

Package ‘dynaTree’

October 19, 2022

Title Dynamic Trees for Learning and Design

Version 1.2-14

Date 2022-10-19

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Depends R (>= 2.14.0), methods

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

Repository CRAN

Date/Publication 2022-10-19 17:05:08 UTC

R topics documented:

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|------------------|----------------------------------------------|
| dynaTree-package | <i>Dynamic trees for learning and design</i> |
|------------------|----------------------------------------------|

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)

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 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 | <i>Calculate the ALC or predictive entropy statistic at the X locations, or ALC at new XX predictive locations</i> |
|---------------|--------------------------------------------------------------------------------------------------------------------|

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

```
## 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 iccept = "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 applies 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)

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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://arxiv.org/abs/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://arxiv.org/abs/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")

## 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 | <i>Class "dynaTree"</i> |
|----------------|-------------------------|

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)

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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)

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, irect = 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,
          irect = 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 <code>nrow(X)</code> 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 ≥ 2 indicating the number of “repeats” or passes through the data, as facilitated by <code>dynaTrees</code> ; see details below |
| sub | Optional argument allowing only a subset of the <code>length(y)</code> X-y pairs to be used in each repeat of <code>dynaTrees</code> ; each repeat will use a different random subset of size <code>sub</code> |
| 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, σ^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 <code>NULL</code> (default) a suitable minimum is calculated based on <code>dim(X)</code> and the type of <code>model</code> 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 <code>X</code> on which treed partitioning is allowed, and the last column of <code>X</code> 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 |
| irect | indicates the type of intercept term used (only applies to <code>model="linear"</code>). The default, “implicit” causes the inputs <code>X</code> to be centered so the intercept can be implied as an afterthought; “augmented” causes the inputs <code>X</code> 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 <code>X</code> 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 $\text{ncol}(XX) == \text{ncol}(X)$) 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 $\text{ncol}(x\$X) > 1$ and $\text{plotit} = \text{TRUE}$ 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 $\text{nrow}(X)$ -by- $(R-1)$ matrix of orderings (permutations of $1:\text{nrow}(X)$) |
| 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 <code>minp</code> (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 <code>minp</code> 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 $\text{verb} = 0$ 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 $\text{pverb} = 0$ 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 ($1:\text{max}(y)$). 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 $ab=c(\alpha, \beta)$ 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

| | |
|---------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>m</code> | <code>ncol(X)</code> |
| <code>T</code> | <code>nrow(X)</code> |
| <code>N</code> | the number of particles used |
| <code>X</code> | a copy of the design matrix X |
| <code>y</code> | a copy of the responses y |
| <code>model</code> | a copy of the specified leaf model |
| <code>params</code> | a vector containing <code>c(nu0s20, alpha, beta, minp, sb, icept, rprop)</code> , where the latter two are in integer form |
| <code>verb</code> | a copy of the verbosity argument |
| <code>lpred</code> | a vector of log posterior probabilities for each observation, conditional on the ones previous, for all time $(2*\text{minp}):T$; see <code>getBF</code> for calculating Bayes factors from these |
| <code>icept</code> | a copy of the intercept argument |
| <code>time</code> | the total computing time used to build the particle cloud |
| <code>num</code> | 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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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
```

```

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 Plumptre, (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)

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. Gavaldá 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 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

```
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)

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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)

## 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

```
## 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 <code>ncol(x\$X) > 1</code> this argument can be used to plot a 1-d projection by specifying which column of <code>x\$X</code> 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)

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
```

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

```
## 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 <code>ncol(XX) == ncol(X)</code>) |
| 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 <code>verb = 0</code> 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:

| | |
|---------------------|--------------------------------------------------------------------------------------------------------------------------------------------|
| <code>mean</code> | a vector containing an estimate of the predictive mean at the XX locations |
| <code>vmean</code> | a vector containing an estimate of the variance of predictive mean at the XX locations |
| <code>var</code> | a vector containing an estimate of the predictive variance (average variance plus variance of mean) at the XX locations |
| <code>df</code> | a vector containing the average degrees of freedom at the XX locations |
| <code>q1</code> | a vector containing an estimate of the 5% quantile of the predictive distribution at the XX locations, unless <code>quants = FALSE</code> |
| <code>q2</code> | a vector containing an estimate of the 95% quantile of the predictive distribution at the XX locations, unless <code>quants = FALSE</code> |
| <code>yypred</code> | if <code>yy != NULL</code> then this contains the predictive probability of the true <code>yy</code> values at the XX locations |
| <code>ei</code> | a vector containing an estimate of the EI statistic, unless <code>ei = FALSE</code> |

;

For classification:

| | |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>p</code> | a <code>nrow(XX)</code> -by- <code>max(object\$y)</code> matrix of mean class probabilities for each of <code>max(object\$y)</code> classes at the predictive data locations |
| <code>entropy</code> | a <code>nrow(XX)</code> 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

| | |
|-------------------|-------------------------------------------------------------------------------------------------------------|
| <code>coef</code> | a <code>nrow(XX)</code> -by- <code>m+1</code> cept 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/

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 $2 * \text{object}\$N$. The new $\text{object}\$N$ 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 $\text{object}\$N$ 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, $\text{object}\$X$ - $\text{object}\$y$ 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 $2 * \text{object}\$N$ 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

