Package ‘dbarts’

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Description Fits Bayesian additive regression trees (BART; Chipman, George, and McCulloch (2010) <doi:10.1214/09-AOAS285>) while allowing the updating of predictors or response so that BART can be incorporated as a conditional model in a Gibbs/Metropolis-Hastings sampler. Also serves as a drop-in replacement for package 'BayesTree'.

License GPL (>= 2)
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**Description**

BART is a Bayesian “sum-of-trees” model in which each tree is constrained by a prior to be a weak learner.

- For numeric response $y = f(x) + \epsilon$, where $\epsilon \sim N(0, \sigma^2)$.
- For binary response $y$, $P(Y = 1 \mid x) = \Phi(f(x))$, where $\Phi$ denotes the standard normal cdf (probit link).

**Usage**

```r
bart(x.train, y.train, x.test = matrix(0.0, 0, 0),
     sigest = NA, sigdf = 3, sigquant = 0.90,
     k = 2.0,
     power = 2.0, base = 0.95,
     binaryOffset = 0.0, weights = NULL,
     ntree = 200,
     ndpost = 1000, nskip = 100,
     printevery = 100, keepevery = 1, keeptrainfits = TRUE,
```

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Arguments

**x.train**  
Explanatory variables for training (in sample) data. May be a matrix or a data frame, with rows corresponding to observations and columns to variables. If a variable is a factor in a data frame, it is replaced with dummies. Note that $q$ dummies are created if $q > 2$ and one dummy is created if $q = 2$, where $q$ is the number of levels of the factor.
**y.train** Dependent variable for training (in sample) data. If `y.train` is numeric a continuous response model is fit (normal errors). If `y.train` is a binary factor or has only values 0 and 1, then a binary response model with a probit link is fit.

**x.test** Explanatory variables for test (out of sample) data. Should have same column structure as `x.train`. `bart` will generate draws of $f(x)$ for each $x$ which is a row of `x.test`.

**sigest** For continuous response models, an estimate of the error variance, $\sigma^2$, used to calibrate an inverse-chi-squared prior used on that parameter. If not supplied, the least-squares estimate is derived instead. See `sigquant` for more information. Not applicable when $y$ is binary.

**sigdf** Degrees of freedom for error variance prior. Not applicable when $y$ is binary.

**sigquant** The quantile of the error variance prior that the rough estimate (`sigest`) is placed at. The closer the quantile is to 1, the more aggressive the fit will be as you are putting more prior weight on error standard deviations ($\sigma$) less than the rough estimate. Not applicable when $y$ is binary.

**k** For numeric $y$, $k$ is the number of prior standard deviations $E(Y|x) = f(x)$ is away from $\pm 0.5$. The response ($y.train$) is internally scaled to range from $-0.5$ to $0.5$. For binary $y$, $k$ is the number of prior standard deviations $f(x)$ is away from $\pm 3$. In both cases, the bigger $k$ is, the more conservative the fitting will be. The value can be either a fixed number, or the a hyperprior of the form $\chi(degreesOfFreedom = 1.25, scale = Inf)$. For bart2, the default of `NULL` uses the value 2 for continuous responses and a $\chi$ hyperprior for binary ones. The default $\chi$ hyperprior is improper, and slightly penalizes small values of $k$.

**power** Power parameter for tree prior.

**base** Base parameter for tree prior.

**binaryOffset** Used for binary $y$. When present, the model is $P(Y = 1 \mid x) = \Phi(f(x) + \text{binaryOffset})$, allowing fits with probabilities shrunk towards values other than 0.5.

**weights** An optional vector of weights to be used in the fitting process. When present, BART fits a model with observations $y \mid x \sim N(f(x), \sigma^2/w)$, where $f(x)$ is the unknown function.

**ntree, n.trees** The number of trees in the sum-of-trees formulation.

**ndpost, n.samples** The number of posterior draws after burn in, `ndpost / keepevery` will actually be returned.

**nskip, n.burn** Number of MCMC iterations to be treated as burn in.

**printevery, printEvery** As the MCMC runs, a message is printed every `printevery` draws.

**keepevery, n.thin** Every `keepevery` draw is kept to be returned to the user. Useful for “thinning” samples.

**keeptrainfits, keepTrainingFits** If TRUE the draws of $f(x)$ for $x$ corresponding to the rows of `x.train` are returned.
usequants, useQuantiles
When TRUE, determine tree decision rules using estimated quantiles derived from the x.train variables. When FALSE, splits are determined using values equally spaced across the range of a variable. See details for more information.

numcut, n.cuts
The maximum number of possible values used in decision rules (see usequants, details). If a single number, it is recycled for all variables; otherwise must be a vector of length equal to ncol(x.train). Fewer rules may be used if a covariate lacks enough unique values.

printcutoffs, printCutoffs
The number of cutoff rules to printed to screen before the MCMC is run. Given a single integer, the same value will be used for all variables. If 0, nothing is printed.

verbose
Logical; if FALSE supress printing.

nchain, n.chains
Integer specifying how many independent tree sets and fits should be calculated.

nthread, n.threads
Integer specifying how many threads to use. Depending on the CPU architecture, using more than the number of chains can degrade performance for small/medium data sets. As such some calculations may be executed single threaded regardless.

combinechains, combineChains
Logical; if TRUE, samples will be returned in arrays of dimensions equal to nchain × ndpost × number of observations.

keeptrees, keepTrees
Logical; must be TRUE in order to use predict with the result of a bart fit. Note that for models with a large number of observations or a large number of trees, keeping the trees can be very memory intensive.

keepcall, keepCall
Logical; if FALSE, returned object will have call set to call("NULL"), otherwise the call used to instantiate BART.

formula
The same as x.train, the name reflecting that a formula object can be used instead.

data
The same as y.train, the name reflecting that a data frame can be specified when a formula is given instead.

test
The same as x.train. Can be missing.

subset
A vector of logicals or indicies used to subset of the data. Can be missing.

offset
The same as binaryOffset. Can be missing.

offset.test
A vector of offsets to be used with test data, in case it is different than the training offset. If offset is missing, defaults to NULL.

object
An object of class bart, returned from either the function bart or bart2.

newdata
Test data for prediction. Obey all the same rules as x.train but cannot be missing.

sampleronly, samplerOnly
Builds the sampler from its arguments and returns it without running it. Useful to use the bart2 interface in more complicated models.
x: Object of class `bart`, returned by function `bart`, which contains the information to be plotted.

plquants: In the plots, beliefs about $f(x)$ are indicated by plotting the posterior median and a lower and upper quantile. `plquants` is a double vector of length two giving the lower and upper quantiles.

cols: Vector of two colors. First color is used to plot the median of $f(x)$ and the second color is used to plot the lower and upper quantiles.

type: The quantity to be returned by generic functions. Options are "ev" - samples from the posterior of the individual level expected value, "bart" - the sum of trees component; same as "ev" for linear models but on the probit scale for binary ones, and "ppd" - samples from the posterior predictive distribution. To synergize with `predict.glm`, "response" can be used as a synonym for "value" and "link" can be used as a synonym for "bart".

sample: Either "train" or "test".

