## Package 'dynaTree'

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Title Dynamic Trees for Learning and Design

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Suggests interp, tgp, plgp, MASS

**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 (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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URL https://bobby.gramacy.com/r\_packages/dynaTree/

NeedsCompilation yes

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dynaTree-package Dynamic trees for learning and design

## 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").

## Author(s)

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

## References

Taddy, M.A., Gramacy, R.B., and Polson, N. (2011). "Dynamic trees for learning and design" Journal of the American Statistical Association, 106(493), pp. 109-123; arXiv:0912.1586

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

#### Arguments

| object | a "dynaTree"-class object built by dynaTree   |
|--------|---|
| rect   | for alcX, a matrix with two columns and ncol(object\$X) rows describing<br>the bounding rectangle for the ALC integration; the default that is used when<br>rect = NULL is the bounding rectangle obtained by applying range to each col-<br>umn of object\$X (taking care to remove the first/intercept column of object\$X<br>if icept = "augmented"; only applies to regression models (object\$model !=<br>"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, dimen-<br>sions of the input space should be treated as categorical; this input is used to help<br>with the analytic integrals from a rect-based calculation, which means it should<br>not specified along with Xref; the default categ argument is NULL meaning that<br>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<br>the numerical ALC calculation - a matrix with ncol(X) columns. If NULL, the<br>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;<br>usually these weights are class probabilities for response surfaces under con-<br>straints  |

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

Taddy, M.A., Gramacy, R.B., and Polson, N. (2011). "Dynamic trees for learning and design" Journal of the American Statistical Association, 106(493), pp. 109-123; arXiv:0912.1586

Anagnostopoulos, C., Gramacy, R.B. (2013) "Information-Theoretic Data Discarding for Dynamic Trees on Data Streams." Entropy, 15(12), 5510-5535; arXiv:1201.5568

https://bobby.gramacy.com/r\_packages/dynaTree/

## See Also

dynaTree, predict.dynaTree, and retire.dynaTree

#### Examples

```
## 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")</pre>
## calculate the alcX
```

verb

## dynaTree-class

```
out <- alcX(out, rect=rect)</pre>
## to compare to analytic
out <- alc(out, XX=out$X[,-1], rect=rect)</pre>
## plot comparison between alcX and predict-ALC
plot(out$X[,-1], out$alcX)
o <- order(out$X[,2])</pre>
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)</pre>
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"): ...
```

#### Author(s)

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

## References

Taddy, M.A., Gramacy, R.B., and Polson, N. (2011). "Dynamic trees for learning and design" Journal of the American Statistical Association, 106(493), pp. 109-123; arXiv:0912.1586

Gramacy, R.B., Taddy, M.A., and S. Wild (2011). "Variable Selection and Sensitivity Analysis via Dynamic Trees with an Application to Computer Code Performance Tuning" arXiv:1108.4739

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)

## dynaTrees

## 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, icept = 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,
    icept = 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

| Х      | A design matrix of real-valued predictors   |
|--------|---|
| У      | A vector of length nrow(X) containing real-valued responses (for regression) or positive integer-valued class labels (for classification)   |
| Ν      | a positive scalar integer indicating the number of particles to be used   |
| R      | a scalar integer >= 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<br>in each repeat of dynaTrees; each repeat will use a different random subset of<br>size sub  |
| model  | indicates the type of model to be used at the leaves of the tree; "constant"<br>and "linear" apply to regression, and "class" to multinomial classification;<br>finally "prior" was recently added to explore sampled without data  |
| nu0s20 | a two-vector indicating Inverse Gamma prior parameters $c(nu0, sigma20)$ for<br>the variance in each leaf node, $\sigma^2$ . A $c(0,0)$ setting indicates a default, scale-<br>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(splitmin, basemax) for the "linear" model. It gives the first column of X on which treed partition-<br>ing 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 >= minp indicating the time index at which treed parti-<br>tioning is allowed to start  |
| icept  | indicates the type of intertcept 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<br>that the former can default to a constant model fit if leaf design matrices become<br>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;<br>also see predict.dynaTree and some explanation in the details below   |
| уу       | 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 func-<br>tions to be called on after each repetition to collect the usage proportions of each<br>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;<br>only applies to 1-d data and dynaTrees   |
| proj     | when ncol(x\$X) > 1 and plotit = TRUE this argument is passed to plot.dynaTree<br>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"<br>uses the lower (L) and upper (U) rectangle method based on minp (above) as de-<br>scribed in the seminal reference in which the growing location and dimension is<br>sampled uniformly. It can be computationally intensive for large input spaces.<br>A thriftier option (the default) in this case is "luvar" which uniformly chooses<br>the splitting variable first and then uses the LU method marginally. Thriftier still<br>is "reject" which just proposes uniformly in the bounding leaf rectangle and<br>rejects subsequent grows that lead to partitions with too few data points; (see the<br>minp argument) |
| verb     | a positive scalar integer indicating how many time steps (iterations) should pass<br>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

