# Package 'dbarts'

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     Hastings sampler. Also serves as a drop-in replacement for package 'BayesTree'.
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Bayesian Additive Regression Trees

# **Description**

bart

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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

```
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, splitprobs = 1 / numvars,
    binaryOffset = 0.0, weights = NULL,
    ntree = 200,
    ndpost = 1000, nskip = 100,
```

```
printevery = 100, keepevery = 1, keeptrainfits = TRUE,
    usequants = FALSE, numcut = 100, printcutoffs = 0,
    verbose = TRUE, nchain = 1, nthread = 1, combinechains = TRUE,
    keeptrees = FALSE, keepcall = TRUE, sampleronly = FALSE,
    seed = NA_integer_,
    proposalprobs = NULL,
    keepsampler = keeptrees)
bart2(
    formula, data, test, subset, weights, offset, offset.test = offset,
    sigest = NA_real_, sigdf = 3.0, sigquant = 0.90,
    k = NULL,
    power = 2.0, base = 0.95, split.probs = 1 / num.vars,
    n.trees = 75L,
    n.samples = 500L, n.burn = 500L,
    n.chains = 4L, n.threads = min(dbarts::guessNumCores(), n.chains),
    combineChains = FALSE,
    n.cuts = 100L, useQuantiles = FALSE,
    n.thin = 1L, keepTrainingFits = TRUE,
    printEvery = 100L, printCutoffs = 0L,
    verbose = TRUE, keepTrees = FALSE,
   keepCall = TRUE, samplerOnly = FALSE,
    seed = NA_integer_,
    proposal.probs = NULL,
    keepSampler = keepTrees,
    ...)
## S3 method for class 'bart'
plot(
    plquants = c(0.05, 0.95), cols = c('blue', 'black'),
    ...)
## S3 method for class 'bart'
predict(
    object, newdata, offset, weights,
    type = c("ev", "ppd", "bart"),
    combineChains = TRUE, ...)
extract(object, ...)
## S3 method for class 'bart'
extract(
    object,
    type = c("ev", "ppd", "bart", "trees"),
    sample = c("train", "test"),
    combineChains = TRUE, ...)
## S3 method for class 'bart'
```

```
fitted(
   object,
   type = c("ev", "ppd", "bart"),
   sample = c("train", "test"),
   ...)

## S3 method for class 'bart'
residuals(object, ...)
```

### **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 continous 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 aggresive 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 reponses 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.

splitprobs, split.probs

Prior and transition probabilities of variables used to generate splits. Can be missing/empty/NULL for equiprobability, a numeric vector of length equal to the number variables, or a named numeric vector with only a subset of the variables specified and a .default named value. Values given for factor variables are replicated for each resulting column in the generated model matrix.

numvars and num. vars symbols will be rebound before execution to the number of columns in the model matrix.

binaryOffset Used for binary y. When present, the model is  $P(Y = 1 \mid x) = \Phi(f(x) + x)$ 

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  $\prime$  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  ${\bf x}$ . 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  $nchain \times ndpost \times number$  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.

Optional integer specifying the desired pRNG seed. It should not be needed when running single-threaded - set.seed will suffice, and can be used to obtain reproducible results when multi-threaded. See Reproducibility section below.

proposalprobs, proposal.probs

Named numeric vector or NULL, optionally specifying the proposal rules and their probabilities. Elements should be "birth\_death", "change", and "swap" to control tree change proposals, and "birth" to give the relative frequency of birth/death in the "birth\_death" step. Defaults are 0.5, 0.1, 0.4, and 0.5 respectively.

keepsampler, keepSampler

Logical that can be used to save the underlying dbartsSampler-class object even if keepTrees is false.

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 offest is missing, defaults to NULL.

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

newdata Test data for prediction. Obeys 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, "ppd" - samples from the posterior predictive distribution, and "trees" - a data frame with tree information for when model was fit with keepTrees equal to TRUE. To synergize with predict.glm, "response" can be used as a synonym for "ev" and "link" can be used as a synonym for "bart". For information on extracting trees, see the subsection below.

sample Either "train" or "test".