Details

BART is an Bayesian MCMC method. At each MCMC iteration, we produce a draw from the joint posterior $(f, \sigma) \mid (x, y)$ in the numeric $y$ case and just $f$ in the binary $y$ case.

Thus, unlike a lot of other modeling methods in R, `bart` does not produce a single model object from which fits and summaries may be extracted. The output consists of values $f^\star(x)$ (and $\sigma^\star$ in the numeric case) where $\star$ denotes a particular draw. The $x$ is either a row from the training data ($x.\text{train}$) or the test data ($x.\text{test}$).

**Decision Rules:** Decision rules for any tree are of the form $x \leq c$ vs. $x > c$ for each 'x' corresponding to a column of $x.\text{train}$. `usequants` determines the means by which the set of possible $c$ is determined. If `usequants` is TRUE, then the $c$ are a subset of the values interpolated half-way between the unique, sorted values obtained from the corresponding column of $x.\text{train}$. If `usequants` is FALSE, the cutoffs are equally spaced across the range of values taken on by the corresponding column of $x.\text{train}$.

The number of possible values of $c$ is determined by `numcut`. If `usequants` is FALSE, `numcut` equally spaced cutoffs are used covering the range of values in the corresponding column of $x.\text{train}$. If `usequants` is TRUE, then for a variable the minimum of `numcut` and one less than the number of unique elements for that variable are used.

`k`: The amount of shrinkage of the node parameters is controlled by `k`. `k` can be given as either a fixed, positive number, or as any value that can be used to build a supported hyperprior. At present, only $\chi_\nu s$ priors are supported, where $\nu$ is a degrees of freedom and $s$ is a scale. Both values must be positive, however the scale can be infinite which yields an improper prior, interpreted as just the polynomial part of the distribution. If $\nu$ is 1 and $s$ is $\infty$, the prior is “flat”.

For BART on binary outcomes, the degree of overfitting can be highly sensitive to `k` so it is encouraged to consider a number of values. The default hyperprior for binary BART, $\chi(1.25, 1/\infty)$, has been shown to work well in a large number of datasets, however crossvalidation may be helpful. Running for a short time with a flat prior may be helpful to see the range of values of `k` that are consistent with the data.
Generics: `bart` and `rbart_vi` support `fitted` to return the posterior mean of a predicted quantity, as well as `predict` to return a set of posterior samples for a different sample. In addition, the `extract` generic can be used to obtain the posterior samples for the training data or test data supplied during the initial fit.

Using `predict` with a `bart` object requires that it be fitted with the option `keeptrees/keepTrees` as `TRUE`. Keeping the trees for a fit can require a sizeable amount of memory and is off by default.

All generics return values on the scale of expected value of the response by default. This means that `predict`, `extract`, and `fitted` for binary outcomes return probabilities unless specifically the sum-of-trees component is requested (type = "bart"). This is in contrast to `yhat.train/yhat.test` that are returned with the fitted model.

Saving: saving and loading fitted BART objects for use with `predict` requires that R’s serialization mechanism be able to access the underlying trees, in addition to being fit with `keeptrees/keepTrees` as `TRUE`. For memory purposes, the trees are not stored as R objects unless specifically requested. To do this, one must “touch” the sampler’s state object before saving, e.g. for a fitted object `bartFit`, execute `invisible(bartFit$fit$state)`.

Value

`bart` returns a list assigned class `bart`. For applicable quantities, `ndpost` / `keepevery` samples are returned. In the numeric `y` case, the list has components:

- `yhat.train` A array/matrix of posterior samples. The `(i,j,k)` value is the jth draw of the posterior of f evaluated at the kth row of `x.train` (i.e. `f^*(x_k)`) corresponding to chain i. When `nchain` is one or `combinechains` is `TRUE`, the result is a collapsed down to a matrix.

- `yhat.test` Same as `yhat.train` but now the `x`s are the rows of the test data.

- `yhat.train.mean` Vector of means of `yhat.train` across columns and chains, with length equal to the number of training observations.

- `yhat.test.mean` Vector of means of `yhat.test` across columns and chains.

- `sigma` Matrix of posterior samples of `sigma`, the residual/error standard deviation. Dimensions are equal to the number of chains times the numbers of samples unless `nchain` is one or `combinechains` is `TRUE`.

- `first.sigma` Burn-in draws of `sigma`.

- `varcount` A matrix with number of rows equal to the number of kept draws and each column corresponding to a training variable. Contains the total count of the number of times that variable is used in a tree decision rule (over all trees).

- `sigest` The rough error standard deviation (σ) used in the prior.

- `y` The input dependent vector of values for the dependent variable. This is used in `plot.bart`.

- `fit` Optional sampler object which stores the values of the tree splits. Required for using `predict` and only stored if `keeptrees` is `TRUE`.

- `n.chains` Information that can be lost if `combinechains` is `TRUE` is tracked here.

- `k` Optional matrix of posterior samples of k. Only present when k is modeled, i.e. there is a hyperprior.
In the binary $y$ case, the returned list has the components `yhat.train`, `yhat.test`, and `varcount` as above. In addition the list has a `binaryOffset` component giving the value used.

Note that in the binary $y$, case `yhat.train` and `yhat.test` are $f(x) + \text{binaryOffset}$. For draws of the probability $P(Y = 1|x)$, apply the normal cdf (`pnorm`) to these values.

