# Package 'bartMachine'

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automobile

Data concerning automobile prices.

# Description

The automobile data frame has 201 rows and 25 columns and concerns automobiles in the 1985 Auto Imports Database. The response variable, price, is the log selling price of the automobile. There are 7 categorical predictors and 17 continuous / integer predictors which are features of the automobiles. 41 automobiles have missing data in one or more of the feature entries. This dataset is true to the original except with a few of the predictors dropped.

# Usage

data(automobile)

# Source

K Bache and M Lichman. UCI machine learning repository, 2013. http://archive.ics.uci.edu/ml/datasets/Automobile

bartMachine

Build a BART Model

# **Description**

Builds a BART model for regression or classification.

# Usage

```
bartMachine(X = NULL, y = NULL, Xy = NULL,
num\_trees = 50,
num_burn_in = 250,
num_iterations_after_burn_in = 1000,
alpha = 0.95, beta = 2, k = 2, q = 0.9, nu = 3,
prob_rule_class = 0.5,
mh_prob_steps = c(2.5, 2.5, 4)/9,
debug_log = FALSE,
run_in_sample = TRUE,
s_sq_y = "mse"
sig_sq_est = NULL,
cov_prior_vec = NULL,
use_missing_data = FALSE,
covariates_to_permute = NULL,
num_rand_samps_in_library = 10000,
use_missing_data_dummies_as_covars = FALSE,
replace_missing_data_with_x_j_bar = FALSE,
impute_missingness_with_rf_impute = FALSE,
impute_missingness_with_x_j_bar_for_lm = TRUE,
mem_cache_for_speed = TRUE,
flush_indices_to_save_RAM = TRUE,
serialize = FALSE,
seed = NULL,
verbose = TRUE)
build_bart_machine(X = NULL, y = NULL, Xy = NULL,
num\_trees = 50,
num_burn_in = 250,
num_iterations_after_burn_in = 1000,
alpha = 0.95, beta = 2, k = 2, q = 0.9, nu = 3,
prob_rule_class = 0.5,
mh_prob_steps = c(2.5, 2.5, 4)/9,
debug_log = FALSE,
run_in_sample = TRUE,
s_sq_y = "mse",
sig_sq_est = NULL,
cov_prior_vec = NULL,
use_missing_data = FALSE,
```

```
covariates_to_permute = NULL,
num_rand_samps_in_library = 10000,
use_missing_data_dummies_as_covars = FALSE,
replace_missing_data_with_x_j_bar = FALSE,
impute_missingness_with_rf_impute = FALSE,
impute_missingness_with_x_j_bar_for_lm = TRUE,
mem_cache_for_speed = TRUE,
flush_indices_to_save_RAM = TRUE,
serialize = FALSE,
seed = NULL,
verbose = TRUE)
```

#### **Arguments**

k

X Data frame of predictors. Factors are automatically converted to dummies inter-

nally.

y Vector of response variable. If y is numeric or integer, a BART model for re-

gression is built. If y is a factor with two levels, a BART model for classification

is built.

Xy A data frame of predictors and the response. The response column must be

named "y".

num\_trees The number of trees to be grown in the sum-of-trees model.

num\_burn\_in Number of MCMC samples to be discarded as "burn-in".

num\_iterations\_after\_burn\_in

Number of MCMC samples to draw from the posterior distribution of f(x).

alpha Base hyperparameter in tree prior for whether a node is nonterminal or not.

beta Power hyperparameter in tree prior for whether a node is nonterminal or not.

Tower hyperparameter in tree prior for whether a node is noncernman or not.

For regression, k determines the prior probability that E(Y|X) is contained in the interval  $(y_{min}, y_{max})$ , based on a normal distribution. For example, when k=2, the prior probability is 95%. For classification, k determines the prior probability that E(Y|X) is between (-3,3). Note that a larger value of k results

in more shrinkage and a more conservative fit.

q Quantile of the prior on the error variance at which the data-based estimate is

placed. Note that the larger the value of q, the more aggressive the fit as you are placing more prior weight on values lower than the data-based estimate. Not

used for classification.

nu Degrees of freedom for the inverse  $\chi^2$  prior. Not used for classification.

prob\_rule\_class

Threshold for classification. Any observation with a conditional probability greater than prob\_class\_rule is assigned the "positive" outcome. Note that the first level of the response is treated as the "negative" outcome and the sec-

ond is treated as the "positive" outcome.

mh\_prob\_steps Vector of prior probabilities for proposing changes to the tree structures: (GROW,

PRUNE, CHANGE)

file in the working directory.

run\_in\_sample If TRUE, in-sample statistics such as  $\hat{f}(x)$ , Pseudo- $R^2$ , and RMSE are computed. Setting this to FALSE when not needed can decrease computation time.

s\_sq\_y If "mse", a data-based estimated of the error variance is computed as the MSE from ordinary least squares regression. If "var"., the data-based estimate is computed as the variance of the response. Not used in classification.

Pass in an estimate of the maximum sig\_sq of the model. This is useful to cache somewhere and then pass in during cross-validation since the default method of estimation is a linear model. In large dimensions, linear model estimation is slow.

cov\_prior\_vec Vector assigning relative weights to how often a particular variable should be proposed as a candidate for a split. The vector is internally normalized so that the weights sum to 1. Note that the length of this vector must equal the length of the design matrix after dummification and augmentation of indicators of missingness (if used). To see what the dummified matrix looks like, use dummify\_data. See Bleich et al. (2013) for more details on when this feature is most appropriate.

If TRUE, the missing data feature is used to automatically handle missing data without imputation. See Kapelner and Bleich (2013) for details.

covariates\_to\_permute

Private argument for cov\_importance\_test. Not needed by user.

num\_rand\_samps\_in\_library Before building a BART model, samples from the Standard Normal and  $\chi^2(\nu)$  are drawn to be used in the MCMC steps. This parameter determines the number of samples to be taken.

use\_missing\_data\_dummies\_as\_covars

If TRUE, additional indicator variables for whether or not an observation in a particular column is missing are included. See Kapelner and Bleich (2013) for

details.
replace\_missing\_data\_with\_x\_j\_bar

impute\_missingness\_with\_rf\_impute

If TRUE, missing entries are filled in using the rf.impute() function from the randomForest library.

If TRUE, missing entries in X are imputed with average value or modal category.

impute\_missingness\_with\_x\_j\_bar\_for\_lm

If TRUE, when computing the data-based estimate of  $\sigma^2$ , missing entries are imputed with average value or modal category.

mem\_cache\_for\_speed

sig\_sq\_est

Speed enhancement that caches the predictors and the split values that are available at each node for selecting new rules. If the number of predictors is large, the memory requirements become large. We recommend keeping this on (default) and turning it off if you experience out-of-memory errors.

flush\_indices\_to\_save\_RAM

Setting this flag to TRUE saves memory with the downside that you cannot use the functions node\_prediction\_training\_data\_indices nor get\_projection\_weights.

serialize Setting this option to TRUE will allow serialization of bartMachine objects which

allows for persistence between R sessions if the object is saved and reloaded. Note that serialized objects can take up a large amount of memory. Thus, the

default is FALSE.

seed Optional: sets the seed in both R and Java. Default is NULL which does not set

the seed in R nor Java.

verbose Prints information about progress of the algorithm to the screen.

#### Value

Returns an object of class "bartMachine". The "bartMachine" object contains a list of the following components:

java\_bart\_machine

A pointer to the BART Java object.

train\_data\_features

The names of the variables used in the training data.

training\_data\_features\_with\_missing\_features.