... Additional arguments passed on to plot, dbartsControl, or extract when type is "trees". Not used in predict.

#### **Details**

BART is an Bayesian MCMC method. At each MCMC interation, 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  $f^*(x)$  (and  $\sigma^*$  in the numeric case) where \* denotes a particular draw. The x is either a row from the training data (x.train) or the test data (x.test).

**Decision Rules:** Decision rules for any tree are of the form  $x \le c$  vs. x > c for each 'x' corresponding to a column of x.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.train. If usequants is FALSE, the cutoffs are equally spaced across the range of values taken on by the corresponding column of x.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.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.

End-node prior parameter 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, which is interpretted 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, Inf), 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:** saveing 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).

**Reproducibility:** Behavior differs when running multi- and single-threaded, as the pseudo random number generators (pRNG) used by R are not thread safe. When single-threaded, R's built-in generator is used; if set at the start, the global .Random.seed will be used and its value updated as samples are drawn. When multi-threaded, the default behavior is to draw new random seeds for each thread using the clock and use thread-specific pRNGs.

This behavior can be modified by setting seed, or by using . . . to pass arguments to dbartsControl. For the single-threaded case, a new pRNG is built using that seed that is separate from R's native generator. As such, the global state will not be modified by subsequent calls to the generator. For multi-threaded, the seeds for threads are drawn sequentially using the supplied seed, and will again be separate from R's native generator.

Consequently, the seed argument is not needed when running single-threaded - set.seed will suffice. However, when multi-threaded the seed argument can be used to obtain reproducible results.

**Extracting Trees:** When a model is fit with keeptrees (bart) or keepTrees (bart2) equal to TRUE, the generic extract can be used to retrieve a data frame containing the tree fit information. In this case, extract will accept the additional, optional arguments: chainNums, sampleNums, and treeNums. Each should be an integer vector detailing the desired trees to be returned.

The result of extract will be a data frame with columns:

- sample, chain, tree index variables
- n number of observations in node
- var either the index of the variable used for splitting or -1 if the node is a leaf
- value either the value such that observations less than or equal to it are sent down the left path of the tree or the predicted value for a leaf node

The order of nodes in the result corresponds to a depth-first traversal, going down the left-side first. The names of variables used in splitting can be recovered by examining the column names of the fit\$data@x element of a fitted bart or bart2 model. See the package vignette "Working with dbarts Saved Trees".

#### Value

bart and bart2 return lists assigned the 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 xs 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. Di-

mensions 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).

signst The rough error standard deviation ( $\sigma$ ) 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 or keepsampler 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.

first.k Burn-in draws of k, if modeled.

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) + 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 a good 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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Vincent Dorie: <vdorie@gmail.com>.

#### References

Chipman, H., George, E., and McCulloch, R. (2009) BART: Bayesian Additive Regression Trees.

Chipman, H., George, E., and McCulloch R. (2006) Bayesian Ensemble Learning. Advances in Neural Information Processing Systems 19, Scholkopf, Platt and Hoffman, Eds., MIT Press, Cambridge, MA, 265-272.

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

Friedman, J.H. (1991) Multivariate adaptive regression splines. The Annals of Statistics, 19, 1–67.

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## See Also

pdbart

#### **Examples**

```
## simulate data (example from Friedman MARS paper)
## y = f(x) + epsilon - N(0, sigma)
\#\# x consists of 10 variables, only first 5 matter
f <- function(x) {</pre>
    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
      <- 100
x <- matrix(runif(n * 10), n, 10)</pre>
Ey \leftarrow f(x)
y <- rnorm(n, Ey, sigma)
## run BART
set.seed(99)
bartFit <- bart(x, y)</pre>
plot(bartFit)
## compare BART fit to linear matter and truth = Ey
lmFit \leftarrow lm(y \sim ., data.frame(x, y))
fitmat <- cbind(y, Ey, lmFit$fitted, bartFit$yhat.train.mean)</pre>
colnames(fitmat) <- c('y', 'Ey', 'lm', 'bart')</pre>
print(cor(fitmat))
```

