Package ‘dynaTree’

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Description Inference by sequential Monte Carlo for
dynamic tree regression and classification models
with hooks provided for sequential design and optimization,
fully online learning with drift, variable selection, and
sensitivity analysis of inputs. Illustrative
effects from the original dynamic trees paper
(Gramacy, Taddy & Polson (2011); <doi:10.1198/jasa.2011.ap09769>) are facilitated
by demos in the package; see demo(package="dynaTree").
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dynaTree-package

Description

Inference by sequential Monte Carlo for dynamic tree regression and classification models with hooks provided for sequential design and optimization, fully online learning with drift, variable selection, and sensitivity analysis of inputs. Illustrative examples from the original dynamic trees paper are facilitated by demos in the package; see demo(package="dynaTree")

Details

For a fuller overview including a complete list of functions, and demos, please use help(package="dynaTree").

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References


https://bobby.gramacy.com/r_packages/dynaTree/

See Also

plgp, tgp
**alcX.dynaTree**

*Calculate the ALC or predictive entropy statistic at the X locations, or ALC at new XX predictive locations*

---

**Description**

Uses analytic integration (at the leaves) to calculate the (regression) ALC statistic, or calculates the predictive (class) entropy at the input (X) locations; or calculate ALC at new predictive locations either analytically or numerically.

**Usage**

```r
## S3 method for class 'dynaTree'
alcX(object, rect = NULL, categ = NULL,
     approx = FALSE, verb = 0)
## S3 method for class 'dynaTree'
entropyX(object, verb = 0)
## S3 method for class 'dynaTree'
alc(object, XX, rect = NULL, categ = NULL,
     approx = FALSE, Xref = NULL, probs = NULL, verb = 0)
```

**Arguments**

- `object` a "dynaTree"-class object built by `dynaTree`
- `rect` for `alcX`, a matrix with two columns and `ncol(object$X)` rows describing the bounding rectangle for the ALC integration; the default that is used when `rect = NULL` is the bounding rectangle obtained by applying `range` to each column of `object$X` (taking care to remove the first/intercept column of `object$X` if `icept = "augmented"`; only applies to regression models (`object$model != "class"`); for `alc`, `rect` must be a scalar logical: see `Xref` below
- `categ` A vector of logicals of length `ncol(object$X)` indicating which, if any, dimensions of the input space should be treated as categorical; this input is used to help with the analytic integrals from a `rect`-based calculation, which means it should not specified along with `Xref`; the default `categ` argument is NULL meaning that the categorical inputs are derived from `object$X` in a sensible way
- `approx` a scalar logical that, when TRUE, causes the number of data points in a node/leaf to be used as a proxy for its area in the analytic calculations
- `XX` a design matrix of predictive locations (where `ncol(XX) == ncol(X)`: only used by `alc`
- `Xref` `Xref` input can be optionally used to specify a grid of reference locations for the numerical ALC calculation - a matrix with `ncol(X)` columns. If NULL, the default, then the `XX` is taken as both candidate and reference locations.
- `probs` weights for the reference locations to be used in a Monte Carlo approximation; usually these weights are class probabilities for response surfaces under constraints
verb a positive scalar integer indicating how many predictive locations (iterations) after which a progress statement should be printed to the console; a (default) value of verb = 0 is quiet

Details

This function is most useful for selecting object$X locations to remove from the analysis, perhaps in an online inference setting. See retire.dynaTree for more details. The output is the same as using predict.dynaTree using XX = object$X, alc = "rect". and Xref = rect

entropyX only apples to classification models (object$model != "class"), and alcX applies (only) to the other, regression, models

The alc function is more generic and allows ALC calculations at new, predictive, XX locations. This functionality used to be part of the predict.dynaTree function, but were separated out for computational reasons. The previous version was Monte Carlo-based (using Xref) whereas the new version also allows analytic calculation (now the default, via rect)

Value

The entire object is returned with a new entry called alcX containing a vector of length nrow(X) with the ALC values, or entropyX containing the entropy values, or alc if general ALC calculations at new XX locations

Author(s)

Robert B. Gramacy <rbg@vt>,
Matt Taddy, and Christoforos Anagnostopoulos

References


https://bobby.gramacy.com/r_packages/dynaTree/

See Also

dynaTree, predict.dynaTree, and retire.dynaTree

Examples

```r
## fit the model to the parabola data
n <- 100
Xp <- runif(n,-3,3)
Yp <- Xp + Xp^2 + rnorm(n, 0, .2)
rect <- c(-3,3)
out <- dynaTree(Xp, Yp, model="linear", icept="augmented")

## calculate the alcX
```
out <- alcX(out, rect=rect)

## to compare to analytic
out <- alc(out, XX=out$X[, -1], rect=rect)

## plot comparison between alcX and predict-ALC
plot(out$X[, -1], out$alcX)
o <- order(out$X[, 2])
lines(out$X[o, -1], out$alc[o], col=2, lty=2)

## now compare to approximate analytic
## (which writes over out$alc)
out <- alc(out, XX=out$X[, -1], rect=rect, approx=TRUE)
lines(out$X[o, -1], out$alc[o], col=3, lty=3)

## clean up
deletecloud(out)

## similarly with entropyX for classification models

## see demo("design") for more iterations and
## design under other active learning heuristics
## like ALC, and EI for optimization; also see
## demo("online") for an online learning example where
## ALC is used for retirement

dynaTree-class

Class "dynaTree"

Description
A stub for class dynaTree and its custom generic methods

Details
This is just a stub file. See sens.dynaTree and retire.dynaTree for more information on the
generic methods used in this package

Objects from the Class
A virtual Class: No objects may be created from it.

Methods
retire signature(object = "dynaTree"): ...
sens signature(object = "dynaTree"): ...
copy signature(object = "dynaTree"): ...
alc signature(object = "dynaTree"): ...
alcX  signature(object = "dynaTree"): ...
entropyX  signature(object = "dynaTree"): ...
ieci  signature(object = "dynaTree"): ...
classprobs  signature(object = "dynaTree"): ...
rejuvenate  signature(object = "dynaTree"): ...
relevance  signature(object = "dynaTree"): ...
varpropuse  signature(object = "dynaTree"): ...
varproptotal  signature(object = "dynaTree"): ...
treestats  signature(object = "dynaTree"): ...
sameleaf  signature(object = "dynaTree"): ...