The `plot` method sets `mfrow` to `c(1,2)` and makes two plots. The first plot is the sequence of kept draws of $\sigma$ including the burn-in draws. Initially these draws will decline as BART finds fit and then level off when the MCMC has burnt in. The second plot has $y$ on the horizontal axis and posterior intervals for the corresponding $f(x)$ on the vertical axis.

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**References**

both of the above at: [http://www.rob-mcculloch.org](http://www.rob-mcculloch.org)

**See Also**

`pdbart`

**Examples**

```r
## simulate data (example from Friedman MARS paper)
## y = f(x) + epsilon , epsilon ~ N(0, sigma)
## x consists of 10 variables, only first 5 matter

f <- function(x) {
  10 * sin(pi * x[,1] * x[,2]) + 20 * (x[,3] - 0.5)^2 +
  10 * x[,4] + 5 * x[,5]
}

set.seed(99)
sigma <- 1.0
n <- 100

x <- matrix(runif(n * 10), n, 10)
Ey <- f(x)
y <- rnorm(n, Ey, sigma)
```
## run BART
set.seed(99)
bartFit <- bart(x, y)

plot(bartFit)

## compare BART fit to linear matter and truth = Ey
lmFit <- lm(y ~ ., data.frame(x, y))

fitmat <- cbind(y, Ey, lmFit$fitted, bartFit$yhat.train.mean)
colnames(fitmat) <- c('y', 'Ey', 'lm', 'bart')
print(cor(fitmat))

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### dbarts

**Discrete Bayesian Additive Regression Trees Sampler**

**Description**

Creates a sampler object for a given problem which fits a Bayesian Additive Regression Trees model. Internally stores state in such a way as to be mutable.

**Usage**

```r
dbarts(formula, data, test, subset, weights, offset, offset.test = offset, verbose = FALSE, n.samples = 800L, tree.prior = cgm, node.prior = normal, resid.prior = chisq, control = dbartsControl(), sigma = NA_real_)
```

**Arguments**

- `formula`: An object of class `formula` following an analogous model description syntax as `lm`. For backwards compatibility, can also be the `bart` matrix `x.train`.
- `data`: An optional data frame, list, or environment containing predictors to be used with the model. For backwards compatibility, can also be the `bart` vector `y.train`.
- `test`: An optional matrix or data frame with the same number of predictors as `data`, or `formula` in backwards compatibility mode. If column names are present, a matching algorithm is used.
- `subset`: An optional vector specifying a subset of observations to be used in the fitting process.
- `weights`: An optional vector of weights to be used in the fitting process. When present, BART fits a model with observations $y \mid x \sim N(f(x), \sigma^2/w)$, where $f(x)$ is the unknown function.
- `offset`: An optional vector specifying an offset from 0 for the relationship between the underlying function, $f(x)$, and the response $y$. Only is useful for binary responses, in which case the model fit is to assume $P(Y = 1 \mid X = x) = \Phi(f(x) + \text{offset})$, where $\Phi$ is the standard normal cumulative distribution function.
offset.test The equivalent of offset for test observations. Will attempt to use offset when applicable.

verbose A logical determining if additional output is printed to the console. See dbartsControl.

n.samples A positive integer setting the default number of posterior samples to be returned for each run of the sampler. Can be overridden at run-time. See dbartsControl.

tree.prior An expression of the form cgm or cgm(power, base) setting the tree prior used in fitting.

node.prior An expression of the form normal or normal(k) that sets the prior used on the averages within nodes.

resid.prior An expression of the form chisq or chisq(df, quant) that sets the prior used on the residual/error variance.

control An object inheriting from dbartsControl, created by the dbartsControl function.

sigma A positive numeric estimate of the residual standard deviation. If NA, a linear model is used with all of the predictors to obtain one.

Details

“Discrete sampler” refers to that dbarts is implemented using ReferenceClasses, so that there exists a mutable object constructed in C++ that is largely obscured from R. The dbarts function is the primary way of creating a dbartsSampler, for which a variety of methods exist.

Value

A reference object of dbartsSampler.

dbartsControl Discrete Bayesian Additive Regression Trees Sampler Control

Description

Convenience function to create a control object for use with a dbarts sampler.

Usage

dbartsControl( verbose = FALSE, keepTrainingFits = TRUE, useQuantiles = FALSE, keepTrees = FALSE, n.samples = NA_integer_, n.cuts = 100L, n.burn = 200L, n.trees = 75L, n.chains = 4L, n.threads = guessNumCores(), n.thin = 1L, printEvery = 100L, printCutoffs = 0L, rngKind = "default", rngNormalKind = "default", rngSeed = NA_integer_, updateState = TRUE)
Arguments

verbose  Logical controlling sampler output to console.

keepTrainingFits  Logical controlling whether or not training fits are returned when the sampler runs. These are always computed as part of the fitting procedure, so disabling will not substantially impact running time.

useQuantiles  Logical to determine if the empirical quantiles of a columns of predictors should be used to determine the tree decision rules. If FALSE, the rules are spaced uniformly throughout the range of covariate values.

keepTrees  A logical that determines whether or not trees are cached as they are sampled. In all cases, the current state of the sampler is stored as a single set of n.trees. When keepTrees is TRUE, a set of n.trees * n.samples trees are set aside and populated as the sampler runs. If the sampler is stopped and restarted, samples proceed from the previously stored tree, looping over if necessary.

n.samples  A non-negative integer giving the default number of samples to return each time the sampler is run. Generally specified by dbarts instead, and can be overridden on a per-use basis whenever the sampler is run.

n.cuts  A positive integer or integer vector giving the number of decision rules to be used for each given predictor. If of length less than the number of predictors, earlier values are recycled. If for any predictor more values are specified than are coherent, fewer may be used. See details for more information.

n.burn  A non-negative integer determining how many samples, if any, are thrown away at the beginning of a run of the sampler.

n.trees  A positive integer giving the number of trees used in the sum-of-trees formulation.

n.chains  A positive integer detailing the number of independent chains for the sampler to use.

n.threads  A positive integer controlling how many threads will be used for various internal calculations, as well as the number of chains. Internal calculations are highly optimized so that single-threaded performance tends to be superior unless the number of observations is very large (>10k), so that it is often not necessary to have the number of threads exceed the number of chains.

n.thin  A positive integer determining how many iterations the MCMC chain should jump on the decision trees alone before recording a sample. Serves to “thin” the samples against serial correlation. n.samples are returned regardless of the value of n.thin.

printEvery  If verbose is TRUE, every printEvery potential samples (after thinning) will issue a verbal statement. Must be a positive integer.

printCutoffs  A non-negative integer specifying how many of the decision rules for a variable are printed in verbose mode.

rngKind  Random number generator kind, as used in set.seed. For type "default", the built-in generator will be used if possible. Otherwise, will attempt to match the built-in generator’s type. Success depends on the number of threads.
**rngNormalKind**
Random number generator normal kind, as used in set.seed. For type "default", the built-in generator will be used if possible. Otherwise, will attempt to match the built-in generator's type. Success depends on the number of threads and the rngKind.