## dynaTrees

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=c(alpha, beta) via the and minp. It was originally described by Chipman et al., (1998, 2002)

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

and subsequently augmented to enforce a minimum number of points (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)   |
|--------|---|
| Т      | nrow(X)   |
| Ν      | the number of particles used  |
| Х      | a copy of the design matrix X   |
| У      | a copy of the responses y   |
| model  | a copy of the specified leaf model  |
| params | a vector containing c(nu0s20, alpha, beta, minp, sb, 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*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

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)

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

#### References

Taddy, M.A., Gramacy, R.B., and Polson, N. (2011). "Dynamic trees for learning and design" Journal of the American Statistical Association, 106(493), pp. 109-123; arXiv:0912.1586

Gramacy, R.B., Taddy, M.A., and S. Wild (2011). "Variable Selection and Sensitivity Analysis via Dynamic Trees with an Application to Computer Code Performance Tuning" arXiv:1108.4739

Carvalho, C., Johannes, M., Lopes, H., and Polson, N. (2008). "Particle Learning and Smoothing". Discussion Paper 2008-32, Duke University Dept. of Statistical Science.

Chipman, H., George, E., & McCulloch, R. (1998). *Bayesian CART model search (with discussion)*. Journal of the American Statistical Association, **93**, 935–960.

Chipman, H., George, E., & McCulloch, R. (2002). *Bayesian treed models*. Machine Learning, **48**, 303–324.

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
```

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## Note

## dynaTrees

```
parab.fit <- predict(parab.fit, XX=seq(-3, 3, length=100))</pre>
plot(parab.fit)
## try duplicating the object
parab.fit.copy <- copy(parab.fit)</pre>
## must delete the cloud or memory may leak
deletecloud(parab.fit); parab.fit$num <- NULL</pre>
## to delete all clouds, do:
deleteclouds()
## for more examples of dynaTree see update.dynaTree
## Motorcycle accident data
if(require("MASS")) {
  data(mcycle)
  Xm <- mcycle[,1]</pre>
  Ym <- mcycle[,2]</pre>
  XXm <- seq(min(mcycle[,1]), max(mcycle[,1]), length=100)</pre>
  R <- 2 \#\# use R >= 10 for better results
  ## small R is for faster CRAN checks
  ## fit constant model with R=2 repeats and predictions
  moto.fit <- dynaTrees(Xm, Ym, XX=XXm, R=R, plotit=TRUE)</pre>
  ## plot the averages
  plot(moto.fit, ptype="mean")
  ## clouds automatically deleted by dynaTrees
}
## Not run:
## 2-d/3-class classification data
library(plgp)
library(tgp)
xx <- seq(-2, 2, length=20)</pre>
XX <- expand.grid(xx, xx)</pre>
X <- dopt.gp(125, Xcand=XX)$XX
C <- exp2d.C(X)
## fit a classification model with R=10 repeats,
class.fit <- dynaTrees(X, C, XX=XX, model="class")</pre>
## for plot the output (no generic plotting available)
cols <- c(gray(0.85), gray(0.625), gray(0.4))</pre>
par(mfrow=c(1,2))
library(interp)
## plot R-averaged predicted class
mclass <- apply(class.fit$p, 1, which.max)</pre>
image(interp(XX[,1], XX[,2], mclass), col=cols,
      xlab="x1", ylab="x2", main="repeated class mean")
points(X)
```

## 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

M. Harries. "Splice-2 Comparative Evaluation: Electricity Pricing". University of New South Wales, School of Computer Science and Engineering technical report (1999)

elec2

## References

Anagnostopoulos, C., Gramacy, R.B. (2013) "Information-Theoretic Data Discarding for Dynamic Trees on Data Streams." Entropy, 15(12), 5510-5535; arXiv:1201.5568

M. Baena-Garcia, J. del Campo-Avila, R., Fidalgo, A. Bifet, R. Gavalda and R. Morales-Bueno. "Early drift detection method". *ECML PKDD 2006 Workshop on Knowledge Discovery from Data Streams*, pp. 77-86 (2006)

L.I. Kuncheva C.O. and Plumpton. "Adaptive Learning Rate for Online Linear Discriminant Classifiers". *SSPR and SPR 2008, Lecture Notes in Computer Science (LNCS)*, 5342, pp. 510-519 (2008)

#### Examples