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References
https://bobby.gramacy.com/r_packages/dynaTree/

See Also
dynaTree, predict.dynaTree, update.dynaTree, retire.dynaTree, sens.dynaTree, alcX.dynaTree

Examples

showClass("dynaTree")

dynaTrees  Fitting Dynamic Tree Models

Description
A function to initialize and fit dynamic tree models to regression and classification data by the
sequential Monte Carlo (SMC) method of particle learning (PL)
**Usage**

dynaTree(X, y, N = 1000, model = c("constant", "linear", "class", "prior"),
        nu0s20 = c(0,0), ab = c(0.95, 2), minp = NULL, sb = NULL,
        nstart = minp, icate = c("implicit", "augmented", "none"),
        rprop = c("luvar", "luall", "reject"), verb = round(length(y)/10))
dynaTrees(X, y, N = 1000, R = 10, sub = length(y),
        model = c("constant", "linear", "class", "prior"), nu0s20 = c(0,0),
        ab=c(0.95, 2), minp = NULL, sb = NULL, nstart = minp,
        icate = c("implicit", "augmented", "none"),
        rprop = c("luvar", "luall", "reject"), XX = NULL, yy = NULL,
        varstats = FALSE, lhs = NULL, plotit = FALSE, proj = 1,
        rorder = TRUE, verb = round(sub/10), pverb=round(N/10), ...)

**Arguments**

- **X**: A design matrix of real-valued predictors
- **y**: A vector of length nrow(X) containing real-valued responses (for regression) or positive integer-valued class labels (for classification)
- **N**: a positive scalar integer indicating the number of particles to be used
- **R**: a scalar integer \( \geq 2 \) indicating the number of “repeats” or passes through the data, as facilitated by dynaTrees; see details below
- **sub**: Optional argument allowing only a subset of the length(y) X-y pairs to be used in each repeat of dynaTrees; each repeat will use a different random subset of size sub
- **model**: indicates the type of model to be used at the leaves of the tree; "constant" and "linear" apply to regression, and "class" to multinomial classification; finally "prior" was recently added to explore sampled without data
- **nu0s20**: a two-vector indicating Inverse Gamma prior parameters \( c(\nu_0, \sigma^2) \) for the variance in each leaf node, \( \sigma^2 \). A \( c(0,0) \) setting indicates a default, scale-invariant, prior; does not apply to the "class" model
- **ab**: tree prior parameter \( c(\alpha, \beta) \); see details below
- **minp**: a positive scalar integer describing the smallest allowable region in the treed partition; if NULL (default) a suitable minimum is calculated based on dim(X) and the type of model being fit
- **sb**: an optional two-vector of positive integers indicating \( c(\text{splitmin}, \text{basemax}) \) for the "linear" model. It gives the first column of X on which treed partitioning is allowed, and the last column of X to use as covariates in the linear model at the leaves, respectively
- **nstart**: a positive scalar integer \( \geq \text{minp} \) indicating the time index at which treed partitioning is allowed to start
- **icate**: indicates the type of intercept term used (only applies to model="linear"). The default, "implicit" causes the inputs X to be centered so the intercept can be implied as an afterthought; "augmented" causes the inputs X to automatically gain a leading column of ones in a way that is transparent to the user; and "none" assumes that no intercept is being used, or that the user has pre-treated X to have...
a column of ones. The main advantage of "implicit" over "augmented" is that the former can default to a constant model fit if leaf design matrices become rank deficient. The latter defaults to the zero-model in such cases.

**XX** a design matrix of predictive locations (where ncol(XX) == ncol(X)) for dynaTrees; also see `predict.dynaTree` and some explanation in the details below.

**yy** an optional vector of "true" responses at the XX predictive locations at which the log posterior probability are to be reported.

**varstats** if TRUE causes the `varpropuse`, `varproptotal`, and `relevance.dynaTree` functions to be called on after each repetition to collect the usage proportions of each input variable (column of X); see those documentation files for more details.

**lhs** an optional lhs argument to `sens.dynaTree` if a sensitivity analysis step is desired after each restart (XX="sens")

**plotit** a scalar logical indicating if the fit should be plotted after each of the R repeats; only applies to 1-d data and dynaTrees.

**proj** when ncol(x$X) > 1 and plotit = TRUE this argument is passed to `plot.dynaTree` to make a 1-d projection using x$X[,proj]

**rorder** a scalar logical indicating if the rows of X (and corresponding components of y) should be randomly re-ordered for repeats 2:R in order to assess the how the time-ordering of the SMC effects the Monte Carlo error; only applies to dynaTrees. Alternatively, one can specify an nrow(X)-by-(R-1) matrix of orderings (permutations of 1:nrow(X))

**rprop** indicates the scheme used to construct a grow proposal. The best setting, "luall" uses the lower (L) and upper (U) rectangle method based on minp (above) as described in the seminal reference in which the growing location and dimension is sampled uniformly. It can be computationally intensive for large input spaces. A thriftier option (the default) in this case is "luvar" which uniformly chooses the splitting variable first and then uses the LU method marginally. Thriftier still is "reject" which just proposes uniformly in the bounding leaf rectangle and rejects subsequent grows that lead to partitions with too few data points; (see the minp argument)

**verb** a positive scalar integer indicating how many time steps (iterations) should pass before a progress statement is printed to the console; a value of verb = 0 is quiet.

**pverb** a positive scalar integer indicating after many particles should be processed for prediction before a progress statement is printed to the console; a value of pverb = 0 is quiet.

... extra arguments to `predict.dynaTree` passed from dynaTrees

### Details

The dynaTree function processes the X and y pairs serially via PL. It builds up a particle cloud which is stored as an object in C. A "pointer" to that object is the primary return value. The dynaTrees function fits several (R) different dynamic tree models on different time-orderings of the data indices and also obtains samples from the posterior predictive distribution at new XX locations. These predictions can be averaged over each repeat, or used to assess the Monte Carlo predictive error.