**rngSeed**
Random number generator seed, as used in set.seed. If the sampler is running single-threaded or has one chain, the behavior will be as any other sequential algorithm. If the sampler is multithreaded, the seed will be used to create an additional pRNG object, which in turn will be used sequentially seed the thread-specific pRNGs. If equal to NA, the clock will be used to seed pRNGs when applicable.

**updateState**
Logical setting the default behavior for many sampler methods with regards to the immediate updating of the cached state of the object. A current, cached state is only useful when saving/loading the sampler.

**Value**
An object of class dbartControl.

**See Also**
dbars

dbarsData
*Discrete Bayesian Additive Regression Trees Sampler Data*

**Description**
Convenience function to create a data object for use with a dbarts sampler.

**Usage**
dbarsData(formula, data, test, subset, weights, offset, offset.test = offset)

**Arguments**

- *formula*, *data*, *test*, *subset*, *weights*, *offset*, *offset.test*

  As in dbarts. Retains backwards compatibility with bart, so that formula/data can be a formula/data.frame pair, or a pair of x.train/y.train matrices/vector.

**Value**
An object of class dbartData.

**See Also**
dbars
dbartsSampler-class

Class "dbartsSampler" of Discrete Bayesian Additive Regression Trees Sampler

Description

A reference class object that contains a Bayesian Additive Regression Trees sampler in such a way that it can be modified, stopped, and started all while maintaining its own state.

Usage

```r
## S4 method for signature 'dbartsSampler'
run(numBurnIn, numSamples, updateState = NA)
## S4 method for signature 'dbartsSampler'
sampleTreesFromPrior(updateState = NA)
## S4 method for signature 'dbartsSampler'
sampleNodeParametersFromPrior(updateState = NA)
## S4 method for signature 'dbartsSampler'
copy(shallow = FALSE)
## S4 method for signature 'dbartsSampler'
show()
## S4 method for signature 'dbartsSampler'
predict(x.test, offset.test)
## S4 method for signature 'dbartsSampler'
setControl(control)
## S4 method for signature 'dbartsSampler'
setModel(model)
## S4 method for signature 'dbartsSampler'
dataSet(data)
## S4 method for signature 'dbartsSampler'
setResponse(y, updateState = NA)
## S4 method for signature 'dbartsSampler'
setOffset(offset, updateState = NA)
## S4 method for signature 'dbartsSampler'
setSigma(sigma, updateState = NA)
## S4 method for signature 'dbartsSampler'
setPredictor(x, column, updateState = NA)
## S4 method for signature 'dbartsSampler'
setTestPredictor(x.test, column, updateState = NA)
## S4 method for signature 'dbartsSampler'
setTestOffset(offset.test, updateState = NA)
## S4 method for signature 'dbartsSampler'
printTrees(treeNums)
## S4 method for signature 'dbartsSampler'
plotTree(treeNum, treePlotPars = list(nodeHeight = 12, nodeWidth = 40, nodeGap = 8), ...)
```
Arguments

numBurnIn  A non-negative integer determining how many iterations the sampler should skip before storing results. If missing or NA, the default is filled in from the sampler’s control object.

numSamples A positive integer determining how many posterior samples should be returned. If missing or NA, the default is also filled in from the control object.

updateState A logical determining if the local cache of the sampler’s state should be updated after the completion of the run. If NA, the default is also filled in from the control object.

shallow A logical determining if the copy should retain the underlying data of the sampler (TRUE) or have its own copies (FALSE).

control An object inheriting from dbartsControl.

model An object inheriting from dbartsModel.

data An object inheriting from dbartsData.

y A numeric response vector of length equal to that with which the sampler was created.

x A numeric predictor vector of length equal to that with which the sampler was created. Can be an entirely matrix of new number of rows for setTestPredictor.

x.test A new matrix of test predictors, of the number of columns equal to that in the current model.

offset A numeric vector of length equal to that with which the sampler was created, or NULL. If offset.test was set from offset, will attempt to update that as well.

updateScale Logical indicating whether BART’s internal scale should update with the new offset. Should only be TRUE during burn-in.

offset.test A numeric vector of length equal to that of the test matrix, or NULL. Can be missing for setTestPredictors.

sigma Numeric vector of residual standard deviations, one for each chain.

column An integer or character string vector specifying which column/columns of the predictor matrix is to be replaced. If missing, the entire matrix is substitute.

treeNode An integer vector listing the indices of the trees to print.

treeNode An integer listing the indices of the tree to plot.

treeNode A list containing the number quantities nodeHeight, nodeWidth, and nodeGap, all of which control aspects of the resulting plot.

... Extra arguments to plot.

Details

A dbartsSampler is a “mutable” object which contains information pertaining to fitting a Bayesian additive regression tree model. The sampler is first created and then, in a separate instruction, run or modified. In this way, MCMC samplers can be constructed with BART components filling arbitrary roles.
Saving: saving and loading a dbarts sampler for future use requires that R’s serialization mechanism be able to access the state of the sampler which, for memory purposes, is only made available to R on request. To do this, one must “touch” the sampler’s state object before saving, e.g. for the object sampler, execute invisible(sampler$state). This is in addition to guaranteeing that the state object is not NULL, which can be done by setting the sampler’s control to an object with updateState as TRUE or passing TRUE as the updateState argument to any of the sampler’s applicable methods.

Value

For run, a named-list with contents sigma, train, test, and varcount.