dbarts

Discrete Bayesian Additive Regression Trees Sampler

# Description

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

#### Usage

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

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```
proposal.probs = c(
    birth_death = 0.5, swap = 0.1, change = 0.4, birth = 0.5),
control = dbarts::dbartsControl(), sigma = NA_real_)
```

# Arguments

- 2	,	
	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 overriden at run-time. See dbartsControl.
	tree.prior	An expression of the form cgm or cgm(power, base, split.probs) 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.
	proposal.probs	Named numeric vector or NULL, optionally specifying the proposal rules and their probabilities. Elements should be "birth_death", "change", and "swap" to control tree change proposals, and "birth" to give the relative frequency of birth/death in the "birth_death" step.
	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.

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#### **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 = dbarts::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.

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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. A non-negative integer determining how many samples, if any, are thrown away n.burn at the beginning of a run of the sampler. A positive integer giving the number of trees used in the sum-of-trees formulan.trees tion. n.chains A positive integer detailing the number of independent chains for the sampler to 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. If verbose is TRUE, every printEvery potential samples (after thinning) will printEvery issue a verbal statement. Must be a positive integer. A non-negative integer specifying how many of the decision rules for a variable printCutoffs are printed in verbose mode. Random number generator kind, as used in set. seed. For type "default", the rngKind 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 threadspecific 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

dbarts

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dbartsData

Discrete Bayesian Additive Regression Trees Sampler Data

#### **Description**

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

# Usage

```
dbartsData(
   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

dbarts

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

```
## 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)
```

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```
## 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'
setData(data)
## S4 method for signature 'dbartsSampler'
setResponse(y, updateState = NA)
## S4 method for signature 'dbartsSampler'
setOffset(offset, updateScale = FALSE, 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'
setTestPredictorAndOffset(x.test, offset.test, 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 = c(
        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.

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у	A numeric response vector of length equal to that with which the sampler was created.
Х	A numeric predictor vector of length equal to that with which the sampler was created. Can be of a distinct 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 substituted.
treeNums	An integer vector listing the indices of the trees to print.
treeNum	An integer listing the indices of the tree to plot.
treePlotPars	A named numeric vector containing the 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:** save-ing 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.

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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.

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.

#### Author(s)

Vincent Dorie: <vdorie@gmail.com>.

makeModelMatrixFromDataFrame

Make Model Matrix from Data Frame

#### **Description**

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

## Usage

```
makeModelMatrixFromDataFrame(x, drop = TRUE)
makeind(x, all = TRUE)
makeTestModelMatrix(data, newdata)
```

#### **Arguments**

x Data frame of explanatory variables.

drop Logical or list controling 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 x. Elements correspond to x according to:

• vector - single logical

• matrix - vector of logicals, one per column

• factor - table of factor levels to be referenced; levels with counts of 0 are to be dropped

all Not currently implemented.
data An existing dbartsData object.

newdata Test data frame.

#### **Details**

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

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

Use of these functions is not required when using bart, bart2, or 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**

```
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"))</pre>
```

pdbart

Partial Dependence Plots for BART

### **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

```
pdbart(
    x.train, y.train,
    xind = NULL,
    levs = NULL, levguants = 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(
    xind = seq_len(length(x$fd)),
    plquants = c(0.05, 0.95), cols = c('black', 'blue'),
    ...)
pd2bart(
    x.train, y.train,
    xind = NULL,
    levs = NULL, levguants = 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(
    plquants = c(0.05, 0.95), contour.color = 'white',
    justmedian = TRUE,
    ...)
```

#### **Arguments**

xind

levs

pl

Χ

levquants

plquants

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.

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.

Gives the values of a variable at which the plot is to be constructed. Must be a list, where the *i*th component gives the values for the *i*th variable. In pdbart, it should have same length as xind. In pd2bart, it should have length 2. See also argument 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.

For pdbart and pd2bart, if TRUE, plot is subsequently made (by calling plot.\*). 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

and a lower and upper quantile. piquants 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.

For plot.\*, object returned from pdbart or pd2bart.

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 pdbart  $x_s$  consists of a single variable in x and in pd2bart it is a pair of variables.

This is a computationally intensive procedure. For example, in 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 keepevery larger than 1 (eg. 10) makes the procedure much faster.