Three different leaf models are supported: two for regression and one for classification. If model == "class" then the y values must contain representatives from every class (1:max(y)). For details...
of these models and the complete description of their use at the leaves of the dynamic trees, see the Taddy, et al., (2009) reference, below.

The tree prior is specified by $ab\text{=}c(\alpha, \beta)$ via the and $\text{minp}$. It was originally described by Chipman et al., (1998, 2002)

$$p_{\text{split}}(\eta, T) = \alpha \ast (1 + \eta)^\beta$$

and subsequently augmented to enforce a minimum number of points ($\text{minp}$) in each region.

Once a "dynaTree"-class object has been built (by dynaTree), predictions and estimates of sequential design and optimization criteria can be obtained via predict.dynaTree, a generic prediction method. These values can be used to augment the design, and the update.dynaTree function can be used to quickly update the fit with the augmenting data.

**Value**

Both functions return an object of class "dynaTree", which is a list containing the following fields:

- `m`: ncol(X)
- `T`: nrow(X)
- `N`: the number of particles used
- `X`: a copy of the design matrix X
- `y`: a copy of the responses y
- `model`: a copy of the specified leaf model
- `params`: a vector containing $c(\nu_0s20, \alpha, \beta, \text{minp}, \text{sb}, \text{icept, rprop})$, where the latter two are in integer form
- `verb`: a copy of the verbosity argument
- `lpred`: a vector of log posterior probabilities for each observation, conditional on the ones previous, for all time $(2\ast\text{minp}):T$; see getBF for calculating Bayes factors from these
- `icept`: a copy of the intercept argument
- `time`: the total computing time used to build the particle cloud
- `num`: a “pointer” to the C-side particle cloud; see the note below

The dynaTrees function can obtain predictive samples (via predict.dynaTree) at each of the R repeats. Therefore, the "dynaTree" object returned contains extra fields collecting these predictive samples, primarily comprising of R columns of information for each of the fields returned by predict.dynaTree; see that function for more details. Likewise, when varstats = TRUE the returned object also contains vpu, vpt and parde[ fields whose columns contain the varpropuse and varproptotal outputs.

Likewise, dynaTrees, can provide variable usage summaries if varstats = TRUE, in which case the output includes vpu and vpt fields; See varpropuse and varproptotal for more details.

The dynaTrees function does not return num since it does not leave any allocated particle clouds on the C-side.
Note
As mentioned in the details section, above, the dynaTree function returns a pointer to a particle cloud allocated in C. This pointer is used for prediction, via predict.dynaTree and for later updating/augmentation of data, via update.dynaTree. This information will not be “freed” unless the user specifically calls deletecloud(num) or deleteclouds(). Failing to call one of these functions (when done with the corresponding object(s)) could result in a memory leak; see their documentation for more details.

The C-side memory cannot be saved in the workspace, so they cannot persist across R sessions.

To copy a "dynaTree"-class object, use copy.dynaTree, which will also copy the C-side memory allocated to the object.

Author(s)
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Matt Taddy and Christoforos Anagnostopoulos

References
https://bobby.gramacy.com/r_packages/dynaTree/

See Also
predict.dynaTree, update.dynaTree, plot.dynaTree, deletecloud, copy.dynaTree, getBF, varpropuse, varproptotal, sens.dynaTree, relevance.dynaTree

Examples
## simple parabolic data
n <- 100
Xp <- sort(runif(n,-3,3))
Yp <- Xp + Xp^2 + rnorm(n, 0, .2)

## fit a piece-wise linear model
parab.fit <- dynaTree(Xp, Yp, model="linear")

## obtain predictions at a new set of locations
## and plot
parab.fit <- predict(parab.fit, XX=seq(-3, 3, length=100))
plot(parab.fit)

## try duplicating the object
parab.fit.copy <- copy(parab.fit)

## must delete the cloud or memory may leak
deletecloud(parab.fit); parab.fit$num <- NULL
## to delete all clouds, do:
deleteclouds()

## for more examples of dynaTree see update.dynaTree

## Motorcycle accident data
if(require("MASS")) {
  data(mcycle)
  Xm <- mcycle[,1]
  Ym <- mcycle[,2]
  XXm <- seq(min(mcycle[,1]), max(mcycle[,1]), length=100)

  R <- 2  ## use R >= 10 for better results
  ## small R is for faster CRAN checks
  ## fit constant model with R=2 repeats and predictions
  moto.fit <- dynaTrees(Xm, Ym, XX=XXm, R=R, plotit=TRUE)

  ## plot the averages
  plot(moto.fit, ptype="mean")

  ## clouds automatically deleted by dynaTrees
}

## Not run:
## 2-d/3-class classification data
library(plgp)
library(tgp)
xx <- seq(-2, 2, length=20)
XX <- expand.grid(xx, xx)
X <- dopt.gp(125, Xcand=XX)$XX
C <- exp2d.C(X)

## fit a classification model with R=10 repeats,
class.fit <- dynaTrees(X, C, XX=XX, model="class")

## for plot the output (no generic plotting available)
cols <- c(gray(0.85), gray(0.625), gray(0.4))
par(mfrow=c(1,2))
library(interp)

## plot R-averaged predicted class
mclass <- apply(class.fit$p, 1, which.max)
image(interp(XX[,1], XX[,2], mclass), col=cols,
      xlab="x1", ylab="x2", main="repeated class mean")
points(X)
## plot R-averaged entropy
ment <- apply(class.fit$entropy, 1, mean)
image(interp(XX[,1], XX[,2], ment),
       xlab="x1", ylab="x2", main="repeated entropy mean")

## End(Not run)

elec2  The ELEC2 Data Set

Description

Electricity Pricing Data Set Exhibiting Concept Drift

Usage

data(elec2)

Format

A data frame with 27552 observations on the following 5 variables.

x1 a numeric vector
x2 a numeric vector
x3 a numeric vector
x4 a numeric vector
y class label

Details

This data has become a benchmark of sorts in streaming classification. It was first described by Harries (1999) and used thereafter for several performance comparisons [e.g., Baena-Garcia et al. (2006); Kuncheva and Plumpton, (2008)]. It holds information for the Australian New South Wales (NSW) Electricity Market, containing 27552 records dated from May 1996 to December 1998, each referring to a period of 30 minutes subsampled as the completely observed portion of 45312 total records with missing values. These records have seven fields: a binary class label, two time stamp indicators (day of week, time), and four covariates capturing aspects of electricity demand and supply.