For setPredictor, TRUE/FALSE depending on whether or not the operation was successful. The operation can fail if the new predictor results in a tree with an empty leaf-node. If only single columns were replaced, on the update is rolled-back so that the sampler remains in a valid state.

predict keeps the current test matrix in place and uses the current set of tree splits. This function has two use cases. The first is when keepTrees of dbartsControl is TRUE, in which case the sampler should be run to completion and the function can be used to interrogate the existing fit. When keepTrees is FALSE, the function can be used to obtain the likelihood as part of a proposed new set of covariates in a Metropolis-Hastings step in a full-Bayes sampler. This would typically be followed by a call to setPredictor if the step is accepted.

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guessNumCores  Guess Number of Cores

Description

Attempts to guess the number of CPU ‘cores’, both physical and logical.

Usage

guessNumCores(logical = FALSE)

Arguments

logical  A logical value. When FALSE, an estimate of the number of physical cores is returned. When TRUE, so-called “logical” cores as also included.

Details

Because of different definitions of cores used by different manufacturers, the distinction between logical and physical cores is not universally recognized. This function will attempt to use operating system definitions when available, which should usually match the CPU itself.

Value

An integer, or NA if no clear answer was obtained.
makeModelMatrixFromDataFrame

Make Model Matrix from Data Frame

Description

Converts a data frame with numeric and factor contents into a matrix, suitable for use with \texttt{bart}. Unlike in linear regression, factors containing more than two levels result in dummy variables being created for each level.

Usage

\begin{verbatim}
makeModelMatrixFromDataFrame(x, drop = TRUE)
makeInd(x, all = TRUE)
makeTestModelMatrix(data, newdata)
\end{verbatim}

Arguments

\begin{itemize}
  \item \texttt{x} Data frame of explanatory variables.
  \item \texttt{drop} Logical or list controlling whether or not columns that are constants or factor levels with no instances are omitted from the result. When a list, must be of length equal to \texttt{x}. Elements correspond to \texttt{x} according to:
    \begin{itemize}
      \item vector - single logical
      \item matrix - vector of logicals, one per column
      \item factor - table of factor levels to be referenced; levels with counts of 0 are to be dropped
    \end{itemize}
  \item \texttt{all} Not currently implemented.
  \item \texttt{data} An existing \texttt{dbartsData} object.
  \item \texttt{newdata} Test data frame.
\end{itemize}

Details

Character vectors are included as factors. If you have numeric data coded as characters, convert it using \texttt{as.numeric} first.

Note that if you have train and test data frames, it may be best to \texttt{rbind} the two together, apply \texttt{makeModelMatrixFromDataFrame} to the result, and then pull them back apart. Alternatively, save the drop attribute used in creating the train data and use it when creating a matrix from the test data. Example given below.

Use of these functions is not required when using \texttt{bart}, \texttt{bart2}, or \texttt{dbartsSampler}; they exist to allow the user finer control and to assist with writing packages that separate the creation of training from test data.
Value

A matrix with columns corresponding to the elements of the data frame. If drop = TRUE or is a list, the attribute drop on the result is set to the list used when creating the matrix.

Author(s)

Vincent Dorie: <vdorie@gmail.com>.

Examples

```r
iv <- 1:10
rv <- runif(10)
f <- factor(rep(seq.int(3), c(4L, 4L, 2L)),
        labels = c("alice", "bob", "charlie"))
df <- data.frame(iv, rv, f)

mm <- makeModelMatrixFromDataFrame(df)

# create test and train matrices with disjoint factor levels
train.df <- df[1:8,]
test.df <- df[9:10,]
train.mm <- makeModelMatrixFromDataFrame(train.df)
test.mm <- makeModelMatrixFromDataFrame(test.df, attr(train.mm, "drop"))
```

Description

Run `bart` at test observations constructed so that a plot can be created displaying the effect of a single variable (`pdbart`) or pair of variables (`pd2bart`). Note that if $y$ is a binary with $P(Y = 1|x) = F(f(x))$, $F$ the standard normal cdf, then the plots are all on the $f$ scale.

Usage

```r
pdbart(x.train, y.train,
      xind = NULL,
      levs = NULL, levquants = c(0.05, seq(0.1, 0.9, 0.1), 0.95),
      pl = TRUE, plquants = c(0.05, 0.95),
      ...
)

# S3 method for class 'pdbart'
plot(x,
      xind = seq_len(length(x$fd)),
      plquants = c(0.05, 0.95), cols = c('black', 'blue'),
      ...
)

pd2bart(x.train, y.train,
```

 pdbart **Partial Dependence Plots for BART**
xind = NULL,
levs = NULL, levquants = c(0.05, seq(0.1, 0.9, 0.1), 0.95),
pl = TRUE, plquants = c(0.05, 0.95),
...

## S3 method for class 'pd2bart'
plot(x,
plquants = c(0.05, 0.95), contour.color = 'white',
justmedian = TRUE,
...

Arguments

x.train       Explanatory variables for training (in sample) data. Can be any valid input to bart, such as a matrix or a formula. Also accepted are fitted bart models or dbartsSampler with keepTrees equal to TRUE.
y.train       Dependent variable for training (in sample) data. Can be a numeric vector or, when passing x.train as a formula, a data.frame or other object used to find variables. Not required if x.train is a fitted model or sampler.
xind          Integer, character vector, or the right-hand side of a formula indicating which variables are to be plotted. In pdbart, corresponds to the variables (columns of x.train) for which a plot is to be constructed. In plot.pdbart, corresponds to the indices in list returned by pdbart for which plot is to be constructed. In pd2bart, the indicies of a pair of variables (columns of x.train) to plot. If NULL a default of all columns is used for pdbart and the first two columns is used for pd2bart.
levs           Gives the values of a variable at which the plot is to be constructed. Must be a list, where the ith component gives the values for the ith variable. In pdbart, it should have same length as xind. In pd2bart, it should have length 2. See also argument levquants.
levquants      If levs in NULL, the values of each variable used in the plot is set to the quantiles (in x.train) indicated by levquants. Must be a vector of numeric type.
pl             For pdbart and pd2bart, if TRUE, plot is subsequently made (by calling plot.*).
plquants       In the plots, beliefs about \( f(x) \) are indicated by plotting the posterior median and a lower and upper quantile. plquants is a double vector of length two giving the lower and upper quantiles.
...
    Additional arguments. In pdbart and pd2bart, arguments are passed on to bart. In plot.pdbart, they are passed on to plot. In plot.pd2bart, they are passed on to image.
x             For plot.*, object returned from pdbart or pd2bart.
cols          Vector of two colors. The first color is for the median of \( f \), while the second color is for the upper and lower quantiles.
contour.color  Color for contours plotted on top of the image.
justmedian     A logical where if TRUE just one plot is created for the median of \( f(x) \) draws. If FALSE, three plots are created one for the median and two additional ones for the lower and upper quantiles. In this case, mfrow is set to c(1,3).
Details