The names of the variables used in the training data. If use\_missing\_data\_dummies\_as\_covars

= TRUE, this also includes dummies for any predictors that contain at least one

missing entry (named "M\_<feature>").

y The values of the response for the training data.

y\_levels The levels of the response (for classification only).

pred\_type Whether the model was build for regression of classification.

model\_matrix\_training\_data

The training data with factors converted to dummies.

num\_cores The number of cores used to build the BART model.

sig\_sq\_est The data-based estimate of  $\sigma^2$  used to create the prior on the error variance for

the BART model.

time\_to\_build Total time to build the BART model.

y\_hat\_train The posterior means of  $\hat{f}(x)$  for each observation. Only returned if run\_in\_sample

= TRUE.

residuals The model residuals given by y - y\_hat\_train. Only returned if run\_in\_sample

= TRUE.

L1\_err\_train L1 error on the training set. Only returned if run\_in\_sample = TRUE.

L2\_err\_train L2 error on the training set. Only returned if run\_in\_sample = TRUE.

PseudoRsq Calculated as 1 - SSE / SST where SSE is the sum of square errors in the training

data and SST is the sample variance of the response times n-1. Only returned

if run\_in\_sample = TRUE.

rmse\_train Root mean square error on the training set. Only returned if run\_in\_sample =

TRUE.

Additionally, the parameters passed to the function bartMachine are also components of the list.

#### Note

This function is parallelized by the number of cores set by set\_bart\_machine\_num\_cores. Each core will create an independent MCMC chain of size num\_burn\_in + num\_iterations\_after\_burn\_in / bart\_machine\_num\_cores.

#### Author(s)

Adam Kapelner and Justin Bleich

#### References

Adam Kapelner, Justin Bleich (2016). bartMachine: Machine Learning with Bayesian Additive Regression Trees. Journal of Statistical Software, 70(4), 1-40. doi:10.18637/jss.v070.i04

HA Chipman, EI George, and RE McCulloch. BART: Bayesian Additive Regressive Trees. The Annals of Applied Statistics, 4(1): 266–298, 2010.

A Kapelner and J Bleich. Prediction with Missing Data via Bayesian Additive Regression Trees. Canadian Journal of Statistics, 43(2): 224-239, 2015

J Bleich, A Kapelner, ST Jensen, and EI George. Variable Selection Inference for Bayesian Additive Regression Trees. ArXiv e-prints, 2013.

#### See Also

bartMachineCV

```
##regression example
##generate Friedman data
set.seed(11)
n = 200
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * \sin(pi* X[,1] * X[,2]) + 20 * (X[,3] -.5)^2 + 10 * X[,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)
summary(bart_machine)
## Not run:
##Build another BART regression model
bart_machine = bartMachine(X,y, num_trees = 200, num_burn_in = 500,
num_iterations_after_burn_in = 1000)
##Classification example
#get data and only use 2 factors
data(iris)
iris2 = iris[51:150,]
iris2$Species = factor(iris2$Species)
```

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```
#build BART classification model
bart_machine = build_bart_machine(iris2[ ,1:4], iris2$Species)
##get estimated probabilities
phat = bart_machine$p_hat_train
##look at in-sample confusion matrix
bart_machine$confusion_matrix
## End(Not run)
```

bartMachineArr

Create an array of BART models for the same data.

# Description

If BART creates models that are variable, running many on the same dataset and averaging is a good strategy. This function is a convenience method for this procedure.

# Usage

```
bartMachineArr(bart_machine, R = 10)
```

# Arguments

bart\_machine An object of class "bartMachine".

R The number of replicated BART models in the array.

#### Value

A bartMachineArr object which is just a list of the R bartMachine models.

# Author(s)

Adam Kapelner

```
#Regression example
## Not run:
#generate Friedman data
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
```

```
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)
bart_machine_arr = bartMachineArr(bart_machine)

#Classification example
data(iris)
iris2 = iris[51 : 150, ] #do not include the third type of flower for this example
iris2$Species = factor(iris2$Species)
bart_machine = bartMachine(iris2[ ,1:4], iris2$Species)
bart_machine_arr = bartMachineArr(bart_machine)

## End(Not run)
```

bartMachineCV

Build BART-CV

# **Description**

Builds a BART-CV model by cross-validating over a grid of hyperparameter choices.

# Usage

```
bartMachineCV(X = NULL, y = NULL, Xy = NULL,
num_tree_cvs = c(50, 200), k_cvs = c(2, 3, 5),
nu_q_cvs = NULL, k_folds = 5, verbose = FALSE, ...)
build_bart_machine_cv(X = NULL, y = NULL, Xy = NULL,
num_tree_cvs = c(50, 200), k_cvs = c(2, 3, 5),
nu_q_cvs = NULL, k_folds = 5, verbose = FALSE, ...)
```

# **Arguments**

X	Data frame of predictors. Factors are automatically converted to dummies interally.
у	Vector of response variable. If y is numeric or integer, a BART model for regression is built. If y is a factor with two levels, a BART model for classification is built.
Ху	A data frame of predictors and the response. The response column must be named "y".
num_tree_cvs	Vector of sizes for the sum-of-trees models to cross-validate over.
k_cvs	Vector of choices for the hyperparameter k to cross-validate over.
nu_q_cvs	Only for regression. List of vectors containing (nu, q) ordered pair choices to cross-validate over. If NULL, then it defaults to the three values list(c(3,0.9),c(3,0.99),c(10,0.75))

k_folds	Number of folds for cross-validation
verbose	Prints information about progress of the algorithm to the screen.
	Additional arguments to be passed to bartMachine.

#### Value

Returns an object of class "bartMachine" with the set of hyperparameters chosen via cross-validation. We also return a matrix "cv\_stats" which contains the out-of-sample RMSE for each hyperparameter set tried and "folds" which gives the fold in which each observation fell across the k-folds.

#### Note

This function may require significant run-time. This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores via calling bartMachine.

# Author(s)

Adam Kapelner and Justin Bleich

# References

Adam Kapelner, Justin Bleich (2016). bartMachine: Machine Learning with Bayesian Additive Regression Trees. Journal of Statistical Software, 70(4), 1-40. doi:10.18637/jss.v070.i04

#### See Also

bartMachine

```
## Not run:
#generate Friedman data
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine_cv = bartMachineCV(X, y)
#information about cross-validated model
summary(bart_machine_cv)
## End(Not run)
```

bart\_machine\_get\_posterior

Get Full Posterior Distribution

# Description

Generates draws from posterior distribution of  $\hat{f}(x)$  for a specified set of observations.

# Usage

```
bart_machine_get_posterior(bart_machine, new_data)
```

# **Arguments**

bart\_machine An object of class "bartMachine".

new\_data A data frame containing observations at which draws from posterior distribution

of f(x) are to be obtained.

# Value

Returns a list with the following components:

y\_hat Posterior mean estimates. For regression, the estimates have the same units as

the response. For classification, the estimates are probabilities.

Column names should match that of the training data.

y\_hat\_posterior\_samples

The full set of posterior samples of size num\_iterations\_after\_burn\_in for each observation. For regression, the estimates have the same units as the re-

sponse. For classification, the estimates are probabilities.

#### Note

This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores.

# Author(s)

Adam Kapelner and Justin Bleich

#### See Also

calc\_credible\_intervals, calc\_prediction\_intervals

# **Examples**

```
## Not run:
#Regression example
#generate Friedman data
set.seed(11)
n = 200
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * \sin(pi* X[,1] * X[,2]) + 20 * (X[,3] -.5)^2 + 10 * X[,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)
#get posterior distribution
posterior = bart_machine_get_posterior(bart_machine, X)
print(posterior$y_hat)
#Classification example
#get data and only use 2 factors
data(iris)
iris2 = iris[51:150,]
iris2$Species = factor(iris2$Species)
#build BART classification model
bart_machine = bartMachine(iris2[ ,1 : 4], iris2$Species)
#get posterior distribution
posterior = bart_machine_get_posterior(bart_machine, iris2[ ,1 : 4])
print(posterior$y_hat)
## End(Not run)
```

bart\_machine\_num\_cores

Get Number of Cores Used by BART

# **Description**

Returns number of cores used by BART

# Usage