```
## this is a snipet 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])</pre>
## predictive likelihood for repated 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")</pre>
w <- 1
for(t in (n+1):T) {
  ## predict the next data point
  ## full model
  fit <- predict(fit, XX=X[t,], yy=y[t])</pre>
  hits[t] <- which.max(fit$p) == y[t]</pre>
  ## sanity check retiring index
  if(any(fit$X[w,] != X[t-n,])) stop("bad retiring")
  ## retire
  fit <- retire(fit, w)</pre>
  ## update retiring index
  w <- w + 1; if(w >= n) w <- 1
  ## update with new point
  fit <- update(fit, X[t,], y[t], verb=100)</pre>
```

## 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="1", main="moving window of hit rates",
        ylab="hit rates", xlab="t")</pre>
```

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

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

#### plot.dynaTree

#### References

Taddy, M.A., Gramacy, R.B., and Polson, N. (2011). "Dynamic trees for learning and design" Journal of the American Statistical Association, 106(493), pp. 109-123; arXiv:0912.1586

Gramacy, R.B., Taddy, M.A., and S. Wild (2011). "Variable Selection and Sensitivity Analysis via Dynamic Trees with an Application to Computer Code Performance Tuning" arXiv:1108.4739

https://bobby.gramacy.com/r\_packages/dynaTree/

#### See Also

dynaTree, update.dynaTree, link{logpost}

#### Examples

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

```
## 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

#### Arguments

| х     | 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 spec-<br>ifying 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:<br>"each" shows each surface with its own set of three lines, and "mean" shows<br>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)

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

#### References

Taddy, M.A., Gramacy, R.B., and Polson, N. (2011). "Dynamic trees for learning and design" Journal of the American Statistical Association, 106(493), pp. 109-123; arXiv:0912.1586

https://bobby.gramacy.com/r\_packages/dynaTree/

#### See Also

predict.dynaTree, dynaTree, update.dynaTree

#### Examples

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

## Description

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

#### Usage

## Arguments

| object | a "dynaTree"-class object built by dynaTree   |
|--------|---|
| XX     | a design matrix of predictive locations (where ncol(XX) == ncol(X))   |
| уу     | 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 visu-<br>alization, but less so for active learning); calculating predictive quantiles is ex-<br>pensive and should be turned off if prediction is not being used for visualization,<br>e.g., if used for active learning |
| ei     | a scalar logical indicating if the expected improvement statistic (for optimiza-<br>tion) 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 |
| yypred | 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:

| р       | 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 XXc field is created so as not to trample on XXs that may have been used in a previous predict, plus

coef 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

Taddy, M.A., Gramacy, R.B., and Polson, N. (2011). "Dynamic trees for learning and design" Journal of the American Statistical Association, 106(493), pp. 109-123; arXiv:0912.1586

https://bobby.gramacy.com/r\_packages/dynaTree/

#### rejuvenate.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

#### 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<br>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 \* object\$N particles. Note that 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 (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

Taddy, M.A., Gramacy, R.B., and Polson, N. (2011). "Dynamic trees for learning and design" Journal of the American Statistical Association, 106(493), pp. 109-123; arXiv:0912.1586

Anagnostopoulos, C., Gramacy, R.B. (2013) "Information-Theoretic Data Discarding for Dynamic Trees on Data Streams." Entropy, 15(12), 5510-5535; arXiv:1201.5568

Carvalho, C., Johannes, M., Lopes, H., and Polson, N. (2008). "Particle Learning and Smoothing". Discussion Paper 2008-32, Duke University Dept. of Statistical Science.

https://bobby.gramacy.com/r\_packages/dynaTree/

## See Also

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

#### Examples

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

relevance.dynaTree Calculate relevance statistics for input coordinates

## 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

#### Arguments

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

## References

Gramacy, R.B., Taddy, M.A., and S. Wild (2011). "Variable Selection and Sensitivity Analysis via Dynamic Trees with an Application to Computer Code Performance Tuning" arXiv:1108.4739

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; "retireed" pairs ar absorbed into the leaf prior(s)

## Usage

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

#### Arguments

| object  | a "dynaTree"-class object built by dynaTree   |
|---------|---|
| indices | a vector of positive integers in 1:nrow(object\$X) indicating which X-y pairs to "retire"; must have length(indices) <= nrow(object\$X) |
| lambda  | a scalar proportion (forgetting factor) used to downweight the previous prior summary statistics  |
| verb    | a nonzero scalar causes info about the "retireed" indices, i.e., their X-y values, to be printed to the screen as they are "retireed"   |

#### 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.

#### retire.dynaTree

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 link{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

Anagnostopoulos, C., Gramacy, R.B. (2013) "Information-Theoretic Data Discarding for Dynamic Trees on Data Streams." Entropy, 15(12), 5510-5535; arXiv:1201.5568

https://bobby.gramacy.com/r\_packages/dynaTree/

#### See Also

dynaTree, alcX.dynaTree, entropyX.dynaTree, update.dynaTree, rejuvenate.dynaTree

#### Examples