We divide the predictor vector \( x \) into a subgroup of interest, \( x_s \) and the complement \( x_c = x \setminus x_s \). A prediction \( f(x) \) can then be written as \( f(x_s, x_c) \). To estimate the effect of \( x_s \) on the prediction, Friedman suggests the partial dependence function

\[
    f_s(x_s) = \frac{1}{n} \sum_{i=1}^{n} f(x_s, x_{ic})
\]

where \( x_{ic} \) is the \( i \)th observation of \( x_c \) in the data. Note that \( (x_s, x_{ic}) \) will generally not be one of the observed data points. Using BART it is straightforward to then estimate and even obtain uncertainty bounds for \( f_s(x_s) \). A draw of \( f^*_s(x_s) \) from the induced BART posterior on \( f_s(x_s) \) is obtained by simply computing \( f^*_s(x_s) \) as a byproduct of each MCMC draw \( f^* \). The median (or average) of these MCMC draws \( f^*_s(x_s) \) then yields an estimate of \( f_s(x_s) \), and lower and upper quantiles can be used to obtain intervals for \( f_s(x_s) \).

In \texttt{pdbart} \( x_s \) consists of a single variable in \( x \) and in \texttt{pd2bart} it is a pair of variables.

This is a computationally intensive procedure. For example, in \texttt{pdbart}, to compute the partial dependence plot for 5 \( x_s \) values, we need to compute \( f(x_s, x_c) \) for all possible \((x_s, x_{ic})\) and there would be \( 5n \) of these where \( n \) is the sample size. All of that computation would be done for each kept BART draw. For this reason running BART with \texttt{keepevery} larger than 1 (e.g. 10) makes the procedure much faster.

Value

The plot methods produce the plots and don’t return anything. \texttt{pdbart} and \texttt{pd2bart} return lists with components given below. The list returned by \texttt{pdbart} is assigned class \texttt{pdbart} and the list returned by \texttt{pd2bart} is assigned class \texttt{pd2bart}.

- \texttt{fd} A matrix whose \((i, j)\) value is the \( i \)th draw of \( f_s(x_s) \) for the \( j \)th value of \( x_s \). “fd” is for “function draws”.
  
  For \texttt{pdbart} \( fd \) is actually a list whose \( k \)th component is the matrix described above corresponding to the \( k \)th variable chosen by argument \texttt{xind}. The number of columns in each matrix will equal the number of values given in the corresponding component of argument \texttt{levs} (or number of values in \texttt{levquants}).
  
  For \texttt{pd2bart}, \( fd \) is a single matrix. The columns correspond to all possible pairs of values for the pair of variables indicated by \texttt{xind}. That is, all possible \((x_i, x_j)\) where \( x_i \) is a value in the \texttt{levs} component corresponding to the first \( x \) and \( x_j \) is a value in the \texttt{levs} components corresponding to the second one. The first \( x \) changes first.

- \texttt{levs} The list of levels used, each component corresponding to a variable. If argument \texttt{levs} was supplied it is unchanged. Otherwise, the levels in \texttt{levs} are as constructed using argument \texttt{levquants}.

- \texttt{xlbs} A vector of character strings which are the plotting labels used for the variables.

The remaining components returned in the list are the same as in the value of \texttt{bart}. They are simply passed on from the BART run used to create the partial dependence plot. The function \texttt{plot.bart} can be applied to the object returned by \texttt{pdbart} or \texttt{pd2bart} to examine the BART run.
Author(s)

Hugh Chipman: <hugh.chipman@acadiau.ca>.
Robert McCulloch: <robert.mcculloch@chicagogsb.edu>.

References

both of the above at: http://www.rob-mcculloch.org/

Examples

```r
## Not run:
## simulate data
f <- function(x) { return(0.5 * x[,1] + 2 * x[,2] * x[,3]) }
sigma <- 0.2
n <- 100
set.seed(27)
x <- matrix(2 * runif(n * 3) -1, ncol = 3)
colnames(x) <- c("Var rob", "Var hugh", "Var ed")
Ey <- f(x)
y <- rnorm(n, Ey, sigma)
## first two plot regions are for pdbart, third for pd2bart
par(mfrow = c(1, 3))
## pdbart: one dimensional partial dependence plot
set.seed(99)
pdb1 <-
pdbart(x, y, xind = c(1, 2),
   levs = list(seq(-1, 1, 0.2), seq(-1, 1, 0.2)),
   pl = FALSE, keepevery = 10, ntree = 100)
plot(pdb1, ylim = c(-0.6,.6))
## pd2bart: two dimensional partial dependence plot
set.seed(99)
pdb2 <-
pd2bart(x, y, xind = c(2, 3),
   levquants = c(0.05, 0.1, 0.25, 0.5, 0.75, 0.9, 0.95),
   pl = FALSE, ntree = 100, keepevery = 10, verbose = FALSE)
plot(pdb2)
## compare BART fit to linear model and truth = Ey
lmFit <- lm(y ~., data.frame(x, y))
fitmat <- cbind(y, Ey, lmFit$fitted, pdb1$yhat.train.mean)
```
```r
colnames(fitmat) <- c('y', 'Ey', 'lm', 'bart')
print(cor(fitmat))

## example showing the use of a pre-fitted model
df <- data.frame(y, x)
set.seed(99)
bartFit <- bart(y ~ rob +Hugh + ed, df,
    keepevery = 10, ntree = 100, keeptrees = TRUE)
pdb1 <- pdbart(bartFit, xind = rob + ed, pl = FALSE)

## End(Not run)
```

---

**rbart**  
*Bayesian Additive Regression Trees with Random Effects*

## Description

Fits a varying intercept/random effect BART model.