An appealing property of this dataset is that it is expected to contain drifting data distributions since, during the recording period, the electricity market was expanded to include adjacent areas. This allowed for the production surplus of one region to be sold in the adjacent region, which in turn dampened price levels.

Source

References


Examples

```r
## this is a snippet from the "elec2" demo; see that demo
## for a full comparison to dynaTree models which can
## cope with drifting concepts

## set up data
data(elec2)
X <- elec2[,1:4]
y <- drop(elec2[,5])

## predictive likelihood for repeated trials
T <- 200 # use nrow(X) for a longer version,
## short T is for faster CRAN checks
hits <- rep(NA, T)

## fit the initial model
n <- 25; N <- 1000
fit <- dynaTree(X[1:n,], y[1:n], N=N, model="class")
w <- 1
for(t in (n+1):T) {
  ## predict the next data point
  ## full model
  fit <- predict(fit, XX=X[t,], yy=y[t])
  hits[t] <- which.max(fit$p) == y[t]

  ## sanity check retiring index
  if(any(fit$X[w,] != X[t-n,])) stop("bad retiring")

  ## retire
  fit <- retire(fit, w)

  ## update retiring index
  w <- w + 1; if(w >= n) w <- 1

  ## update with new point
  fit <- update(fit, X[t,], y[t], verb=100)
}

## free C-side memory
```
deleteclouds()

## plotting a moving window of hit rates over time
rhits <- rep(0, length(hits))
for(i in (n+1):length(hits)) {
  rhits[i] <- 0.05*as.numeric(hits[i]) + 0.95*rhits[i-1]
}

## plot moving window of hit rates
plot(rhits, type="l", main="moving window of hit rates",
     ylab="hit rates", xlab="t")

---

**getBF**

*Extract a Path of (log) Bayes Factors*

**Description**

Extract a path (log) Bayes factors (BFs) from the log marginal posterior probabilities of two "dynaTree"-class objects

**Usage**

```r
getBF(obj1, obj2)
```

**Arguments**

- `obj1` a "dynaTree"-class object built by `dynaTree`
- `obj2` another "dynaTree"-class object built by `dynaTree`

**Details**

Simply calculates a difference in log marginal posterior probabilities, setting BFs to zero for initial elements of the path where one of the objects has more zero marginal probabilities than the other. The BF is for the model in `obj1` over `obj2`. If the objects are the output of repeated fits as obtained from `dynaTrees`, then multiple traces are returned

**Value**

Returns a vector or matrix of a trace(s) of Bayes factors that can be plotted; see examples below

**Author(s)**

Robert B. Gramacy `<rbg@vt.edu>`,
Matt Taddy and Christoforos Anagnostopoulos
References


https://bobby.gramacy.com/r_packages/dynaTree/

See Also
dynaTree, update.dynaTree, link{logpost}

Examples

```r
## parabola data
n <- 100
Xp <- sort(runif(n,-3,3))
Yp <- Xp + Xp^2 + rnorm(n, 0, .2)
XXp <- seq(-3,3,length=100)

## comparison by log Bayes Factor
R <- 2 ## use R >= 10 for better results
## small R is for faster CRAN checks
o <- apply(matrix(runif(n*(R-1)), ncol=R-1), 2, order)
lpc.p <- dynaTrees(Xp, Yp, R=R, rorder=o, verb=0)
lpl.p <- dynaTrees(Xp, Yp, model="linear", R=R, rorder=o, verb=0)
bf.p <- getBF(lpl.p, lpc.p)

## plot the log Bayes factors
matplot(bf.p, type="l", lty=1, col="gray", main="parabola",
       xlab="time", ylab="log Bayes factor")

## see demo("reg1d") for further examples
```

---

### plot.dynaTree

Plotting Predictive Distributions of Dynamic Tree models

**Description**

Plotting predictive distributions constructed from dynamic tree (regression) models for 1-d data – provided primarily for use in our 1-d examples and for illustrative purposes

**Usage**

```r
## S3 method for class 'dynaTree'
plot(x, proj = 1, add = FALSE, ylim = NULL,
     col = 2, lwd = 1, ptype = c("each", "mean"), ...)
```
Arguments

- **x**: a "dynaTree"-class object built by `dynaTree`
- **add**: a scalar logical indicating if the lines/points should be “added” to an existing plot
- **proj**: when `ncol(x$X) > 1` this argument can be used to plot a 1-d projection by specifying which column of `x$X` should be used to make the plot
- **ylim**: user-specified y-axis limits values; see `plot`
- **col**: user-specified color value; see `plot`
- **lwd**: user-specified line-width value; see `plot`
- **ptype**: type of plot used to visualize several predictive samples obtained from `dynaTrees`: "each" shows each surface with its own set of three lines, and "mean" shows the three lines obtained by averaging
  ...  other arguments to the generic `plot` method

Details

This plotting function only handles the predictive output from 1-dimensional regression `dynaTree` models as obtained by first calling `dynaTree` and then `predict.dynaTree` on the resulting output at new `XX` locations. It is provided to help make the illustration of our 1-d examples easier and to serve as an aid in a user’s development of custom plotting functions in higher dimensions.