```
bart_machine_num_cores()
```

# **Details**

Returns the number of cores currently being used by parallelized BART functions

# Value

Number of cores currently being used by parallelized BART functions.

# Author(s)

Adam Kapelner and Justin Bleich

# See Also

```
set_bart_machine_num_cores
```

# **Examples**

```
## Not run:
bart_machine_num_cores()
## End(Not run)
```

```
bart_predict_for_test_data
```

Predict for Test Data with Known Outcomes

# Description

Utility wrapper function for computing out-of-sample metrics for a BART model when the test set outcomes are known.

# Usage

```
bart_predict_for_test_data(bart_machine, Xtest, ytest, prob_rule_class = NULL)
```

# Arguments

bart\_machine An object of class "bartMachine".

Xtest Data frame for test data containing rows at which predictions are to be made.

Colnames should match that of the training data.

ytest Actual outcomes for test data.

prob\_rule\_class

Threshold for classification.

# Value

For regression models, a list with the following components is returned:

y\_hat Predictions (as posterior means) for the test observations.

L1\_err L1 error for predictions.
L2\_err L2 error for predictions.
rmse RMSE for predictions.

For classification models, a list with the following components is returned:

y\_hat Class predictions for the test observations.
p\_hat Probability estimates for the test observations.
confusion\_matrix

A confusion matrix for the test observations.

# Author(s)

Adam Kapelner and Justin Bleich

#### See Also

predict

```
#generate Friedman data
set.seed(11)
n = 250
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[,4] + 5 * X[,5] + rnorm(n)
##split into train and test
train_X = X[1 : 200, ]
test_X = X[201 : 250, ]
train_y = y[1 : 200]
test_y = y[201 : 250]
##build BART regression model
bart_machine = bartMachine(train_X, train_y)
#explore performance on test data
oos_perf = bart_predict_for_test_data(bart_machine, test_X, test_y)
print(oos_perf$rmse)
```

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benchmark\_datasets benchmark\_datasets

# **Description**

Nine diverse datasets which were used for benchmarking bartMachine's out of sample performance in the vignette for this package.

# Usage

```
data(benchmark_datasets)
```

# **Source**

See vignette for details.

```
calc_credible_intervals
```

Calculate Credible Intervals

# Description

Generates credible intervals for  $\hat{f}(x)$  for a specified set of observations.

# Usage

```
calc_credible_intervals(bart_machine, new_data,
ci_conf = 0.95)
```

# **Arguments**

bart\_machine An object of class "bartMachine".

new\_data A data frame containing observations at which credible intervals for  $\hat{f}(x)$  are to

be computed.

ci\_conf Confidence level for the credible intervals. The default is 95%.

# **Details**

This interval is the appropriate quantiles based on the confidence level, ci\_conf, of the predictions for each of the Gibbs samples post-burn in.

#### Value

Returns a matrix of the lower and upper bounds of the credible intervals for each observation in new\_data.

#### Note

This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores.

#### Author(s)

Adam Kapelner and Justin Bleich

#### See Also

```
calc_prediction_intervals, bart_machine_get_posterior
```

# **Examples**

```
#generate Friedman data
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)

#get credible interval
cred_int = calc_credible_intervals(bart_machine, X)
print(head(cred_int))
```

calc\_prediction\_intervals

Calculate Prediction Intervals

# Description

Generates prediction intervals for  $\hat{y}$  for a specified set of observations.

# Usage

```
calc_prediction_intervals(bart_machine, new_data,
pi_conf = 0.95, num_samples_per_data_point = 1000)
```

# **Arguments**

bart\_machine An object of class "bartMachine".

new\_data A data frame containing observations at which prediction intervals for  $\hat{y}$  are to

be computed.

pi\_conf Confidence level for the prediction intervals. The default is 95%.

num\_samples\_per\_data\_point

The number of samples taken from the predictive distribution. The default is 1000.

#### **Details**

Credible intervals (see calc\_credible\_intervals) are the appropriate quantiles of the prediction for each of the Gibbs samples post-burn in. Prediction intervals also make use of the noise estimate at each Gibbs sample and hence are wider. For each Gibbs sample, we record the  $\hat{y}$  estimate of the response and the  $\hat{\sigma^2}$  estimate of the noise variance. We then sample normal\_samples\_per\_gibbs\_sample times from a  $N(\hat{y}, \hat{\sigma^2})$  random variable to simulate many possible disturbances for that Gibbs sample. Then, all normal\_samples\_per\_gibbs\_sample times the number of Gibbs sample post burnin are collected and the appropriate quantiles are taken based on the confidence level, pi\_conf.

#### Value

Returns a matrix of the lower and upper bounds of the prediction intervals for each observation in new\_data.

# Note

This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores.

#### Author(s)

Adam Kapelner and Justin Bleich

#### References

Adam Kapelner, Justin Bleich (2016). bartMachine: Machine Learning with Bayesian Additive Regression Trees. Journal of Statistical Software, 70(4), 1-40. doi:10.18637/jss.v070.i04

# See Also

calc\_credible\_intervals, bart\_machine\_get\_posterior

```
## Not run:
#generate Friedman data
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)
#get prediction interval
pred_int = calc_prediction_intervals(bart_machine, X)
print(head(pred_int))
## End(Not run)
```

# **Description**

Diagnostic tools to assess whether the errors of the BART model for regression are normally distributed and homoskedastic, as assumed by the model. This function generates a normal quantile plot of the residuals with a Shapiro-Wilks p-value as well as a residual plot.

# Usage

```
check_bart_error_assumptions(bart_machine, hetero_plot = "yhats")
```

# **Arguments**

 ${\tt bart\_machine} \qquad {\tt An\ object\ of\ class\ "bartMachine"}.$ 

hetero\_plot If "yhats", the residuals are plotted against the fitted values of the response. If

"ys", the residuals are plotted against the actual values of the response.

#### Value

None.

# Author(s)

Adam Kapelner and Justin Bleich

# See Also

```
plot_convergence_diagnostics
```

```
## Not run:
#generate Friedman data
set.seed(11)
n = 300
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)
#check error diagnostics
check_bart_error_assumptions(bart_machine)
## End(Not run)
```

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cov\_importance\_test

Importance Test for Covariate(s) of Interest

# **Description**

This function tests the null hypothesis  $H_0$ : These covariates of interest do not affect the response under the assumptions of the BART model.

#### Usage

```
cov_importance_test(bart_machine, covariates = NULL,
num_permutation_samples = 100, plot = TRUE)
```

# **Arguments**

bart\_machine An object of class "bart\_machine".

covariates A vector of names of covariates of interest to be tested for having an effect on the

response. A value of NULL indicates an omnibus test for all covariates having an effect on the response. If the name of a covariate is a factor, the entire factor will be permuted. We do not recommend entering the names of factor covariate

dummies.

num\_permutation\_samples

The number of times to permute the covariates of interest and create a corre-

sponding new BART model (see details).

plot If TRUE, this produces a histogram of the Pseudo-Rsq's / total misclassifca-

tion error rates from the num\_permutations BART models created with the covariates permuted. The plot also illustrates the observed Pseudo-Rsq's / total misclassification error rate from the original training data and indicates the

test's p-value.

#### **Details**

To test the importance of a covariate or a set of covariates of interest on the response, this function generates num\_permutations BART models with the covariate(s) of interest permuted (differently each time). On each run, a measure of fit is recorded. For regression, the metric is Pseudo-Rsq; for classification, it is total misclassification error.

A p-value can then be generated as follows. For regression, the p-value is the number of permutation-sampled Pseudo-Rsq's greater than the observed Pseudo-Rsq divided by num\_permutations + 1. For classification, the p-value is the number of permutation-sampled total misclassification errors less than the observed total misclassification error divided by num\_permutations + 1.

# Value

