perform quadratic programming, which can be controlled by the argument solver. By default the function solve_osqp (solver = "osqp") is used. Alternatively the more established but slower function solve.QP (solver = "quadprog") as well as qprog (solver = "coneproj") functions can be used. Although default parameters are internally

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set for these function, they can entirely be controlled through the argument qp_pars. See their specific help pages for details.

In some cases, minimal numerical imprecision in the repeated call to quadratic program, along with the normalization of alpha coefficients, can lead to unfeasible alphas at convergence. To avoid this, these imprecision are compensated by adding a small tolerance ctol to the constraints, defaulting to 0.001. If no tolerance is wanted, it can be set to 0.

By default, the package automatically checks that Cmat is irreducible, i.e. that no constraint is redundant. A constraint is redundant if it can be expressed as a non-negative linear combination of other constraints. If check. Cmat = TRUE, such constraints are removed with a warning.

Value

A named list containing all arguments to be used in cgaim.

References

Bates, D.M., Watts, D.G., 1981. A Relative Off set Orthogonality Convergence Criterion for Nonlinear least Squares. Technometrics 23, 179–183.

Bates, D.M., Watts, D.G., 1988. Nonlinear Regression Analysis and Its Applications, Wiley Series in Probability and Statistics. Wiley.

See Also

These parameters control the fitting of cgaim.

confint.cgaim

Confidence intervals

Description

Computes confidence intervals for the CGAIM components.

Usage

```
## S3 method for class 'cgaim'
confint(object, parm, level = 0.95, type = c("normal",
   "bootstrap"), B = 100, ...)
## S3 method for class 'boot.cgaim'
confint(object, parm, level = 0.95, ...)
```

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Arguments

object	A cgaim or boot.cgaim object.
parm	The model components for which to get confidence intervals. One or several of: "alpha" for index weights, "beta" for scaling coefficients and "g" for ridge function. By default, returns confidence intervals for all components.
level	The level of confidence intervals. Default to 0.95.
type	The type of confidence intervals. Either "normal" (the default) or "bootstrap". See details.
В	The number of samples to be simulated.
	Additional parameters to be passed to boot.cgaim for bootstrap confidence intervals.

Details

Two types of confidence intervals are currently implemented in the function. When type = "normal", confidence intervals are computed assuming components are normally distributed. Beta coefficients are treated as regular linear regression coefficients and g as regular smooth functions estimated by (shape-constrained) generalized additive models. For alpha coefficients, we consider a linear transformation mapping them to a Truncated Multivariate Normal distribution (i.e. with only bound constraints). Simulation from the TMVN are performed (see tmvnorm) and transformed back into the original coefficient space (i.e. with linear constraints). The parameter B controls the number of simulations from the TMVN. Confidence intervals are computed as the percentiles of these simulated coefficients, ensuring the confidence region is entirely within the feasible region defined by the constraints.

When type = "bootstrap", confidence intervals are estimated by percentile bootstrap. boot.cgaim is called internally to create B samples of model components, and confidence intervals are then computed as the percentiles of bootstrap samples. Alternatively, the user can directly call boot.cgaim and feed the result into confint.boot.cgaim.

Value

A list of confidence intervals. Contains one element per model component in the parm argument.

Note

Confidence intervals for the g functions are evaluated on the same n index values as the functions in object.

References

Masselot, P. and others, 2022. Constrained groupwise additive index models. Biostatistics.

Pya, N., Wood, S.N., 2015. Shape constrained additive models. Stat. Comput. 25, 543-559.

Wood, S.N., 2017. Generalized Additive Models: An Introduction with R, 2nd ed, Texts in Statistical Science. Chapman and Hall/CRC.

DiCiccio, T.J., Efron, B., 1996. Bootstrap Confidence Intervals. Statistical Science 11, 189–212.

Carpenter, J., Bithell, J., 2000. Bootstrap confidence intervals: when, which, what? A practical guide for medical statisticians. Statistics in Medicine 19, 1141–1164.

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See Also

boot.cgaim for bootstrapping.

Examples

```
# A simple CGAIM
n <- 200
x1 <- rnorm(n)</pre>
x2 <- x1 + rnorm(n)
z < -x1 + x2
y \leftarrow z + rnorm(n)
df1 <- data.frame(y, x1, x2)</pre>
ans <- cgaim(y \sim g(x1, x2, acons = list(monotone = 1)), data = df1)
# Normal confidence intervals
set.seed(1)
ci1 \leftarrow confint(ans, B = 1000)
ci1$alpha
ci1$beta
# Select only alphas: identical to above result
set.seed(1)
confint(ans, B = 1000, parm = "alpha")
# Select only betas: identical to above result
set.seed(1)
confint(ans, B = 1000, parm = "beta")
# Confidence intervals by bootstrap (more computationally intensive, B should be increased)
set.seed(2)
ci2 <- confint(ans, type = "boot", B = 10)</pre>
# Alternatively, bootstrap samples can be performed beforehand
set.seed(2)
boot1 <- boot.cgaim(ans, B = 10)</pre>
ci3 <- confint(boot1)</pre>
```

Defining terms in CGAIM formula

Description

g

Functions used to define terms within a cgaim formula. g defines an index with ridge function and s a smooth covariate.