## Usage

rbart_vi(
    formula, data, test, subset, weights, offset, offset.test = offset,
    group.by, group.by.test, prior = cauchy,
    sigest = NA_real_, sigdf = 3.0, sigquant = 0.90,
    k = 2.0,
    power = 2.0, base = 0.95,
    n.trees = 75L,
    n.samples = 1500L, n.burn = 1500L,
    n.chains = 4L, n.threads = min(guessNumCores(), n.chains), combineChains = FALSE,
    n.cuts = 100L, useQuantiles = FALSE,
    n.thin = 5L, keepTrainingFits = TRUE,
    printEvery = 100L, printCutoffs = 0L,
    verbose = TRUE,
    keepTrees = TRUE, keepCall = TRUE, ...
)

```

```
## S3 method for class 'rbart'
predict(object, newdata, group.by, offset,
       type = c("ev", "ppd", "bart", "ranef"),
       combineChains = TRUE,
       ...
)
## S3 method for class 'rbart'
residuals(object, ...)

Arguments

- **group.by**
  - Grouping factor. Can be an integer vector/factor, or a reference to such in `data`.
- **group.by.test**
  - Grouping factor for test data, of the same type as `group.by`. Can be missing.
- **prior**
  - A function or symbolic reference to built-in priors. Determines the prior over the standard deviation of the random effects. Supplied functions take two arguments, `x` - the standard deviation, and `rel.scale` - the standard deviation of the response variable before random effects are fit. Built in priors are cauchy with a scale of 2.5 times the relative scale and gamma with a shape of 2.5 and scale of 2.5 times the relative scale.
- **n.thin**
  - The number of tree jumps taken for every stored sample, but also the number of samples from the posterior of the standard deviation of the random effects before one is kept.
- **formula, data, test, subset, weights, offset, offset.test, sigest, sigdf, sigquant, k, power, base, n.trees, n.samples**
  - Same as in `bart2`.
- **object**
  - A fitted `rbart` model.
- **newdata**
  - Same as `test`, but named to match `predict` generic.
- **type**
  - One of "ev", "ppd", "bart", "ranef" for the posterior of the expected value, posterior predictive distribution, non-parametric/BART component, or random effect respectively. The expected value is the sum of the BART component and the random effects, while the posterior predictive distribution is a response sampled with that mean. To synergize with `predict.glm`, "response" can be used as a synonym for "value" and "link" can be used as a synonym for "bart".
- **sample**
  - One of "train" or "test", referring to the training or tests samples respectively.
- **x, plquants, cols**
  - Same as in `plot.bart`.

Details

Fits a BART model with additive random intercepts, one for each factor level of `group.by`. For continuous responses:

- \( y_i \sim N(f(x_i) + \alpha_j, \sigma^2) \)
- \( \alpha_j \sim N(0, \tau^2). \)

For binary outcomes the response model is changed to \( P(Y_i = 1) = \Phi(f(x_i) + \alpha_j). \) \( i \) indexes observations, \( g[i] \) is the group index of observation \( i \), \( f(x) \) and \( \sigma_y \) come from a BART model, and \( \alpha_j \) are the independent and identically distributed random intercepts.
Out Of Sample Groups: Predicting random effects for groups not in the training sample is supported by sampling from their posterior predictive distribution, that is a draw is taken from 
\[ p(\alpha | y) = \int p(\alpha | \tau)p(\tau | y) d\alpha. \]
For out-of-sample groups in the test data, these random effect draws can be kept with the saved object. For those supplied to predict, they cannot and may change for subsequent calls.

Generics: See the generics section of `bart`.

Value

An object of class `rbart`. Contains all of the same elements of an object of class `bart`, as well as the elements

- `ranef` Samples from the posterior of the random effects. A array/matrix of posterior samples. The \((k,l,j)\) value is the \(l\)th draw of the posterior of the random effect for group \(j\) (i.e. \(\alpha^*_j\)) corresponding to chain \(k\). When \(n.chains\) is one or `combineChains` is `TRUE`, the result is a collapsed down to a matrix.

- `ranef.mean` Posterior mean of random effects, derived by taking mean across group index of samples.

- `tau` Matrix of posterior samples of \(\tau\), the standard deviation of the random effects. Dimensions are equal to the number of chains times the numbers of samples unless \(n.chains\) is one or `combineChains` is `TRUE`.

- `first.tau` Burn-in draws of \(\tau\).

Author(s)

Vincent Dorie: <vdorie@gmail.com>

See Also

`bart`, `dbarts`

Examples

```r
f <- function(x) {
  10 * sin(pi * x[,1] * x[,2]) + 20 * (x[,3] - 0.5)^2 +
  10 * x[,4] + 5 * x[,5]
}

set.seed(99)
sigma <- 1.0
n <- 100
x <- matrix(runif(n * 10), n, 10)
Ey <- f(x)
y <- rnorm(n, Ey, sigma)

n.g <- 10
g <- sample(n.g, length(y), replace = TRUE)
sigma.b <- 1.5
```
b <- rnorm(n.g, 0, sigma.b)

y <- y + b[g]

df <- as.data.frame(x)
colnames(df) <- paste0("x", seq_len(ncol(x)))
df$y <- y
df$g <- g

## low numbers to reduce run time
rbartFit <- rbart_vi(y ~ . - g, df, group.by = g,
    n.samples = 40L, n.burn = 10L, n.thin = 2L, n.chains = 1L,
    n.trees = 25L, n.threads = 1L)

### Crossvalidation For Bayesian Additive Regression Trees

**Description**

Fits the BART model against varying k, power, base, and ntree parameters using $K$-fold or repeated random subsampling crossvalidation, sharing burn-in between parameter settings. Results are given an array of evaluations of a loss functions on the held-out sets.

**Usage**

```r
xbart(formula, data, subset, weights, offset, verbose = FALSE, n.samples = 200L,
    method = c("k-fold", "random subsample"), n.test = c(5, 0.2),
    n.reps = 40L, n.burn = c(200L, 150L, 50L),
    loss = c("rmse", "log", "mcr"), n.trees = guessNumCores(), n.trees = 75L,
    k = NULL, power = 2, base = 0.95, drop = TRUE,
    resid.prior = chisq, control = dbartsControl(), sigma = NA_real_)
```

**Arguments**

- **formula**: An object of class `formula` following an analogous model description syntax as `lm`. For backwards compatibility, can also be the `bart` matrix `x.train`. See `dbarts`.