```
permutation_samples_of_error
```

A vector which records the error metric of the BART models with the covariates permuted (see details).

observed\_error\_estimate

For regression, this is the Pseudo-Rsq on the original training data set. For classification, this is the observed total misclassification error on the original training data set.

pval

The approximate p-value for this test (see details).

#### Note

This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores.

#### Author(s)

Adam Kapelner and Justin Bleich

#### References

Adam Kapelner, Justin Bleich (2016). bartMachine: Machine Learning with Bayesian Additive Regression Trees. Journal of Statistical Software, 70(4), 1-40. doi:10.18637/jss.v070.i04

# **Examples**

```
## Not run:
##regression example

##generate Friedman data
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)

##build BART regression model
bart_machine = bartMachine(X, y)

##now test if X[, 1] affects Y nonparametrically under the BART model assumptions
cov_importance_test(bart_machine, covariates = c(1))
## note the plot and the printed p-value

## End(Not run)
```

destroy\_bart\_machine Destroy BART Model (deprecated — do not use!)

#### **Description**

A deprecated function that previously was responsible for cleaning up the RAM associated with a BART model. This is now handled natively by R's garbage collection.

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# Usage

```
destroy_bart_machine(bart_machine)
```

#### **Arguments**

```
bart_machine deprecated — do not use!
```

# **Details**

Removing a "bart\_machine" object from R previously did not free heap space from Java. Since BART objects can consume a large amount of RAM, it is important to remove these objects by calling this function if they are no longer needed or many BART objects are being created. This operation is now taken care of by R's garbage collection. This function is deprecated and should not be used. However, running it is harmless.

#### Value

None.

# Author(s)

Adam Kapelner and Justin Bleich

# **Examples**

##None

 $dummify\_data$ 

Dummify Design Matrix

# **Description**

Create a data frame with factors converted to dummies.

# Usage

```
dummify_data(data)
```

# **Arguments**

data

Data frame to be dummified.

# **Details**

The column names of the dummy variables are given by the "FactorName\_LevelName" and are augmented to the end of the design matrix. See the example below.

#### Value

Returns a data frame with factors converted to dummy indicator variables.

# Note

BART handles dummification internally. This function is provided as a utility function.

# Author(s)

Adam Kapelner and Justin Bleich

# **Examples**

```
#generate data
set.seed(11)
x1 = rnorm(20)
x2 = as.factor(ifelse(x1 > 0, "A", "B"))
x3 = runif(20)
X = data.frame(x1,x2,x3)
#dummify data
X_dummified = dummify_data(X)
print(X_dummified)
```

```
get_projection_weights
```

Gets Training Sample Projection / Weights

# **Description**

Returns the matrix H where yhat is approximately equal to H y where yhat is the predicted values for new\_data. If new\_data is unspecified, yhat will be the in-sample fits. If BART was the same as OLS, H would be an orthogonal projection matrix. Here it is a projection matrix, but clearly non-orthogonal. Unfortunately, I cannot get this function to work correctly because of three possible reasons (1) BART does not work by averaging tree predictions: it is a sum of trees model where each tree sees the residuals via backfitting (2) the prediction in each node is a bayesian posterior draw which is close to ybar of the observations contained in the node if noise is gauged to be small and (3) there are transformations of the original y variable. I believe I got close and I think I'm off by a constant multiple which is a function of the number of trees. I can use regression to estimate the constant multiple and correct for it. Turn regression\_kludge to TRUE for this. Note that the weights do not add up to one here. The intuition is because due to the backfitting there is multiple counting. But I'm not entirely sure.

# Usage

```
get_projection_weights(bart_machine, new_data = NULL, regression_kludge = FALSE)
```

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# **Arguments**

```
bart_machine An object of class "bartMachine".

new_data Data that you wish to investigate the training sample projection / weights. If NULL, the original training data is used.

regression_kludge See explanation in the description. Default is FALSE.
```

#### Value

Returns a matrix of proportions with number of rows equal to the number of rows of new\_data and number of columns equal to the number of rows of the original training data, n.

```
## Not run:
options(java.parameters = "-Xmx10g")
pacman::p_load(bartMachine, tidyverse)
seed = 1984
set.seed(seed)
n = 100
x = rnorm(n, 0, 1)
sigma = 0.1
y = x + rnorm(n, 0, sigma)
num\_trees = 200
num_iterations_after_burn_in = 1000
bart_mod = bartMachine(data.frame(x = x), y,
flush_indices_to_save_RAM = FALSE,
num_trees = num_trees,
num_iterations_after_burn_in = num_iterations_after_burn_in,
seed = seed)
bart_mod
n_star = 100
x_star = rnorm(n_star)
y_star = as.numeric(x_star + rnorm(n_star, 0, sigma))
yhat_star_bart = predict(bart_mod, data.frame(x = x_star))
Hstar = get_projection_weights(bart_mod, data.frame(x = x_star))
rowSums(Hstar)
yhat_star_projection = as.numeric(Hstar
ggplot(data.frame(
yhat_star = yhat_star_bart,
yhat_star_projection = yhat_star_projection,
y_star = y_star)) +
  geom_point(aes(x = yhat_star_bart, y = yhat_star_projection), col = "green") +
  geom_abline(slope = 1, intercept = 0)
Hstar = get_projection_weights(bart_mod, data.frame(x = x_star), regression_kludge = TRUE)
```

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```
rowSums(Hstar)
yhat_star_projection = as.numeric(Hstar)

ggplot(data.frame(
yhat_star = yhat_star_bart,
yhat_star_projection = yhat_star_projection,
y_star = y_star)) +
    geom_point(aes(x = yhat_star_bart, y = yhat_star_projection), col = "green") +
    geom_abline(slope = 1, intercept = 0)

## End(Not run)
```

get\_sigsqs

Get Posterior Error Variance Estimates

# **Description**

Returns the posterior estimates of the error variance from the Gibbs samples with an option to create a histogram of the posterior estimates of the error variance with a credible interval overlaid.

# Usage

```
get_sigsqs(bart_machine, after_burn_in = T,
plot_hist = F, plot_CI = .95, plot_sigma = F)
```

# **Arguments**

bart\_machine An object of class "bartMachine". after\_burn\_in If TRUE, only the  $\sigma^2$  draws after the burn-in period are returned. plot\_hist If TRUE, a histogram of the posterior  $\sigma^2$  draws is generated. plot\_CI Confidence level for credible interval on histogram. plot\_sigma If TRUE, plots  $\sigma$  instead of  $\sigma^2$ .

# Value

Returns a vector of posterior  $\sigma^2$  draws (with or without the burn-in samples).

# Author(s)

Adam Kapelner and Justin Bleich

#### See Also

```
get_sigsqs
```

# **Examples**

```
## Not run:
#generate Friedman data
set.seed(11)
n = 300
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)

#get posterior sigma^2's after burn-in and plot
sigsqs = get_sigsqs(bart_machine, plot_hist = TRUE)
## End(Not run)
```

```
get_var_counts_over_chain
```

Get the Variable Inclusion Counts

# **Description**

Computes the variable inclusion counts for a BART model.

# Usage

```
get_var_counts_over_chain(bart_machine, type = "splits")
```

# **Arguments**

bart\_machine An object of class "bartMachine".

type If "splits", then the number of times each variable is chosen for a splitting rule

is computed. If "trees", then the number of times each variable appears in a tree

is computed.

#### Value

Returns a matrix of counts of each predictor across all trees by Gibbs sample. Thus, the dimension is num\_interations\_after\_burn\_in by p (where p is the number of predictors after dummifying factors and adding missingness dummies if specified by use\_missing\_data\_dummies\_as\_covars).

# Author(s)

Adam Kapelner and Justin Bleich

# See Also

```
get_var_props_over_chain
```

# **Examples**

```
## Not run:
#generate Friedman data
set.seed(11)
n = 200
p = 10
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y, num_trees = 20)
#get variable inclusion counts
var_counts = get_var_counts_over_chain(bart_machine)
print(var_counts)
## End(Not run)
```

```
get_var_props_over_chain
```

Get the Variable Inclusion Proportions

# **Description**

Computes the variable inclusion proportions for a BART model.