Value

The only output of this function is a pretty plot

Author(s)

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Matt Taddy and Christoforos Anagnostopoulos

References


https://bobby.gramacy.com/r_packages/dynaTree/

See Also

`predict.dynaTree`, `dynaTree`, `update.dynaTree`

Examples

```r
## see dynaTree, dynaTrees and update.dynaTree for examples
## which use this plot function
```
predict.dynaTree

**Prediction for Dynamic Tree Models**

**Description**

Predicting and calculating sequential design and optimization statistics at new design points (i.e., active learning heuristics) for dynamic tree models

**Usage**

```r
## S3 method for class 'dynaTree'
predict(object, XX, yy = NULL, quants = TRUE,
         ei = FALSE, verb = 0, ...)
## S3 method for class 'dynaTree'
coef(object, XX, verb = 0, ...)
```

**Arguments**

- **object**: a "dynaTree"-class object built by `dynaTree`
- **XX**: a design matrix of predictive locations (where `ncol(XX) == ncol(X)`)  
- **yy**: an optional vector of “true” responses at the XX predictive locations at which the log posterior probability are to be reported
- **quants**: a scalar logical indicating if predictive quantiles are desired (useful for visualization, but less so for active learning); calculating predictive quantiles is expensive and should be turned off if prediction is not being used for visualization, e.g., if used for active learning
- **ei**: a scalar logical indicating if the expected improvement statistic (for optimization) should be calculated and returned
- **verb**: a positive scalar integer indicating how many predictive locations (iterations) after which a progress statement should be printed to the console; a (default) value of `verb = 0` is quiet
- **...**: to comply with the generic `predict` method – currently unused

**Details**

`predict` returns predictive summary statistics by averaging over the samples from the posterior predictive distribution obtained from each of the particles in the cloud pointed to by the object (`object`)

`coef` returns a matrix of regression coefficients used in linear model leaves (`model = "linear"`) leaves, averaged over all particles, for each XX location. For other models it prints a warning and defaults to `predict`.

The value(s) calculated are appended to `object`; the new fields are described below

Note that ALC calculations have been moved to the `alc.dynaTree` function(s)
Value

The object returned is of class "dynaTree", which includes a copy of the list elements from the object passed in, with the following (predictive) additions depending on whether object$model is for regression ("constant" or "linear") or classification ("class").

For regression:

mean
- a vector containing an estimate of the predictive mean at the XX locations

vmean
- a vector containing an estimate of the variance of predictive mean at the XX locations

var
- a vector containing an estimate of the predictive variance (average variance plus variance of mean) at the XX locations

df
- a vector containing the average degrees of freedom at the XX locations

q1
- a vector containing an estimate of the 5% quantile of the predictive distribution at the XX locations, unless quants = FALSE

q2
- a vector containing an estimate of the 95% quantile of the predictive distribution at the XX locations, unless quants = FALSE

yy(pred)
- if yy != NULL then this contains the predictive probability of the true yy values at the XX locations

ei
- a vector containing an estimate of the EI statistic, unless ei = FALSE

For classification:

p
- a nrow(XX)-by-max(object$y) matrix of mean class probabilities for each of max(object$y) classes at the predictive data locations

entropy
- a nrow(XX) vector of predictive entropys at the predictive data locations

For coef a new RXXc field is created so as not to trample on XXs that may have been used in a previous predict, plus

ccoef
- a nrow(XX)-by-m+icept

matrix of particle- averaged regression coefficients.

Author(s)

Robert B. Gramacy <rbg@vt.edu>,
Matt Taddy and Christoforos Anagnostopoulos

References

https://bobby.gramacy.com/r_packages/dynaTree/
See Also
dynaTree, update.dynaTree, plot.dynaTree, alc.dynaTree, entropyX.dynaTree

Examples
## see the example(s) section(s) of dynaTree and
## update.dynaTree and the demos (demo(package=dynaTree))

rejuvenate.dynaTree  Rejuvenate particles from the dynaTree posterior

Description
Re-pass the X-y pairs in the object in a random (or specified) order to temporarily double the size
of the particle set

Usage
## S3 method for class 'dynaTree'
rejuvenate(object, odr = order(runif(length(object$y))), verb = round(length(object$y)/10))

Arguments
object  a "dynaTree"-class object built by dynaTree
odr    an integer vector of length(object$y) specifying the order in which the object$X-
        object$y paris should be processed for the rejuvenated particles
verb   a positive scalar integer indicating how many time steps (iterations) should pass
        before a progress statement is printed to the console; a value of verb = 0 is quiet

Details
The rejuvenate function causes the particle set to temporarily double, to have size 2 * object$N. The
new object$N particles represent a discrete approximation to the dynaTree posterior under the
ordering specified by odr, which may be random. Subsequent calls to update.dynaTree cause the
particle set to revert back to object$N particles as only that many are obtained from the particle
learning resample step.

This function can be particularly useful in online learning contexts, where retire.dynaTree is
used to retain information on discarded data, especially when the data is discarded historically
to deal with drifting concepts. Since the new, rejuvenated, particles are based only on the active
data, object$X-object$y pairs (and not the retired data via informative leaf priors), subsequent
update.dynaTree steps allow the data to dictate if old (informative prior) or new (default prior)
particles are best for the new concept
Value

The returned list is the same as `dynaTree` – i.e., a "dynaTree"-class object but with \(2 \times \text{object}\$N\) particles. Note that \text{object}\$N\ is not updated to reflect this fact, but the C-side object will indeed have a double particle set. Repeated calls to `rejuvenate` will cause the particle set to double again.

Note

The object (\text{object}) must contain a pointer to a particle cloud (\text{object}\$num) which has not been deleted by `deletecloud`. In particular, it cannot be an object returned from `dynaTrees`.

Author(s)

Robert B. Gramacy <rbg@vt.edu>,
Matt Taddy and Christoforos Anagnostopoulos

References


https://bobby.gramacy.com/r_packages/dynaTree/

See Also

dynaTree, alcX.dynaTree, entropyX.dynaTree, update.dynaTree, retire.dynaTree

Examples

```r
## see retire.dynaTree for a combined example
## illustrating rejuvenation
```

Description

Computes relevance statistics for each input coordinate by calculating their particle-averaged mean reduction in variance each time that coordinate is used as a splitting variable in (an internal node of) the tree(s).

Usage

```r
relevance.dynaTree(object, rect = NULL, categ = NULL,
                        approx = FALSE, verb = 0)
```
Arguments

- **object**: a "dynaTree"-class object built by `dynaTree`
- **rect**: an optional matrix with two columns and `ncol(object$X)` rows describing the bounding rectangle for the ALC integration; the default that is used when `rect = NULL` is the bounding rectangle obtained by applying `range` to each column of `object$X` (taking care to remove the first/intercept column of `object$X` if `icet = "augmented"`)
- **categ**: A vector of logicals of length `ncol(object$X)` indicating which, if any, dimensions of the input space should be treated as categorical; the default `categ` argument is `NULL` meaning that the categorical inputs are derived from `object$X` in a sensible way
- **approx**: a scalar logical indicating if the count of the number of data points in the leaf should be used in place of its area; this can help with numerical accuracy in high dimensional input spaces
- **verb**: a positive scalar integer indicating how many particles should be processed (iterations) before a progress statement should be printed to the console; a (default) value of `verb = 0` is quiet

Details

Each binary split in the tree (in each particle) emits a reduction in variance (for regression models) or a reduction in entropy (for classification). This function calculates these reductions and attributes them to the variable(s) involved in the split(s). Those with the largest relevances are the most useful for prediction. A sensible variable selection rule based on these relevances is to discard those variables whose median relevance is not positive. See the Gramacy, Taddy, & Wild (2011) reference below for more details.