```
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
```

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

## 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 dimen-<br>sion, upon which main effects will be estimated  |

| span   | 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<br>and mode describing the marginal distributions of the Latin Hypercube; specify<br>NULL for a default specification for method = "boot". The fields should have the<br>following format(s):  |
|        | • rect: Optional rectangle describing the domain of the uncertainty distribu-<br>tion with respect to which the sensitivity is to be determined. This defines<br>the domain from which the LH sample is to be taken. The rectangle should<br>be a matrix or data.frame with ncol(rect) = 2, and number of rows<br>equal to the dimension of the domain. For 1-d data, a vector of length 2 is<br>allowed. The default is the input data range of each column of (object\$X).  |
|        | <ul> <li>shape: Optional vector of shape parameters for Beta marginal distributions having length ncol(object\$X) and elements &gt; 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).</li> </ul> |
|        | • mode: Optional vector of mode values for the Beta uncertainty distribution.<br>Vector of length equal to the dimension of the domain, with elements within<br>the support defined by rect. If shape is specified, but this is not, then the<br>scaled Beta distributions will be symmetric.   |
| categ  | A vector of logicals of length ncol(object\$X) indicating which, if any, dimen-<br>sions of the input space should be treated as categorical; this input is used to<br>help set the default lhs\$shape argument if not specified; the default categ ar-<br>gument is NULL meaning that the categorical inputs are derived from object\$X<br>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

Saltelli (2002) describes a Latin Hypercube sampling based method for estimation of the 'Sobol' sensitivity indices:

1st Order for input *i*,

$$S(i) = \operatorname{Var}(E[f|x_i]) / \operatorname{Var}(f),$$

where  $x_i$  is the *i*-th input.

Total Effect for input *i*,

 $T(i) = E[\operatorname{Var}(f|x_{-i})]/\operatorname{Var}(f),$ 

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\*(nco1(X)+2) function evaluations.

The sens.dynaTree function implements the method for unknown functions f, through prediction via one of the **tgp** regression models conditional on an observed set of X locations. For each particle, treated as sample from the dynaTree model posterior, the nns\*(nco1(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 method = "boot" is used then simply replace LHS above with a bootstrap resample of the object\$X locations.

As with prediction, the 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 object passed in, with the following (sensitivity-analysis specific) additions.

| MEgrid | An nME-by-ncol(object\$X) matrix containing the main effects predictive grid at which the following MEmean, MEq1, and MEq2 quantities were obtained |
|--------|---|
| MEmean | A matrix with ncol(object\$X) columns and nME rows containing the mean main effects for each input dimension  |
| MEq1   | same as MEmean but containing the 5% quantiles  |
| MEq2   | same as MEmean but containing the 95% quantiles   |
| S      | An object\$N-row and ncol(object\$X) matrix containing the posterior (samples) of the 1st Order Sobol sensitivity indices                           |
| Т      | same as S but containing the Total Effect indices   |

In the case of object\$model = "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 NA

#### sens.dynaTree

## Author(s)

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

## References

Saltelli, A. (2002) *Making best use of model evaluations to compute sensitivity indices.* Computer Physics Communications, 145, 280-297.

Gramacy, R.B., Taddy, M.A., and S. Wild (2011). "Variable Selection and Sensitivity Analysis via Dynamic Trees with an Application to Computer Code Performance Tuning" arXiv:1108.4739

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)</pre>
 X <- f[,1:6]
 Z <- f$Y
 ## fit the model and do the sensitivity analysis
 N <- 100 ## use N >= 1000 for better results
 ## small N is for fast CRAN checks
 out <- dynaTree(X=X, y=Z, N=N, ab=c(0.01,2))</pre>
 ## also try with model="linear"
 ## gather relevance statistics
 out <- relevance(out)</pre>
 boxplot(out$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)</pre>
 ## plot the main effects
 r <- range(rbind(c(out$MEmean, out$MEq1, out$MEq2)))</pre>
 par(mfrow=c(1,ncol(out$X)), mar=c(5,3,2,1))
 plot(out$MEgrid[,1], out$MEmean[,1], type="1", 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)) {
```

```
plot(out$MEgrid[,d], out$MEmean[,d], col=d, type="1", ylim=r,
         lwd=2, xlab=colnames(out$MEmean)[d], ylab="")
    lines(out$MEgrid[,d], out$MEq1[,d], col=d, lty=2)
    lines(out$MEgrid[,d], out$MEq2[,d], col=d, lty=2)
 }
}
## Sobol indices
par(mfrow=c(1,2), mar=c(5,4,4,2))
boxplot(out$S, main="first order indices", xlab="inputs")
boxplot(out$T, main="total indices", xlab="inputs")
## these look better when model="linear"
## clean up
deletecloud(out)
## for a classification example using the sensitivity hooks
## in the dynaTrees function, see the class2d demo
## i.e., demo("class2d")
}
```