#### Value

The plot methods produce the plots and don't return anything.

pdbart and pd2bart return lists with components given below. The list returned by pdbart is assigned class pdbart and the list returned by pd2bart is assigned class pd2bart.

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 pdbart fd is actually a list whose kth component is the matrix described above corresponding to the kth variable chosen by argument xind. The number of columns in each matrix will equal the number of values given in the corresponding component of argument levs (or number of values in levquants).

For pd2bart, fd is a single matrix. The columns correspond to all possible pairs of values for the pair of variables indicated by xind. That is, all possible  $(x_i, x_j)$  where  $x_i$  is a value in the levs component corresponding to the first x and  $x_j$  is a value in the levs components corresponding to the second one. The first x changes first.

levs

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

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 bart. They are simply passed on from the BART run used to create the partial dependence plot. The function plot.bart can be applied to the object returned by pdbart or pd2bart to examine the BART run.

#### Author(s)

Hugh Chipman: <hugh.chipman@acadiau.ca>.

Robert McCulloch: <robert.mcculloch@chicagogsb.edu>.

#### References

Chipman, H., George, E., and McCulloch, R. (2006) BART: Bayesian Additive Regression Trees.

Chipman, H., George, E., and McCulloch R. (2006) Bayesian Ensemble Learning.

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

Friedman, J.H. (2001) Greedy function approximation: A gradient boosting machine. *The Annals of Statistics*, **29**, 1189–1232.

# **Examples**

```
## Not run:
## simulate data
f <- function(x)
    return(0.5 * x[,1] + 2 * x[,2] * x[,3])
sigma <- 0.2
   <- 100
set.seed(27)
x \leftarrow matrix(2 * runif(n * 3) - 1, ncol = 3)
colnames(x) <- c('rob', 'hugh', 'ed')</pre>
Ey \leftarrow 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, 0.6))
## 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 \sim ., data.frame(x, y))
fitmat <- cbind(y, Ey, lmFit$fitted, pdb1$yhat.train.mean)</pre>
colnames(fitmat) <- c('y', 'Ey', 'lm', 'bart')</pre>
print(cor(fitmat))
## example showing the use of a pre-fitted model
df <- data.frame(y, x)</pre>
set.seed(99)
bartFit <- bart(</pre>
    y \sim rob + hugh + ed, df,
    keepevery = 10, ntree = 100, keeptrees = TRUE)
pdb1 <- pdbart(bartFit, xind = rob + ed, pl = FALSE)</pre>
```

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```
## 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(dbarts::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,
    seed = NA_integer_,
    keepSampler = keepTrees,
   keepTestFits = TRUE,
    callback = NULL,
    . . . )
## S3 method for class 'rbart'
plot(
    x, plquants = c(0.05, 0.95), cols = c('blue', 'black'), ...)
## S3 method for class 'rbart'
fitted(
    object,
    type = c("ev", "ppd", "bart", "ranef"),
    sample = c("train", "test"),
    ...)
## S3 method for class 'rbart'
extract(
   object,
```

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```
type = c("ev", "ppd", "bart", "ranef", "trees"),
    sample = c("train", "test"),
    combineChains = 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.

keepTestFits Logical where, if false, test fits are obtained while running but not returned.

Useful with callback.

callback Optional function of trainFits, testFits, ranef, sigma, and tau. Called af-

ter every post-burn-in iteration and the results of which are collected and stored

in the final object.

formula, data, test, subset, weights, offset, offset.test, sigest, sigdf, sigquant, k, power, base, n.trees, n.samples, n.burn, n.chains, n.threads, combineChains, n.cuts, useQuantiles, keepTrainingFits, printEvery, printCutoffs, verbose, keepTrees, keepCall, seed, keepSampler, ...

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", or "trees" for the posterior of the

expected value, posterior predictive distribution, non-parametric/BART component, random effect, or saved trees 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"

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can be used as a synonym for "bart". For additional details on tree extraction, see the corresponding subsection in 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:

•  $y_i \sim N(f(x_i) + \alpha_{q[i]}, \sigma^2)$ 

•  $\alpha_j \sim N(0, \tau^2)$ .

For binary outcomes the response model is changed to  $P(Y_i = 1) = \Phi(f(x_i) + \alpha_{g[i]})$ . 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. Draws from the posterior of tau are made using a slice sampler, with a width dynamically determined by assessing the curvature of the posterior distribution at its mode.

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  $p(\alpha \mid y) = \int p(\alpha \mid \tau)p(\tau \mid y)d\alpha$ . 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 lth draw of the posterior of the random effect for group j (i.e.  $\alpha_i^*$ ) 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.

callback Optional results of callback function.

# Author(s)

Vincent Dorie: <vdorie@gmail.com>

#### See Also