The new set of particles is appended to the old set. However after a subsequent `update.dynaTree` call the total number of particles reverts to the original amount.

Note that this does not work well with `dynaTree` objects which were built with `model="linear"`. Rather, a full sensitivity analysis (`sens.dynaTree`) is needed. Usually it is best to first do `model="constant"` and then use `relevance.dynaTree`. Bayes factors (`getBF`) can be used to back up any variable selections implied by the relevance. Then, if desired, one can re-fit on the new (possibly reduced) set of predictors with `model="linear"`.

There are no caveats with `model="class"`

Value

The entire object is returned with a new entry called `relevance` containing a matrix with `ncol(X)` columns. Each row contains the sample from the relevance of each input, and there is a row for each particle.

Author(s)

Robert B. Gramacy <rbg@vt.edu>,
Matt Taddy and Christoforos Anagnostopoulos
retire.dynaTree

References
https://bobby.gramacy.com/r_packages/dynaTree/

See Also
dynaTree, sens.dynaTree, predict.dynaTree varpropuse, varproptotal

Examples
## see the examples in sens.dynaTree for the relevances;
## Also see varpropuse and the class2d demo via
## demo("class2d")

retire.dynaTree  Retire (i.e. remove) data from the a dynaTree model

Description
Allows the removal (or “retireing”) of X-y pairs from a "dynaTree"-class object to facilitate online learning; “retired” pairs ar absorbed into the leaf prior(s)

Usage
## S3 method for class 'dynaTree'
retire(object, indices, lambda = 1, verb = 0)

Arguments
<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>object</td>
<td>a &quot;dynaTree&quot;-class object built by dynaTree</td>
</tr>
<tr>
<td>indices</td>
<td>a vector of positive integers in 1:nrow(object$X) indicating which X-y pairs to “retire”; must have length(indices) &lt;= nrow(object$X)</td>
</tr>
<tr>
<td>lambda</td>
<td>a scalar proportion (forgetting factor) used to downweight the previous prior summary statistics</td>
</tr>
<tr>
<td>verb</td>
<td>a nonzero scalar causes info about the “retired” indices, i.e., their X-y values, to be printed to the screen as they are “retired”</td>
</tr>
</tbody>
</table>

Details
Primarily for use in online learning contexts. After “retireing” the predictive distribution remains unchanged, because the sufficient statistics of the removed pairs enters the prior in the leaves of the tree of each particle. Further update.dynaTree calls (adding data) may cause changes to the posterior predictive as grow moves cannot keep the “retires”; see a forthcoming paper for more details. In many ways, retire.dynaTree is the opposite of update.dynaTree except that the loss of information upon “retireing” is not complete.
Drifting regression or classification relationships may be modeled with a forgetting factor $\lambda$ < 1. The `alcX.dynaTree` provides a good, and computationally efficient, heuristic for choosing which points to “retire” for regression models, and likewise `entropyX.dynaTree` for classification models.

Note that classification models (model = "class") are not supported, and implicit intercepts (icept = "implicit") with linear models (model = "linear") are not supported at this time.

Value
returns a "dynaTree"-class object with updated attributes

Note
In order to use model = "linear" with `dynaTree` and retirement one must also specify icept = "augmented" which automatically augments an extra column of ones onto the input $X$ design matrix/matrices. The `retire` function only supports this icept case.

Author(s)
Robert B. Gramacy <rbg@vt.edu>,
Matt Taddy and Christoforos Anagnostopoulos

References
https://bobby.gramacy.com/r_packages/dynaTree/

See Also
`dynaTree, alcX.dynaTree, entropyX.dynaTree, update.dynaTree, rejuvenate.dynaTree`

Examples
```r
n <- 100
Xp <- runif(n,-3,3)
XX <- seq(-3,3, length=200)
Yp <- Xp + Xp^2 + rnorm(n, 0, .2)
rect <- c(-3,3)
out <- dynaTree(Xp, Yp, model="linear", icept="augmented")

## predict and plot
out <- predict(out, XX)
plot(out, main="parabola data", lwd=2)

## randomly remove half of the data points
out <- retire(out, sample(1:n, n/2, replace=FALSE))

## predict and add to plot -- shouldn't change anything
```
out <- predict(out, XX)
plot(out, add=TRUE, col=3)
points(out$X[, -1], out$y, col=3)

## now illustrating rejuvenation, which should result
## in a change to the predictive surface
out <- rejuvenate(out)
out <- predict(out, XX)
plot(out, add=TRUE, col=4)
legend("top", c("original", "retired", "rejuvenated"),
  col=2:4, lty=1)

## clean up
deletecloud(out)

## see demo("online") for an online learning example
## where ALC is used for retirement

---

**sens.dynaTree**

*Monte Carlo Sensitivity Analysis for dynaTree Models*

**Description**

A Monte Carlo sensitivity analysis using random Latin hypercube samples (LHSs) or bootstrap resamples for each particle to estimate main effects as well as 1st order and total sensitivity indices

**Usage**

```r
## S3 method for class 'dynaTree'
sens(object, class = NULL, nns = 1000, nME = 100,
     span = 0.3, method = c("lhs", "boot"),
     lhs = NULL, categ = NULL, verb = 0)
```