update.dynaTree Updating a Dynamic Tree Model With New Data

## Description

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

## Usage

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

## Arguments

| object | a "dynaTree"-class object built by dynaTree   |
|--------|---|
| Х      | an augmenting design matrix of real-valued predictors with ncol(X) = object\$m  |
| У      | 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

Taddy, M.A., Gramacy, R.B., and Polson, N. (2011). "Dynamic trees for learning and design" Journal of the American Statistical Association, 106(493), pp. 109-123; arXiv:0912.1586

Anagnostopoulos, C., Gramacy, R.B. (2013) "Information-Theoretic Data Discarding for Dynamic Trees on Data Streams." Entropy, 15(12), 5510-5535; arXiv:1201.5568

Carvalho, C., Johannes, M., Lopes, H., and Polson, N. (2008). "Particle Learning and Smoothing". Discussion Paper 2008-32, Duke University Dept. of Statistical Science.

https://bobby.gramacy.com/r\_packages/dynaTree/

#### See Also

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

## Examples

```
## simple function describing (x,y) data
f1d <- 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 <- f1d(X)
## PL fit to initial data
obj <- dynaTree(X=X, y=y, N=1000, model="linear")</pre>
```

```
## a predictive grid
XX <- seq(0,7, length=100)
obj <- predict(obj, XX, quants=FALSE)</pre>
## follow the ALM algorithm and choose the next
## point with the highest predictive variance
m <- which.max(obj$var)</pre>
xstar <- drop(obj$XX[m,])</pre>
ystar <- f1d(xstar)</pre>
## 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)</pre>
## new predictive surface
obj <- predict(obj, XX, quants=FALSE)</pre>
## plotted
plot(obj, ylab="y", xlab="x", main="updated fitted surface")
plot(obj$XX, sqrt(obj$var), type="1", xlab="x",
     ylab="predictive sd", main="active learning")
## delete the cloud to prevent a memory leak
deletecloud(obj); obj$num <- NULL</pre>
## 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'

#### varpropuse

```
varpropuse(object)
## S3 method for class 'dynaTree'
varproptotal(object)
## S3 method for class 'dynaTree'
treestats(object)
```

#### Arguments

object a "dynaTree"-class object built by 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)

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#### References

Gramacy, R.B., Taddy, M.A., and S. Wild (2011). "Variable Selection and Sensitivity Analysis via Dynamic Trees with an Application to Computer Code Performance Tuning" arXiv:1108.4739

https://bobby.gramacy.com/r\_packages/dynaTree/

## See Also

dynaTree, sens.dynaTree, relevance.dynaTree

#### Examples

```
## ffit 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</pre>
```

## varpropuse

```
varproptotal(out)
```

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

## obtain tree statistics
treestats(out)

## clean up
deletecloud(out)

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