- **data**: An optional data frame, list, or environment containing predictors to be used with the model. For backwards compatibility, can also be the `bart` vector `y.train`.

- **subset**: An optional vector specifying a subset of observations to be used in the fitting process.

- **weights**: An optional vector of weights to be used in the fitting process. When present, BART fits a model with observations $y \mid x \sim N(f(x), \sigma^2/w)$, where $f(x)$ is the unknown function.
offset
An optional vector specifying an offset from 0 for the relationship between the underlying function, \( f(x) \), and the response \( y \). Only is useful for binary responses, in which case the model fit is to assume \( P(Y = 1 \mid X = x) = \Phi(f(x) + \text{offset}) \), where \( \Phi \) is the standard normal cumulative distribution function.

verbose
A logical determining if additional output is printed to the console.

n.samples
A positive integer, setting the number of posterior samples drawn for each fit of training data and used by the loss function.

method
Character string, either "k-fold" or "random subsample".

n.test
For each fit, the test sample size or proportion. For method "k-fold", it is expected to be the number of folds, and in \([2, n]\). For method "random subsample", can be a real number in \((0, 1)\) or a positive integer in \((1, n)\). When a given as proportion, the number of test observations used is the proportion times the sample size rounded to the nearest integer.

n.reps
A positive integer setting the number of cross validation steps that will be taken. For "k-fold", each replication corresponds to fitting each of the \( K \) folds in turn, while for "random subsample" a replication is a single fit.

n.burn
Between one and three positive integers, specifying the 1) initial burn-in, 2) burn-in when moving from one parameter setting to another, and 3) the burn-in between each random subsample replication. The third parameter is also the burn in when moving between folds in "k-fold" crossvalidation.

loss
Either a one of the pre-set loss functions as character-strings (mcr - misclassification rate for binary responses, rmse - root-mean-squared-error for continuous response), log - negative log-loss for binary response (rmse serves this purpose for continuous responses), a function, or a function-evaluation environment list-pair. Functions should have prototypes of the form function(y.test, y.test.hat), where y.test is the held out test subsample and y.test.hat is a matrix of dimension length(y.test) * n.samples. See examples.

n.threads
Across different sets of parameters \((k \times \text{power} \times \text{base} \times \text{n.trees})\) and \(\text{n.reps}\), results are independent. For \(\text{n.threads} > 1\), evaluations of the above are divided into approximately equal size evaluations chunks and executed in parallel. The default uses \link{guessNumCores}, which should work across the most common operating system/hardware pairs. A value of \(\text{NA}\) is interpreted as 1.

n.trees
A vector of positive integers setting the BART hyperparameter for the number of trees in the sum-of-trees formulation. See \link{bart}.

k
A vector of positive real numbers, setting the BART hyperparameter for the node-mean prior standard deviation. If \(\text{NULL}\), the default of \(\text{bart2}\) will be used - 2 for continuous response and a Chi hyperprior for binary. Hyperprior crossvalidation not possible at this time.

power
A vector of real numbers greater than one, setting the BART hyperparameter for the tree prior’s growth probability, given by \(\text{base}/(1 + \text{depth})^{\text{power}}\).

base
A vector of real numbers in \((0, 1)\), setting the BART hyperparameter for the tree prior’s growth probability.

drop
Logical, determining if dimensions with a single value are dropped from the result.
resid.prior An expression of the form `chisq` or `chisq(df,quant)` that sets the prior used on the residual/error variance.

control An object inheriting from `dbartsControl`, created by the `dbartsControl` function.

sigma A positive numeric estimate of the residual standard deviation. If `NA`, a linear model is used with all of the predictors to obtain one.

Details

Crossvalidates `n.reps` replications against the crossproduct of given hyperparameter vectors `n.trees \times k \times power \times base`. For each fit, either one fold is withheld as test data and `n.test - 1` folds are used as training data or `n * n.test` observations are withheld as test data and `n * (1 - n.test)` used as training. A replication corresponds to fitting all `K` folds in "k-fold" crossvalidation or a single fit with "random subsample". The training data is used to fit a model and make predictions on the test data which are used together with the test data itself to evaluate the loss function.

Loss functions are either the default of average negative log-loss for binary outcomes and root-mean-squared error for continuous outcomes, misclassification rates for binary outcomes, or a function with arguments `y.test` and `y.test.hat`. `y.test.hat` is of dimensions equal to length(`y.test`) \times `n.samples`. A third option is to pass a list of `list(function,evaluationEnvironment)`, so as to provide default bindings. RMSE is a monotonic transformation of the average log-loss for continuous outcomes, so specifying log-loss in that case calculates RMSE instead.

Value

An array of dimensions `n.reps \times length(n.trees) \times length(k) \times length(power) \times length(base)`. If `drop` is `TRUE`, dimensions of length 1 are omitted. If all hyperparameters are of length 1, then the result will be a vector of length `n.reps`. When the result is an array, the dimnames of the result shall be set to the corresponding hyperparameters.

For method "k-fold", each element is an average across the `K` fits. For "random subsample", each element represents a single fit.

Author(s)

Vincent Dorie: `<vdorie@gmail.com>`

See Also

`bart`, `dbarts`

Examples

```r
f <- function(x) {
  10 * sin(pi * x[,1] * x[,2]) + 20 * (x[,3] - 0.5)^2 +
  10 * x[,4] + 5 * x[,5]
}
set.seed(99)
sigma <- 1.0
n <- 100
```
x <- matrix(runif(n * 10), n, 10)
Ey <- f(x)
y <- rnorm(n, Ey, sigma)

mad <- function(y.train, y.train.hat)
    mean(abs(y.train - apply(y.train.hat, 1L, mean)))

## low iteration numbers to run quickly
xval <- xbart(x, y, n.samples = 15L, n.reps = 4L, n.burn = c(10L, 3L, 1L),
              n.trees = c(5L, 7L),
              k = c(1, 2, 4),
              power = c(1.5, 2),
              base = c(0.75, 0.8, 0.95), n.threads = 1L,
              loss = mad)
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