```
bart, dbarts
```

# **Examples**

```
f <- function(x) {</pre>
    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
      <- 100
x <- matrix(runif(n * 10), n, 10)</pre>
Ey \leftarrow f(x)
y <- rnorm(n, Ey, sigma)
n.g < -10
g <- sample(n.g, length(y), replace = TRUE)</pre>
sigma.b <- 1.5
b <- rnorm(n.g, 0, sigma.b)</pre>
y \leftarrow y + b[g]
df <- as.data.frame(x)</pre>
colnames(df) \leftarrow paste0("x_", seq_len(ncol(x)))
df$y <- y
df$g <- g
## low numbers to reduce run time
rbartFit <- rbart_vi(y \sim . - g, df, group.by = g,
                       n.samples = 40L, n.burn = 10L, n.thin = 2L,
                       n.chains = 1L,
                       n.trees = 25L, n.threads = 1L)
```

xbart

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 evalulations of a loss functions on the held-out sets.

#### Usage

```
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.threads = dbarts::guessNumCores(), n.trees = 75L,
k = NULL, power = 2, base = 0.95, drop = TRUE,
resid.prior = chisq, control = dbarts::dbartsControl(), sigma = NA_real_,
seed = NA_integer_)
```

#### **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

underyling 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 func-

tion.

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", is ex-

pected 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 - missclassifi-

cation rate for binary responses, rmse - root-mean-squared-error for continuous response), log - negative log-loss for binary response (rmse serves this pur-

pose 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, weights), where y.test is the held out test subsample, y.test.hat is a matrix of dimension length(y.test) * n. samples, and weights are an optional vector of user-supplied weights. See examples.
Across different sets of parameters (k $\times$ power $\times$ base $\times$ n.trees) and n.reps, results are independent. For 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 NA is interpretted as 1.
A vector of positive integers setting the BART hyperparameter for the number of trees in the sum-of-trees formulation. See bart.
A vector of positive real numbers, setting the BART hyperparameter for the node-mean prior standard deviation. If NULL, the default of bart2 will be used - 2 for continuous response and a Chi hyperprior for binary. Hyperprior crossvalidation not possible at this time.
A vector of real numbers greater than one, setting the BART hyperparameter for the tree prior's growth probability, given by $base/(1+depth)^{power}$ .
A vector of real numbers in $(0,1)$ , setting the BART hyperparameter for the tree prior's growth probability.
Logical, determining if dimensions with a single value are dropped from the result.
An expression of the form chisq or chisq(df, quant) that sets the prior used on the residual/error variance.
An object inheriting from dbartsControl, created by the dbartsControl function.
A positive numeric estimate of the residual standard deviation. If NA, a linear model is used with all of the predictors to obtain one.
Optional integer specifying the desired pRNG seed. It should not be needed when running single-threaded - set.seed will suffice, and can be used to obtain reproducible results when multi-threaded. See Reproducibility section of bart.

# **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, missclassification 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) × 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)

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#### See Also

```
bart, dbarts
```

# **Examples**

```
f <- function(x) {</pre>
    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
      <- 100
x <- matrix(runif(n * 10), n, 10)</pre>
Ey \leftarrow f(x)
y <- rnorm(n, Ey, sigma)
mad <- function(y.train, y.train.hat, weights) {</pre>
    # note, weights are ignored
    mean(abs(y.train - apply(y.train.hat, 1L, mean)))
}
## low iteration numbers to to run quickly
xval \leftarrow 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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