# Usage

```
get_var_props_over_chain(bart_machine, type = "splits")
```

# **Arguments**

bart\_machine An object of class "bartMachine".

type If "splits", then the proportion of times each variable is chosen for a splitting

rule versus all splitting rules is computed. If "trees", then the proportion of times each variable appears in a tree versus all appearances of variables in trees

is computed.

#### Value

Returns a vector of the variable inclusion proportions.

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# Author(s)

Adam Kapelner and Justin Bleich

#### See Also

```
get_var_counts_over_chain
```

#### **Examples**

```
#generate Friedman data
set.seed(11)
n = 200
p = 10
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y, num_trees = 20)
#Get variable inclusion proportions
var_props = get_var_props_over_chain(bart_machine)
print(var_props)
```

interaction\_investigator

Explore Pairwise Interactions in BART Model

# Description

Explore the pairwise interaction counts for a BART model to learn about interactions fit by the model. This function includes an option to generate a plot of the pairwise interaction counts.

# Usage

```
interaction_investigator(bart_machine, plot = TRUE,
num_replicates_for_avg = 5, num_trees_bottleneck = 20,
num_var_plot = 50, cut_bottom = NULL, bottom_margin = 10)
```

# **Arguments**

```
bart_machine An object of class "bartMachine".

plot If TRUE, a plot of the pairwise interaction counts is generated.

num_replicates_for_avg
```

The number of replicates of BART to be used to generate pairwise interaction inclusion counts. Averaging across multiple BART models improves stability of the estimates.

num\_trees\_bottleneck

Number of trees to be used in the sum-of-trees model for computing pairwise interactions counts. A small number of trees should be used to force the variables to compete for entry into the model.

num\_var\_plot

Number of variables to be shown on the plot. If "Inf," all variables are plotted (not recommended if the number of predictors is large). Default is 50.

cut\_bottom

A display parameter between 0 and 1 that controls where the y-axis is plotted. A value of 0 would begin the y-axis at 0; a value of 1 begins the y-axis at the minimum of the average pairwise interaction inclusion count (the smallest bar in the bar plot). Values between 0 and 1 begin the y-axis as a percentage of that minimum.

bottom\_margin

A display parameter that adjusts the bottom margin of the graph if labels are clipped. The scale of this parameter is the same as set with par(mar = c(...)) in R. Higher values allow for more space if the crossed covariate names are long. Note that making this parameter too large will prevent plotting and the plot function in R will throw an error.

#### **Details**

An interaction between two variables is considered to occur whenever a path from any node of a tree to any of its terminal node contains splits using those two variables. See Kapelner and Bleich, 2013, Section 4.11.

#### Value

interaction\_counts\_avg

For each of the  $p \times p$  interactions, what is the average count across all num\_replicates\_for\_avg BART model replicates' post burn-in Gibbs samples in all trees.

interaction\_counts\_sd

For each of the  $p \times p$  interactions, what is the average sd of the interaction counts across the num\_replicates\_for\_avg BART models replicates.

#### Note

In the plot, the red bars correspond to the standard error of the variable inclusion proportion estimates (since multiple replicates were used).

#### Author(s)

Adam Kapelner and Justin Bleich

# References

Adam Kapelner, Justin Bleich (2016). bartMachine: Machine Learning with Bayesian Additive Regression Trees. Journal of Statistical Software, 70(4), 1-40. doi:10.18637/jss.v070.i04

#### See Also

investigate\_var\_importance

# **Examples**

```
## Not run:
#generate Friedman data
set.seed(11)
n = 200
p = 10
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y, num_trees = 20)
#investigate interactions
interaction_investigator(bart_machine)
## End(Not run)
```

investigate\_var\_importance

Explore Variable Inclusion Proportions in BART Model

# **Description**

Explore the variable inclusion proportions for a BART model to learn about the relative influence of the different covariates. This function includes an option to generate a plot of the variable inclusion proportions.

# Usage

```
investigate_var_importance(bart_machine, type = "splits",
plot = TRUE, num_replicates_for_avg = 5, num_trees_bottleneck = 20,
num_var_plot = Inf, bottom_margin = 10)
```

#### **Arguments**

bart\_machine An object of class "bartMachine".

type If "splits", then the proportion of times each variable is chosen for a splitting

rule is computed. If "trees", then the proportion of times each variable appears

in a tree is computed.

plot If TRUE, a plot of the variable inclusion proportions is generated.

num\_replicates\_for\_avg

The number of replicates of BART to be used to generate variable inclusion proportions. Averaging across multiple BART models improves stability of the

estimates. See Bleich et al. (2013) for more details.

num\_trees\_bottleneck

Number of trees to be used in the sum-of-trees for computing the variable inclusion proportions. A small number of trees should be used to force the variables to compete for entry into the model. Chipman et al. (2010) recommend 20. See this reference for more details.

num\_var\_plot

Number of variables to be shown on the plot. If "Inf", all variables are plotted.

bottom\_margin

A display parameter that adjusts the bottom margin of the graph if labels are clipped. The scale of this parameter is the same as set with par(mar = c(...)) in R. Higher values allow for more space if the covariate names are long. Note that making this parameter too large will prevent plotting and the plot function in R will throw an error.

#### **Details**

In the plot, the red bars correspond to the standard error of the variable inclusion proportion estimates.

#### Value

Invisibly, returns a list with the following components:

avg\_var\_props The average variable inclusion proportions for each variable

(across num\_replicates\_for\_avg)

(across num\_replicates\_for\_avg)

#### Note

This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores.

# Author(s)

Adam Kapelner and Justin Bleich

# References

Adam Kapelner, Justin Bleich (2016). bartMachine: Machine Learning with Bayesian Additive Regression Trees. Journal of Statistical Software, 70(4), 1-40. doi:10.18637/jss.v070.i04

J Bleich, A Kapelner, ST Jensen, and EI George. Variable Selection Inference for Bayesian Additive Regression Trees. ArXiv e-prints, 2013.

HA Chipman, EI George, and RE McCulloch. BART: Bayesian Additive Regressive Trees. The Annals of Applied Statistics, 4(1): 266–298, 2010.

#### See Also

interaction\_investigator

k\_fold\_cv 31

# **Examples**

```
## Not run:
#generate Friedman data
set.seed(11)
n = 200
p = 10
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y, num_trees = 20)
#investigate variable inclusion proportions
investigate_var_importance(bart_machine)
## End(Not run)
```

k\_fold\_cv

Estimate Out-of-sample Error with K-fold Cross validation

# **Description**

Builds a BART model using a specified set of arguments to build\_bart\_machine and estimates the out-of-sample performance by using k-fold cross validation.

# Usage

```
k_fold_cv(X, y, k_folds = 5, folds_vec = NULL, verbose = FALSE, ...)
```

# **Arguments**

Χ	Data frame of predictors. Factors are automatically converted to dummies interally.
У	Vector of response variable. If y is numeric or integer, a BART model for regression is built. If y is a factor with two levels, a BART model for classification is built.
k_folds	Number of folds to cross-validate over. This argument is ignored if folds_vec is non-null.
folds_vec	An integer vector of indices specifying which fold each observation belongs to.
verbose	Prints information about progress of the algorithm to the screen.
	Additional arguments to be passed to build_bart_machine.

#### **Details**

For each fold, a new BART model is trained (using the same set of arguments) and its performance is evaluated on the holdout piece of that fold.

 $k_{fold}cv$ 

#### Value

For regression models, a list with the following components is returned:

y\_hat Predictions for the observations computed on the fold for which the observation

was omitted from the training set.

L1\_err Aggregate L1 error across the folds.

L2\_err Aggregate L1 error across the folds.

rmse Aggregate RMSE across the folds.

folds Vector of indices specifying which fold each observation belonged to.