**Arguments**

- `object` a "dynaTree"-class object built by `dynaTree`
- `class` only valid for `object$model = "class"`, allows the user to specify the subset of class labels in `unique(object$y)` for which sensitivity indices are calculated. The implementation loops over the vector of labels provided. The default of `NULL` results in `class = unique(object$y)`
- `nns` A positive integer scalar indicating the size of each LHS or bootstrap drawn for use in the Monte Carlo integration scheme underlying the sensitivity analysis; the total number of locations is `nn.lhs*(ncol(X)+2)`
- `nME` A positive integer scalar indicating number of grid points, in each input dimension, upon which main effects will be estimated
A positive real-valued scalar giving the smoothing parameter for main effects integration: the fraction of nns points that will be included in a moving average window that is used to estimate main effects at the nME locations in each input dimension.

method indicates whether LHS or bootstrap should be used.

lhs if method = "lhs" then this argument should be a list with entries rect, shape and mode describing the marginal distributions of the Latin Hypercube; specify NULL for a default specification for method = "boot". The fields should have the following format(s):

- rect: Optional rectangle describing the domain of the uncertainty distribution with respect to which the sensitivity is to be determined. This defines the domain from which the LH sample is to be taken. The rectangle should be a matrix or data.frame with ncol(rect) = 2, and number of rows equal to the dimension of the domain. For 1-d data, a vector of length 2 is allowed. The default is the input data range of each column of (object$X).

- shape: Optional vector of shape parameters for Beta marginal distributions having length ncol(object$X) and elements > 1, i.e., concave Beta distributions. If specified, the uncertainty distribution (i.e. the LHS) is proportional to a joint pdf formed by independent Beta distributions in each dimension of the domain, scaled and shifted to have support defined by rect. If unspecified, the uncertainty distribution is uniform over rect. The specification shape[i]=0 instructs sens to treat the i’th dimension as a binary variable. In this case, mode[i] is the probability parameter for a bernoulli uncertainty distribution, and we must also have rect[i,]=c(0,1).

- mode: Optional vector of mode values for the Beta uncertainty distribution. Vector of length equal to the dimension of the domain, with elements within the support defined by rect. If shape is specified, but this is not, then the scaled Beta distributions will be symmetric.

categ A vector of logicals of length ncol(object$X) indicating which, if any, dimensions of the input space should be treated as categorical; this input is used to help set the default lhs$shape argument if not specified; the default categ argument is NULL meaning that the categorical inputs are derived from object$X in a sensible way.

verb a positive scalar integer indicating how many predictive locations (iterations) after which a progress statement should be printed to the console; a (default) value of verb = 0 is quiet.

details


1st Order for input i,

\[ S(i) = \frac{\text{Var}(E[f|x_i])}{\text{Var}(f)} \]

where \( x_i \) is the i-th input.

Total Effect for input i,

\[ T(i) = E[\text{Var}(f|x_{-i})]/\text{Var}(f) \]
where \( x_{-i} \) is all inputs except for the \( i \)-th.

All moments are with respect to the appropriate marginals of the uncertainty distribution \( U \) — that is, the probability distribution on the inputs with respect to which sensitivity is being investigated. Under this approach, the integrals involved are approximated through averages over properly chosen samples based on two LH samples proportional to \( U \). If \( nns \) is the sample size for the Monte Carlo estimate, this scheme requires \( nns \times (\text{ncol}(X)+2) \) function evaluations.

The sens.dynaTree function implements the method for unknown functions \( f \), through prediction via one of the \texttt{tgp} regression models conditional on an observed set of \( X \) locations. For each particle, treated as sample from the \texttt{dynaTree} model posterior, the \( nns \times (\text{ncol}(X)+2) \) locations are drawn randomly from the LHS scheme and realizations of the sensitivity indices are calculated. Thus we obtain a posterior sample of the indices, incorporating variability from both the Monte Carlo estimation and uncertainty about the function output. Since a subset of the predictive locations are actually an LHS proportional to the uncertainty distribution, we can also estimate the main effects through simple non-parametric regression (a moving average).

See the Gramacy, Taddy, & Wild (2011) reference below for more details.

If \( \text{method} = \text{"boot"} \) is used then simply replace LHS above with a bootstrap resample of the \texttt{object$X} locations.

As with prediction, the \texttt{dynaTrees} function enables repeated calls to sens.dynaTree

**Value**

The object returned is of class "dynaTree", which includes a copy of the list elements from the \texttt{object} passed in, with the following (sensitivity-analysis specific) additions.

- **MEgrid**
  - An \( nME \)-by-\( \text{ncol}(\text{object$X}) \) matrix containing the main effects predictive grid at which the following \texttt{MEmean}, \texttt{MEq1}, and \texttt{MEq2} quantities were obtained

- **MEmean**
  - A matrix with \( \text{ncol}(\text{object$X}) \) columns and \( nME \) rows containing the mean main effects for each input dimension

- **MEq1**
  - same as \texttt{MEmean} but containing the 5% quantiles

- **MEq2**
  - same as \texttt{MEmean} but containing the 95% quantiles

- **S**
  - An \texttt{object$N}-row and \texttt{ncol}(\texttt{object$X}) \texttt{matrix} containing the posterior (samples) of the 1st Order Sobol sensitivity indices

- **T**
  - same as \texttt{S} but containing the Total Effect indices

In the case of \texttt{object$model = \text{"class"}} the entries listed above will themselves be lists with an entry for each class specified on input, or all classes as is the default

**Note**

The quality of sensitivity analysis is dependent on the size of the LHSs used for integral approximation; as with any Monte Carlo integration scheme, the sample size (\( nns \)) must increase with the dimensionality of the problem. The total sensitivity indices \( T \) are forced non-negative, and if negative values occur it is necessary to increase \( nnd \). Postprocessing replaces negative values with \texttt{NA}
Author(s)
Robert B. Gramacy <rbg@vt.edu>,
Matt Taddy and Christoforos Anagnostopoulos

References
https://bobby.gramacy.com/r_packages/dynaTree/

See Also
dynaTree, predict.dynaTree, relevance.dynaTree, varpropuse, varproptotal

Examples
## friedman data
if(require("tgp")) {
  f <- friedman.1.data(1000)
  X <- f[,1:6]
  Z <- f$Y

  ## fit the model and do the sensitivity analysis
  N <- 100 ## use N >= 1000 for better results
  ## small N is for fast CRAN checks
  out <- dynaTree(X=X, y=Z, N=N, ab=c(0.01,2))
  ## also try with model="linear"