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Usage

```
g(..., label = NULL, acons = list(), Cmat = NULL, bvec = 0,
fcons = NULL, s_opts = list())
s(x, fcons = NULL, s_opts = list())
```

Arguments

• • •	Variables entering the index. May include vectors and matrices.
label	Character (or any object that can coerced into one) labeling the index. By default, named after the first variable in
acons	A list of character naming common constraints to be applied to the index weights alpha. See build_constraints for allowed constraints.
Cmat	A constraint matrix for alpha coefficients. Number of columns must match the number of variables in the index.
bvec	Numeric vector of constraint bounds. Recycled if necessary.
fcons	The type of shape constraint to be applied on the smooth function. See details.
s_opts	A named list of options to be passed to the smoothing of ridge functions. Depends on the method used to smooth additive models. See details.
Х	Covariate on which the smooth is applied.

Details

These functions define nonlinear terms in the formula, with g defining an index created from a collection of terms passed through the . . . argument while s is applied to a single variable, similarly to s in mgcv.

For indices, g allows the definition of constraints applied to the index only. This is a convenient alternative to passing the whole constraint matrix Cmat in cgaim. Constraints can be defined by a prespecified matrix through the argument Cmat or through the argument acons for common constraints (see build_constraints). Note that any provided Cmat must match the total number of variables in . . . , including potential matrix expansion and factors. Both Cmat and acons can be passed to the function, which will bind them internally.

Both g and s allow the definition of shape constraints for the smooth. Eight shape-constraints are currently available: monotone increasing (fcons = "inc"), monotone decreasing (fcons = "dec"), convex (fcons = "cvx"), concave (fcons = "ccv"), increasing and convex(fcons = "inccvx"), decreasing and convex (fcons = "deccvx"), increasing and concave (fcons = "incccv"), decreasing and concave (fcons = "decccv").

Smoothing can be controlled by the s_opts parameter. It is a list of argument depends on the method used for smoothing. See s for smooth_method = "scam". For smooth_method = "cgam", the parameters allowed may vary according to the shape-constraint chosen. The full list can be found in cgam, but only the constraints beginning with s. are allowed for now. No parameter are necessary when smooth_method = "scar" (see scar).

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Value

A matrix containing the variables passed in . . . with additional attributes:

fcons The shape constraint for smoothing.

s_opts Arguments passed to the smoothing function.

label The label of the term.

The following attributes result from a call to g only:

term The terms in the index.

nterms The number of variables in the index.

Cmat The constraint matrix for alpha coefficients.

bvec The associated boundary vector.

See Also

cgaim for fitting the CGAIM, build_constraints for built-in constraint matrices.

```
## Simulate some data
n <- 200
x1 <- rnorm(n)</pre>
x2 <- rnorm(n)
x3 <- rnorm(n)
x4 <- rnorm(n)
mu \leftarrow 4 * exp(8 * x1) / (1 + exp(8 * x1)) + exp(x3)
y \leftarrow mu + rnorm(n)
df1 <- data.frame(y, x1, x2, x3, x4)
## Fit an unconstrained the model
ans <- cgaim(y \sim g(x1, x2) + g(x3, x4), data = df1)
## Fit constrained model
ans2 <- cgaim(y \sim g(x1, x2, acons = list(monotone = -1)) +
  g(x3, x4, fcons = "cvx"), data = df1)
## Pass constraint matrices instead
ans3 <- cgaim(y \sim g(x1, x2, Cmat = -diff(diag(2))) +
  g(x3, x4, fcons = "cvx"), data = df1)
## Label indices
ans4 <- cgaim(y \sim g(x1, x2, label = "foo") + g(x3, x4, label = "bar"),
  data = df1)
```

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Description

Plot method for the ridge and smooth terms of a cgaim object. If provided, also plots confidence intervals.