For classification models, a list with the following components is returned:

y\_hat Class predictions for the observations computed on the fold for which the obser-

vation was omitted from the training set.

p\_hat Probability estimates for the observations computed on the fold for which the

observation was omitted from the training set.

confusion\_matrix

Aggregate confusion matrix across the folds.

misclassification\_error

Total misclassification error across the folds.

folds Vector of indices specifying which fold each observation belonged to.

#### Note

This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores.

#### Author(s)

Adam Kapelner and Justin Bleich

# See Also

bartMachine

```
## Not run:
#generate Friedman data
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
#evaluate default BART on 5 folds
k_fold_val = k_fold_cv(X, y)
print(k_fold_val$rmse)
## End(Not run)
```

linearity\_test 33

# **Description**

Test to investigate  $H_0$ : the functional relationship between the response and the regressors is linear. We fit a linear model and then test if the residuals are a function of the regressors using the

# Usage

```
linearity_test(lin_mod = NULL, X = NULL, y = NULL,
num_permutation_samples = 100, plot = TRUE, ...)
```

# **Arguments**

	lin_mod	A linear model you can pass in if you do not want to use the default which is $lm(y \sim X)$ . Default is NULL which should be used if you pass in X and y.
	X	Data frame of predictors. Factors are automatically converted to dummies internally. Default is NULL which should be used if you pass in lin_mode.
	у	Vector of response variable. If y is numeric or integer, a BART model for regression is built. If y is a factor with two levels, a BART model for classification is built. Default is NULL which should be used if you pass in lin_mode.
num_permutation_samples		
		This function relies on ${\tt cov\_importance\_test}$ (see documentation there for details).
	plot	This function relies on cov_importance_test (see documentation there for details).
	•••	Additional parameters to be passed to bartMachine, the model constructed on the residuals of the linear model.

# Value

```
permutation_samples_of_error

This function relies on cov_importance_test (see documentation there for details).

observed_error_estimate

This function relies on cov_importance_test (see documentation there for details).

pval

The approximate p-value for this test. See the documentation at cov_importance_test.
```

# Author(s)

Adam Kapelner

# See Also

```
cov_importance_test
```

# **Examples**

```
## Not run:
##regression example
##generate Friedman data i.e. a nonlinear response model
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[,1] * X[,2]) + 20 * (X[,3] -.5)^2 + 10 * X[,4] + 5 * X[,5] + rnorm(n)
##now test if there is a nonlinear relationship between X1, ..., X5 and y.
linearity_test(X = X, y = y)
## note the plot and the printed p-value.. should be approx 0
#generate a linear response model
y = 1 * X[,1] + 3 * X[,2] + 5 * X[,3] + 7 * X[,4] + 9 * X[,5] + rnorm(n)
linearity_test(X = X, y = y)
## note the plot and the printed p-value.. should be > 0.05
## End(Not run)
```

node\_prediction\_training\_data\_indices

Gets node predictions indices of the training data for new data.

# Description

This returns a binary tensor for all gibbs samples after burn-in for all trees and for all training observations.

# Usage

```
node_prediction_training_data_indices(bart_machine, new_data = NULL)
```

# **Arguments**

bart\_machine An object of class "bartMachine".

new\_data Data that you wish to investigate the training sample weights. If NULL, the orig-

inal training data is used.

# Value

Returns a binary tensor indicating whether the prediction node contained a training datum or not. For each observation in new data, the size of this tensor is number of gibbs sample after burn-in times the number of trees times the number of training data observations. This the size of the

pd\_plot 35

full tensor is the number of observations in the new data times the three dimensional object just explained.

pd\_plot

Partial Dependence Plot

# **Description**

Creates a partial dependence plot for a BART model for regression or classification.

# Usage

```
pd_plot(bart_machine, j,
levs = c(0.05, seq(from = 0.1, to = 0.9, by = 0.1), 0.95),
lower_ci = 0.025, upper_ci = 0.975, prop_data = 1)
```

# **Arguments**

bart_machine	An object of class "bartMachine".
j	The number or name of the column in the design matrix for which the partial dependence plot is to be created.
levs	Quantiles at which the partial dependence function should be evaluated. Linear extrapolation is performed between these points.
lower_ci	Lower limit for credible interval
upper_ci	Upper limit for credible interval
prop_data	The proportion of the training data to use. Default is 1. Use a lower proportion for speedier pd_plots. The closer to 1, the more resolution the PD plot will have; the closer to 0, the lower but faster.

# **Details**

For regression models, the units on the y-axis are the same as the units of the response. For classification models, the units on the y-axis are probits.

# Value

Invisibly, returns a list with the following components:

```
x_j_quants Quantiles at which the partial dependence function is evaluated. bart_avg_predictions_by_quantile Posterior means for \hat{f}(x) at x_j_quants.
```

# Note

This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores.

pd\_plot

# Author(s)

Adam Kapelner and Justin Bleich

#### References

Adam Kapelner, Justin Bleich (2016). bartMachine: Machine Learning with Bayesian Additive Regression Trees. Journal of Statistical Software, 70(4), 1-40. doi:10.18637/jss.v070.i04

HA Chipman, EI George, and RE McCulloch. BART: Bayesian Additive Regressive Trees. The Annals of Applied Statistics, 4(1): 266–298, 2010.

```
## Not run:
#Regression example
#generate Friedman data
set.seed(11)
n = 200
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)
#partial dependence plot for quadratic term
pd_plot(bart_machine, "X3")
#Classification example
#get data and only use 2 factors
data(iris)
iris2 = iris[51:150,]
iris2$Species = factor(iris2$Species)
#build BART classification model
bart_machine = bartMachine(iris2[ ,1:4], iris2$Species)
#partial dependence plot
pd_plot(bart_machine, "Petal.Width")
## End(Not run)
```

```
plot_convergence_diagnostics
```

Plot Convergence Diagnostics

## **Description**

A suite of plots to assess convergence diagonstics and features of the BART model.

## Usage

```
plot_convergence_diagnostics(bart_machine,
plots = c("sigsqs", "mh_acceptance", "num_nodes", "tree_depths"))
```

## **Arguments**

bart\_machine An object of class "bartMachine".

plots The list of plots to be displayed. The four options are: "sigsqs", "mh\_acceptance",

"num\_nodes", "tree\_depths".

#### **Details**

The "sigsqs" option plots the posterior error variance estimates by the Gibbs sample number. This is a standard tool to assess convergence of MCMC algorithms. This option is not applicable to classification BART models.

The "mh\_acceptance" option plots the proportion of Metropolis-Hastings steps accepted for each Gibbs sample (number accepted divided by number of trees).

The "num\_nodes" option plots the average number of nodes across each tree in the sum-of-trees model by the Gibbs sample number (for post burn-in only). The blue line is the average number of nodes over all trees.

The "tree\_depths" option plots the average tree depth across each tree in the sum-of-trees model by the Gibbs sample number (for post burn-in only). The blue line is the average number of nodes over all trees.

#### Value

None.

# Note

The "sigsqs" plot separates the burn-in  $\sigma^2$ 's for the first core by post burn-in  $\sigma^2$ 's estimates for all cores by grey vertical lines. The "mh\_acceptance" plot separates burn-in from post-burn in by a grey vertical line. Post burn-in, the different core proportions plot in different colors. The "num\_nodes" plot separates different core estimates by vertical lines (post burn-in only). The 'tree\_depths" plot separates different core estimates by vertical lines (post burn-in only).

## Author(s)

Adam Kapelner and Justin Bleich

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# **Examples**

```
## Not run:
#generate Friedman data
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)

#plot convergence diagnostics
plot_convergence_diagnostics(bart_machine)
## End(Not run)
```

plot\_y\_vs\_yhat

Plot the fitted Versus Actual Response

# **Description**

Generates a plot actual versus fitted values and corresponding credible intervals or prediction intervals for the fitted values.

#### Usage

```
plot_y_vs_yhat(bart_machine, Xtest = NULL, ytest = NULL,
credible_intervals = FALSE, prediction_intervals = FALSE,
interval_confidence_level = 0.95)
```

#### Arguments

bart\_machine An object of class "bartMachine".