```
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 <code>ncol(object\$X)</code> rows describing the bounding rectangle for the ALC integration; the default that is used when <code>rect = NULL</code> is the bounding rectangle obtained by applying range to each column of <code>object\$X</code> (taking care to remove the first/intercept column of <code>object\$X</code> if <code>icpt = "augmented"</code>) |
| categ | A vector of logicals of length <code>ncol(object\$X)</code> indicating which, if any, dimensions of the input space should be treated as categorical; the default <code>categ</code> argument is <code>NULL</code> meaning that the categorical inputs are derived from <code>object\$X</code> 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 <code>verb = 0</code> 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 | <i>Retire (i.e. remove) data from the a dynaTree model</i> |
|-----------------|------------------------------------------------------------|

Description

Allows the removal (or “retiring” 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

| | |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------|
| 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 “retired” indices, i.e., their X-y values, to be printed to the screen as they are “retired” |

Details

Primarily for use in online learning contexts. After “retiring” 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 “retiring” 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 `link{entropyX.dynaTree}` for classification models.

Note that classification models (`model = "class"`) are not supported, and implicit intercepts (`icpt = "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 `icpt = "augmented"` which automatically augments an extra column of ones onto the input X design matrix/matrices. The `retire` function only supports this `icpt` 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", icpt="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

```

## 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 |

| | |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 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 <code>list</code> with entries <code>rect</code> , <code>shape</code> and <code>mode</code> describing the marginal distributions of the Latin Hypercube; specify <code>NULL</code> for a default specification for method = "boot". The fields should have the following format(s): <ul style="list-style-type: none"> • <code>rect</code>: 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 <code>matrix</code> or <code>data.frame</code> with <code>ncol(rect) = 2</code>, 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 <code>(object\$X)</code>. • <code>shape</code>: Optional vector of shape parameters for Beta marginal distributions having length <code>ncol(object\$X)</code> 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 <code>rect</code>. If unspecified, the uncertainty distribution is uniform over <code>rect</code>. The specification <code>shape[i]=0</code> instructs <code>sens</code> to treat the i'th dimension as a binary variable. In this case, <code>mode[i]</code> is the probability parameter for a bernoulli uncertainty distribution, and we must also have <code>rect[i,]=c(0,1)</code>. • <code>mode</code>: 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 <code>rect</code>. If <code>shape</code> is specified, but this is not, then the scaled Beta distributions will be symmetric. |
| categ | A vector of logicals of length <code>ncol(object\$X)</code> indicating which, if any, dimensions of the input space should be treated as categorical; this input is used to help set the default <code>lhs\$shape</code> argument if not specified; the default <code>categ</code> argument is <code>NULL</code> meaning that the categorical inputs are derived from <code>object\$X</code> 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 <code>verb = 0</code> is quiet |

Details

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

1st Order for input i ,

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

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 $nns*(ncol(X)+2)$ 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 $nns*(ncol(X)+2)$ 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 `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 <code>matrix</code> 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 $ncol(object\$X)$ <code>matrix</code> containing the posterior (samples) of the 1st Order Sobol sensitivity indices |
| T | 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

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.l.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)) {
```

```

    plot(out$MEgrid[,d], out$MEmean[,d], col=d, type="l", 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 |
| X | an augmenting design matrix of real-valued predictors with $\text{ncol}(X) = \text{object}\m |
| y | an augmenting vector of real-valued responses or integer categories with $\text{length}(y) = \text{nrow}(X)$ |
| 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 $\text{verb} = 0$ 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)

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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")
```

```

## 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'
```

```

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)

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://arxiv.org/abs/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
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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