Usage

```
## S3 method for class 'cgaim'
plot(x, select = NULL, ci = NULL, ci.plot = c("polygon",
   "lines"), ci.args = list(), add = FALSE, xcenter = FALSE,
   xscale = FALSE, yshift = FALSE, yscale = FALSE, ...)
```

Arguments

X	A cgaim object.
select	A numeric or character vector indicating which terms to plot.
ci	An object returned by a call to ${\tt confint.cgaim}.$ If NULL, no confidence interval is drawn.
ci.plot	Whether to plot the confidence intervals as shaded areas ci.plot = "polygon" or as lines ci.plot = "lines".
ci.args	Additional arguments to be passed to the function used to draw confidence interval. Either polygon or lines.
add	Logical. If TRUE, adds the function to the current active plot.
xcenter, xscale	
	Centering and scaling values for the x axis. See scale.
yshift, yscale	Either logical or numeric values to shift and scale the ridge functions. See details.
	Additional graphical parameters for the drawn function. See par.

Details

The values of yshift and yscale determine how ridge functions are shifted and scaled for plotting. This can be used to display the functions over data points for instance. If numeric, a vector can be passed with one value for each plotted function. The vector is recycled if necessary. This indicate the desired mean and standard deviation of plotted ridge functions. Note that this is inverse to the parameters in scale (and xcenter,xscale). If TRUE is passed instead, functions are shifted to the intercept and scaled to their corresponding beta coefficients, placing them on the response scale.

Value

The function is called to generate plots and returns no value.

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See Also

cgaim for the main fitting function and confint.cgaim for confidence interval computation.

```
## Simulate some data
n <- 200
x1 <- rnorm(n)
x2 <- rnorm(n)
x3 <- rnorm(n)
x4 <- rnorm(n)
mu \leftarrow 4 * exp(8 * x1) / (1 + exp(8 * x1)) + exp(x3)
y < -5 + mu + rnorm(n)
df1 <- data.frame(y, x1, x2, x3, x4)
## Fit a model
ans <- cgaim(y \sim g(x1, x2, label = "foo") + g(x3, x4, label = "bar"),
  data = df1)
## Default plot method
plot(ans)
## Select variable
plot(ans, select = 1)
# Same as
plot(ans, select = "foo")
## Add confidence intervals
ci <- confint(ans)</pre>
plot(ans, select = 1, ci = ci)
## Change scale and location
# On the response scale
plot(ans, select = 1, ci = ci, yshift = TRUE, yscale = TRUE)
# Arbitrary scale
plot(ans, select = 1, ci = ci, yshift = 1000)
## Change look
# Main line
plot(ans, select = 1, ci = ci, col = 2, lwd = 3)
# Confidence intervals
plot(ans, select = 1, ci = ci, col = 2, lwd = 3,
  ci.args = list(col = adjustcolor(2, .5)))
# Confidence interval type
plot(ans, select = 1, ci = ci, ci.plot = "lines", col = 2, lwd = 3,
  ci.args = list(col = 2, lty = 4))
```

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```
## Put curves on the same plot (need to shift and scale)
plot(ans, select = 1, col = 2, ylim = c(-2, 3))
plot(ans, select = 2, col = 4, add = TRUE)
```

predict.cgaim

Predictions from a fitted CGAIM object

Description

Uses a fitted cgaim object and computes prediction for the observed data or new data. Predicts the response, indices or ridge functions values at the provided data.

Usage

```
## $3 method for class 'cgaim'
predict(object, newdata, type = c("response", "terms",
   "scterms", "indices"), select = NULL, na.action = "na.pass", ...)
```

Arguments

object	A gaim object.
newdata	A list or data.frame containing the new data to predict. If missing, fitted values from the model are returned.
type	A character indicating the type of prediction to return. type = "response" returns the predicted response. type = "terms", returns ridge and smooth functions evaluated at index predicted for newdata. type = "scterms" is the same, except that terms are postmultiplied by their scaling coefficients beta. type = "indices" returns predicted indices values.
select	A numeric or character vector indicating terms to return for all types except "response".
na.action	A function indicating how to treat NAs. See na. fail.
	For compatibility with the default predict method. Unused at the moment.

Details

type = "terms" returns the scaled ridge functions, i.e. before being multiplied by scaling coefficients beta.

Value

When type = "response" returns a vector of predicted response. When type = "terms" or "scterms", returns a matrix of evaluated ridge and smooth terms. When type = "indices", returns a matrix of evaluated indices.

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See Also

cgaim for main fitting function