Xtest Optional argument for test data. If included, BART computes fitted values at the

rows of Xtest. Else, the fitted values from the training data are used.

ytest Optional argument for test data. Vector of observed values corresponding to the

rows of Xtest to be plotted against the predictions for the rows of Xtest.

credible\_intervals

If TRUE, Bayesian credible intervals are computed using the quantiles of the posterior distribution of  $\hat{f}(x)$ . See calc\_credible\_intervals for details.

prediction\_intervals

If TRUE, Bayesian predictive intervals are computed using the a draw of from  $\hat{f}(x)$ . See calc\_prediction\_intervals for details.

interval\_confidence\_level

Desired level of confidence for credible or prediction intervals.

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# Value

None.

#### Note

This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores.

## Author(s)

Adam Kapelner and Justin Bleich

# See Also

```
bart\_machine\_get\_posterior, calc\_credible\_intervals, calc\_prediction\_intervals
```

# **Examples**

```
## Not run:
#generate linear data
set.seed(11)
n = 500
p = 3
X = data.frame(matrix(runif(n * p), ncol = p))
y = 3*X[ ,1] + 2*X[ ,2] +X[ ,3] + rnorm(n)

##build BART regression model
bart_machine = bartMachine(X, y)

##generate plot
plot_y_vs_yhat(bart_machine)

#generate plot with prediction bands
plot_y_vs_yhat(bart_machine, prediction_intervals = TRUE)

## End(Not run)
```

predict.bartMachine

Make a prediction on data using a BART object

# **Description**

Makes a prediction on new data given a fitted BART model for regression or classification.

```
## S3 method for class 'bartMachine'
predict(object, new_data, type = "prob", prob_rule_class = NULL, verbose = TRUE, ...)
```

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#### **Arguments**

object An object of class "bartMachine".

new\_data A data frame where each row is an observation to predict. The column names

should be the same as the column names of the training data.

type Only relevant if the bartMachine model is classification. The type can be "prob"

which will return the estimate of P(Y=1) (the "positive" class) or "class" which will return the best guess as to the class of the object, in the original label, based on if the probability estimate is greater than prob\_rule\_class. Default

is "prob."

prob\_rule\_class

The rule to determine when the class estimate is Y=1 (the "positive" class) based on the probability estimate. This defaults to what was originally specified

in the bart\_machine object.

verbose Prints out prediction-related messages. Currently in use only for probability

predictions to let the user know which class is being predicted. Default is TRUE.

... Parameters that are ignored.

#### Value

If regression, a numeric vector of y\_hat, the best guess as to the response. If classification and type = ``prob'', a numeric vector of p\_hat, the best guess as to the probability of the response class being the "positive" class. If classification and type = ''class'', a character vector of the best guess of the response's class labels.

## Author(s)

Adam Kapelner and Justin Bleich

#### See Also

```
bart_predict_for_test_data
```

```
#Regression example
## Not run:
#generate Friedman data
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)
##make predictions on the training data
y_hat = predict(bart_machine, X)
```

```
#Classification example
data(iris)
iris2 = iris[51 : 150, ] #do not include the third type of flower for this example
iris2$Species = factor(iris2$Species)
bart_machine = bartMachine(iris2[ ,1:4], iris2$Species)

##make probability predictions on the training data
p_hat = predict(bart_machine, X)

##make class predictions on test data
y_hat_class = predict(bart_machine, X, type = "class")

##make class predictions on test data conservatively for ''versicolor''
y_hat_class_conservative = predict(bart_machine, X, type = "class", prob_rule_class = 0.9)

## End(Not run)
```

predict\_bartMachineArr

Make a prediction on data using a BART array object

## **Description**

Makes a prediction on new data given an array of fitted BART model for regression or classification. If BART creates models that are variable, running many and averaging is a good strategy. It is well known that the Gibbs sampler gets locked into local modes at times. This is a way to average over many chains.

# Usage

```
predict_bartMachineArr(object, new_data, ...)
```

# Arguments

object An object of class "bartMachineArr".

new\_data A data frame where each row is an observation to predict. The column names

should be the same as the column names of the training data.

... Not supported. Note that parameters type and prob\_rule\_class for predict.bartMachine

are not supported.

#### Value

If regression, a numeric vector of y\_hat, the best guess as to the response. If classification and type = ``prob'', a numeric vector of p\_hat, the best guess as to the probability of the response class being the "positive" class. If classification and type = ''class'', a character vector of the best guess of the response's class labels.

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## Author(s)

Adam Kapelner

#### See Also

```
predict.bartMachine
```

## **Examples**

```
#Regression example
## Not run:
#generate Friedman data
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * \sin(pi * X[,1] * X[,2]) + 20 * (X[,3] -.5)^2 + 10 * X[,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)
bart_machine_arr = bartMachineArr(bart_machine)
##make predictions on the training data
y_hat = predict(bart_machine_arr, X)
#Classification example
data(iris)
iris2 = iris[51 : 150, ] #do not include the third type of flower for this example
iris2$Species = factor(iris2$Species)
bart_machine = bartMachine(iris2[ ,1:4], iris2$Species)
bart_machine_arr = bartMachineArr(bart_machine)
##make probability predictions on the training data
p_hat = predict_bartMachineArr(bart_machine_arr, iris2[ ,1:4])
## End(Not run)
```

print.bartMachine

Summarizes information about a bartMachine object.

## Description

This is an alias for the summary function. See description in that section.

```
## S3 method for class 'bartMachine'
print(x, ...)
```

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# Arguments

x An object of class "bartMachine".

... Parameters that are ignored.

#### Value

None.

# Author(s)

Adam Kapelner and Justin Bleich

# **Examples**

```
#Regression example

#generate Friedman data
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)

##build BART regression model
bart_machine = bartMachine(X, y)

##print out details
print(bart_machine)

##Also, the default print works too
bart_machine
```

rmse\_by\_num\_trees

Assess the Out-of-sample RMSE by Number of Trees

# **Description**

Assess out-of-sample RMSE of a BART model for varying numbers of trees in the sum-of-trees model.

```
rmse_by_num_trees(bart_machine, tree_list = c(5, seq(10, 50, 10), 100, 150, 200),
in_sample = FALSE, plot = TRUE, holdout_pctg = 0.3, num_replicates = 4, ...)
```

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## **Arguments**

bart\_machine An object of class "bartMachine".

tree\_list List of sizes for the sum-of-trees models.

in\_sample If TRUE, the RMSE is computed on in-sample data rather than an out-of-sample holdout.

plot If TRUE, a plot of the RMSE by the number of trees in the ensemble is created.

holdout\_pctg Percentage of the data to be treated as an out-of-sample holdout.

num\_replicates Number of replicates to average the results over. Each replicate uses a randomly sampled holdout of the data, (which could have overlap).

Other arguments to be passed to the plot function.

#### Value

Invisibly, returns the out-of-sample average RMSEs for each tree size.

#### Note

Since using a large number of trees can substantially increase computation time, this plot can help assess whether a smaller ensemble size is sufficient to obtain desirable predictive performance. This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores.

#### Author(s)

Adam Kapelner and Justin Bleich

```
## Not run:
#generate Friedman data
set.seed(11)
n = 200
p = 10
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y, num_trees = 20)
#explore RMSE by number of trees
rmse_by_num_trees(bart_machine)
## End(Not run)
```

```
set_bart_machine_num_cores
```

Set the Number of Cores for BART

# **Description**

Sets the number of cores to be used for all parallelized BART functions.

## Usage

```
set_bart_machine_num_cores(num_cores)
```

## **Arguments**

num\_cores

Number of cores to use

## Value

None.