  ## gather relevance statistics
  out <- relevance(out)
  boxplot(out$relevance)
  abline(h=0, col=2, lty=2)
  ## relevance stats are not as useful when model="linear"
  ## since it will appear that x4 and x5 not helpful; these
  ## interact linearly with the response

  ## full simulation-based sensitivity analysis, the dynaTree::
  ## part is only needed if the tgp package is loaded
  out <- dynaTree::sens(out, verb=100)

  ## plot the main effects
  r <- range(rbind(c(out$MEmean, out$MEq1, out$MEq2)))
  par(mfrow=c(1,ncol(out$X)), mar=c(5,3,2,1))
  plot(out$MEgrid[,1], out$MEmean[,1], type="l", ylim=r, lwd=2, ylab="",
       xlab=colnames(out$MEmean)[1])
  lines(out$MEgrid[,1], out$MEq1[,1], lty=2, lwd=2)
  lines(out$MEgrid[,1], out$MEq2[,1], lty=2, lwd=2)
  if(ncol(out$X) > 1) {
    for(d in 2:ncol(out$X)) {
}
update.dynaTree

Description

Updating an already-initialized dynamic tree model with new input/output pairs, primarily to facilitate sequential design and optimization applications.

Usage

```r
## S3 method for class 'dynaTree'
update(object, X, y, verb = round(length(y)/10), ...)
```

Arguments

- **object**: a "dynaTree"-class object built by `dynaTree`
- **X**: an augmenting design matrix of real-valued predictors with `ncol(X) = object$m`
- **y**: an augmenting vector of real-valued responses or integer categories with `length(y) = nrow(X)`
- **verb**: a positive scalar integer indicating how many time steps (iterations) after which a progress statement should be printed to the console; a value of `verb = 0` is quiet
- **...**: to comply with the generic `predict` method – currently unused
Details

This function updates the dynaTree fit with new (X,y) pairs by the Particle Learning (PL) algorithm. The updated fit will be for data combined as rbind(object$X, X) and c(object$Y, y).

The primary use of this function is to facilitate sequential design by optimization and active learning. Typically one would use predict.dynaTree to estimate active learning statistics at candidate location. These are used to pick new (X,y) locations to add to the design – the new fit being facilitated by this function; see the examples below.

Value

The returned list is the same as dynaTree – i.e., a "dynaTree"-class object

Note

The object (object) must contain a pointer to a particle cloud (object$num) which has not been deleted by deletecloud. In particular, it cannot be an object returned from dynaTrees

Author(s)

Robert B. Gramacy <rbg@vt.edu>,
Matt Taddy and Christoforos Anagnostopoulos

References


https://bobby.gramacy.com/r_packages/dynaTree/

See Also

predict.dynaTree, dynaTree, plot.dynaTree, deletecloud, getBF

Examples

```r
## simple function describing (x,y) data
fld <- function(x, sd=0.1) {
  return( sin(x) - dcauchy(x,1.6,0.15) + rnorm(1,0,sd))
}

## initial (x,y) data
X <- seq(0, 7, length=30)
y <- fld(X)

## PL fit to initial data
obj <- dynaTree(X=X, y=y, N=1000, model="linear")
```
## a predictive grid
XX <- seq(0, 7, length=100)
obj <- predict(obj, XX, quants=FALSE)

## follow the ALM algorithm and choose the next
## point with the highest predictive variance
m <- which.max(obj$var)
xstar <- drop(obj$XX[m,])
ystar <- f1d(xstar)

## plot the next chosen point
par(mfrow=c(2,1))
plot(obj, ylab="y", xlab="x", main="fitted surface")
points(xstar, ystar, col=3, pch=20)
plot(obj$XX, sqrt(obj$var), type="l", xlab="x",
     ylab="predictive sd", main="active learning")

## update the fit with (xstar, ystar)
obj <- update(obj, xstar, ystar)

## new predictive surface
obj <- predict(obj, XX, quants=FALSE)

## plotted
plot(obj, ylab="y", xlab="x", main="updated fitted surface")
plot(obj$XX, sqrt(obj$var), type="l", xlab="x",
     ylab="predictive sd", main="active learning")

## delete the cloud to prevent a memory leak
deletecloud(obj); obj$num <- NULL

## see demo("design") for more iterations and
## design under other active learning heuristics
## like ALC, and EI for optimization; also see
## demo("online") for an online learning example

---

varpropuse Calculate the proportion of variables used in tree splits, and average summary stats of tree heights and leaf sizes

**Description**

Calculates the proportion of particles which use each input to make a tree split and the proportion of all splits in trees of each particle that correspond to each input variable; also provides tree height and leaf size summary information

**Usage**

## S3 method for class 'dynaTree'
### Details

`varpropuse` gives the proportion of times a particle uses each input variable in a tree split; `varproptotal` gives the proportion of total uses by the tree in each particle (i.e., averaged over the total number of splits used in the tree).

Usually, `varpropuse` returns a vector of (nearly) all ones unless there are variables which are not useful in predicting the response. Using `model = "linear"` is not recommended for this sort of variable selection.

`treestats` returns the average tree height, and the average leaf size, both active and retired.

### Value

For `varprop*`, a vector of proportions of length `ncol(object$X)` is returned; for `treestats` a 1-row, 4-column `data.frame` is returned.

### Author(s)

Robert B. Gramacy `<rbg@vt.edu>`,
Matt Taddy and Christoforos Anagnostopoulos

### References


[https://bobby.gramacy.com/r_packages/dynaTree/](https://bobby.gramacy.com/r_packages/dynaTree/)

### See Also

dynaTree, sens.dynaTree, relevance.dynaTree

### Examples

```r
## fit a dynaTree model to the Ozone data
X <- airquality[,2:4]
y <- airquality$Ozone
na <- apply(is.na(X), 1, any) | is.na(y)
out <- dynaTree(X=X[!na,], y=y[!na])

## obtain variable usage proportions
varpropuse(out)
```
varproptotal(out)

## gather relevance statistics which are more meaningful
out <- relevance(out)
boxplot(out$relevance)
abline(h=0, col=2, lty=2)

## obtain tree statistics
treestats(out)

## clean up
deletecloud(out)
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