```
## Simulate some data
n <- 200
x1 <- rnorm(n)
x2 <- rnorm(n)
x3 <- rnorm(n)
x4 <- rnorm(n)
mu \leftarrow 4 * exp(8 * x1) / (1 + exp(8 * x1)) + exp(x3)
y \leftarrow mu + rnorm(n)
df1 \leftarrow data.frame(y, x1, x2, x3, x4)
## Fit an unconstrained the model
ans <- cgaim(y \sim g(x1, x2, label = "foo") + g(x3, x4, label = "bar"),
  data = df1)
## Get fitted values
yhat <- predict(ans)</pre>
## Predict on new data
newdf <- as.data.frame(matrix(rnorm(100), 25, 4))</pre>
names(newdf) <- sprintf("x%i", 1:4)</pre>
# predicted response
ypred <- predict(ans, newdf)</pre>
indices <- predict(ans, newdata = newdf, type = "indices")</pre>
# Ridge functions
funs <- predict(ans, newdata = newdf, type = "terms")</pre>
## Select specific terms
ind1 <- predict(ans, newdata = newdf, select = "foo", type = "indices")</pre>
fun1 <- predict(ans, newdata = newdf, select = "foo", type = "terms")</pre>
# Plot
plot(ans, select = "foo")
points(ind1, fun1)
## Scaled terms
fun2 <- predict(ans, newdata = newdf, select = "foo", type = "scterms")</pre>
# Plot
plot(ans, select = "foo", yscale = TRUE)
points(ind1, fun2)
```

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print.cgaim

Print a cgaim object

Description

Default method to print the results from a call to cgaim. Conveniently prints the formula, beta and alpha coefficients as well as the residual sum of squares.

Usage

```
## S3 method for class 'cgaim'
print(x, ...)
```

Arguments

x A cgaim object.

... For compatibility with the default print method. Unused at the moment.

Value

Function called for its side effect of printing a cgaim object. Returns no value.

See Also

The main fitting function cgaim.

vcov.cgaim

Calculate Variance-Covariance Matrix for a Fitted CGAIM Object

Description

Returns the variance covariance matrix of the main parameters of a fitted cgaim object. These parameters correspond to the index weights alpha and the scaling coefficients beta.

Usage

```
## S3 method for class 'cgaim'
vcov(object, parm = c("alpha", "beta"), type = c("normal",
   "bootstrap"), B = 100, complete = TRUE, ...)

## S3 method for class 'boot.cgaim'
vcov(object, parm = c("alpha", "beta"),
   complete = TRUE, ...)
```

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Arguments

object A cgaim or boot.cgaim object.

parm The model components for which to get confidence intervals. Either "alpha" (the default) for index weights or "beta" for scaling coefficients.

type The type of confidence intervals. Either "normal" (the default) or "bootstrap". See details.

B The number of samples to be simulated.

complete Indicates whether the full variance-covariance matrix should be returned when

some of the parameters could not be estimated. If so, the matrix is padded with

NAs.

... Additional parameters to be passed to boot.cgaim for bootstrap replications.

Details

Two types of computation are currently implemented in the function. When type = "normal", variance-covariance matrices are computed assuming components are normally distributed. Beta coefficients are treated as regular linear regression coefficients and alpha coefficients are assumed to follow a Truncated Multivariate Normal distribution. The latter is obtained by simulating from TMVN (see tmvnorm) and computing the empirical variance covariance matrix from these simulations. The parameter B controls the number of simulations from the TMVN (and is not used when parm = "beta").

When type = "bootstrap", the variance-covariance matrix is computed on Bootstrap replications. In this case boot.cgaim is called internally and B corresponds to the number of replications. Alternatively, the user can directly call boot.cgaim and feed the result into vcov.boot.cgaim (see examples).

Value

A variance-covariance matrix object.

References

Masselot, P. and others, 2022. Constrained groupwise additive index models. Biostatistics.

Pya, N., Wood, S.N., 2015. Shape constrained additive models. Stat. Comput. 25, 543-559.

Wood, S.N., 2017. Generalized Additive Models: An Introduction with R, 2nd ed, Texts in Statistical Science. Chapman and Hall/CRC.

See Also

boot.cgaim for bootstrapping and confint.cgaim for confidence intervals.

```
# A simple CGAIM
n <- 200
x1 <- rnorm(n)
x2 <- x1 + rnorm(n)
```

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```
z < -x1 + x2
y \leftarrow z + rnorm(n)
df1 <- data.frame(y, x1, x2)</pre>
ans <- cgaim(y \sim g(x1, x2, acons = list(monotone = 1)), data = df1)
# (Truncated) Normal variance-covariance matrix
set.seed(1)
vcov(ans, B = 1000)
set.seed(1)
vcov(ans, parm = "alpha", B = 1000) # Same result
vcov(ans, parm = "beta", B = 1000)
# Confidence intervals by bootstrap (more computationally intensive, B should be increased)
vcov(ans, type = "boot", B = 10)
# Alternatively, bootstrap samples can be performed beforehand
set.seed(2)
boot1 <- boot.cgaim(ans, B = 10)</pre>
vcov(boot1)
```

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