# Author(s)

Adam Kapelner and Justin Bleich

#### See Also

```
bart_machine_num_cores
```

# **Examples**

```
## Not run:
## set all parallelized functions to use 4 cores
## set_bart_machine_num_cores(4)
## End(Not run)
```

summary.bartMachine

 $Summarizes\ information\ about\ a\ {\it bartMachine}\ object.$ 

# **Description**

Provides a quick summary of the BART model.

```
## S3 method for class 'bartMachine'
summary(object, ...)
```

## **Arguments**

```
object An object of class "bartMachine".
... Parameters that are ignored.
```

## **Details**

Gives the version number of the bartMachine package used to build this bartMachine object and if the object models either "regression" or "classification." Gives the amount of training data and the dimension of feature space. Prints the amount of time it took to build the model, how many processor cores were used to during its construction, as well as the number of burn-in and posterior Gibbs samples were used.

If the model is for regression, it prints the estimate of  $\sigma^2$  before the model was constructed as well as after so the user can inspect how much variance was explained.

If the model was built using the run\_in\_sample = TRUE parameter in build\_bart\_machine and is for regression, the summary L1, L2, rmse, Pseudo- $R^2$  are printed as well as the p-value for the tests of normality and zero-mean noise. If the model is for classification, a confusion matrix is printed.

#### Value

None.

# Author(s)

Adam Kapelner and Justin Bleich

```
#Regression example
#generate Friedman data
set.seed(11)
n = 200
p = 5
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model
bart_machine = bartMachine(X, y)
##print out details
summary(bart_machine)
##Also, the default print works too
bart_machine
```

```
var_selection_by_permute
```

Perform Variable Selection using Three Threshold-based Procedures

## **Description**

Performs variable selection using the three thresholding methods introduced in Bleich et al. (2013).

# Usage

```
var_selection_by_permute(bart_machine,
num_reps_for_avg = 10, num_permute_samples = 100,
num_trees_for_permute = 20, alpha = 0.05,
plot = TRUE, num_var_plot = Inf, bottom_margin = 10)
```

# **Arguments**

bart\_machine An object of class "bartMachine".

num\_reps\_for\_avg

Number of replicates to over over to for the BART model's variable inclusion proportions.

num\_permute\_samples

Number of permutations of the response to be made to generate the "null" permutation distribution.

num\_trees\_for\_permute

Number of trees to use in the variable selection procedure. As with

investigate\_var\_importance, a small number of trees should be used to force variables to compete for entry into the model. Note that this number is used to estimate both the "true" and "null" variable inclusion proportions.

alpha Cut-off level for the thresholds.

plot If TRUE, a plot showing which variables are selected by each of the procedures

is generated.

num\_var\_plot Number of variables (in order of decreasing variable inclusion proportion) to be

plotted.

bottom\_margin A display parameter that adjusts the bottom margin of the graph if labels are

clipped. The scale of this parameter is the same as set with par(mar = c(...)) in R. Higher values allow for more space if the crossed covariate names are long. Note that making this parameter too large will prevent plotting and the

plot function in R will throw an error.

## Details

See Bleich et al. (2013) for a complete description of the procedures outlined above as well as the corresponding vignette for a brief summary with examples.

#### Value

```
Invisibly, returns a list with the following components:
```

```
important_vars_local_names
```

Names of the variables chosen by the Local procedure.

important\_vars\_global\_max\_names

Names of the variables chosen by the Global Max procedure.

important\_vars\_global\_se\_names

Names of the variables chosen by the Global SE procedure.

important\_vars\_local\_col\_nums

Column numbers of the variables chosen by the Local procedure.

important\_vars\_global\_max\_col\_nums

Column numbers of the variables chosen by the Global Max procedure.

important\_vars\_global\_se\_col\_nums

Column numbers of the variables chosen by the Global SE procedure.

var\_true\_props\_avg

The variable inclusion proportions for the actual data.

permute\_mat The permutation distribution generated by permuting the response vector.

#### Note

Although the reference only explores regression settings, this procedure is applicable to both regression and classification problems. This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores.

# Author(s)

Adam Kapelner and Justin Bleich

## References

J Bleich, A Kapelner, ST Jensen, and EI George. Variable Selection Inference for Bayesian Additive Regression Trees. ArXiv e-prints, 2013.

Adam Kapelner, Justin Bleich (2016). bartMachine: Machine Learning with Bayesian Additive Regression Trees. Journal of Statistical Software, 70(4), 1-40. doi:10.18637/jss.v070.i04

## See Also

```
var_selection_by_permute, investigate_var_importance
```

```
## Not run:
#generate Friedman data
set.seed(11)
n = 300
p = 20 ##15 useless predictors
X = data.frame(matrix(runif(n * p), ncol = p))
```

```
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
##build BART regression model (not actuall used in variable selection)
bart_machine = bartMachine(X, y)

#variable selection
var_sel = var_selection_by_permute(bart_machine)
print(var_sel$important_vars_local_names)
print(var_sel$important_vars_global_max_names)
## End(Not run)
```

var\_selection\_by\_permute\_cv

Perform Variable Selection Using Cross-validation Procedure

# **Description**

Performs variable selection by cross-validating over the three threshold-based procedures outlined in Bleich et al. (2013) and selecting the single procedure that returns the lowest cross-validation RMSE.

#### Usage

```
var_selection_by_permute_cv(bart_machine, k_folds = 5,
num_reps_for_avg = 5, num_permute_samples = 100,
num_trees_for_permute = 20, alpha = 0.05, num_trees_pred_cv = 50)
```

# **Arguments**

bart\_machine An object of class "bartMachine".

k\_folds Number of folds to be used in cross-validation.

num\_reps\_for\_avg

Number of replicates to over over to for the BART model's variable inclusion proportions.

num\_permute\_samples

Number of permutations of the response to be made to generate the "null" permutation distribution.

num\_trees\_for\_permute

Number of trees to use in the variable selection procedure. As with investigate\_var\_importance, a small number of trees should be used to force variables to compete for entry into the model. Note that this number is used to estimate both the "true" and "null" variable inclusion proportions.

alpha Cut-off level for the thresholds.

```
num_trees_pred_cv
```

Number of trees to use for prediction on the hold-out portion of each fold. Once variables have been selected using the training portion of each fold, a new model is built using only those variables with num\_trees\_pred\_cv trees in the sum-of-trees model. Forecasts for the holdout sample are made using this model. A larger number of trees is recommended to exploit the full forecasting power of BART.

#### **Details**

See Bleich et al. (2013) for a complete description of the procedures outlined above as well as the corresponding vignette for a brief summary with examples.

#### Value

Returns a list with the following components:

best\_method The name of the best variable selection procedure, as chosen via cross-validation. important\_vars\_cv

The variables chosen by the best\_method above.

#### Note

This function can have substantial run-time. This function is parallelized by the number of cores set in set\_bart\_machine\_num\_cores.

## Author(s)

Adam Kapelner and Justin Bleich

#### References

J Bleich, A Kapelner, ST Jensen, and EI George. Variable Selection Inference for Bayesian Additive Regression Trees. ArXiv e-prints, 2013.

Adam Kapelner, Justin Bleich (2016). bartMachine: Machine Learning with Bayesian Additive Regression Trees. Journal of Statistical Software, 70(4), 1-40. doi:10.18637/jss.v070.i04

# See Also

```
var_selection_by_permute, investigate_var_importance
```

```
## Not run:
#generate Friedman data
set.seed(11)
n = 150
p = 100 ##95 useless predictors
X = data.frame(matrix(runif(n * p), ncol = p))
y = 10 * sin(pi* X[ ,1] * X[,2]) +20 * (X[,3] -.5)^2 + 10 * X[ ,4] + 5 * X[,5] + rnorm(n)
```

```
##build BART regression model (not actually used in variable selection)
bart_machine = bartMachine(X, y)

#variable selection via cross-validation
var_sel_cv = var_selection_by_permute_cv(bart_machine, k_folds = 3)
print(var_sel_cv$best_method)
print(var_sel_cv$important_vars_cv)

## End(Not run)
```

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