Package 'xgboost'

March 25, 2020

of the gradient boosting framework from Chen & Guestrin (2016) <doi:10.1145/2939672.2939785>. This package is its R interface. The package includes efficient linear model solver and tree learning algorithms. The package can automatically do parallel computation on a single machine which could be more than 10 times faster than existing gradient boosting packages. It supports various objective functions, including regression, classification and ranking. The package is made to be extensible, so that users are also allowed to define their own objectives easily. License Apache License (== 2.0) | file LICENSE URL https://github.com/dmlc/xgboost BugReports https://github.com/dmlc/xgboost/issues NeedsCompilation yes VignetteBuilder knitr Suggests knitr, rmarkdown, ggplot2 (>= 1.0.1), DiagrammeR (>= 0.9.0), Ckmeans.1d.dp (>= 3.3.1), vcd (>= 1.3), testthat, lintr, igraph (>= 1.0.1), jsonlite, float **Depends** R (>= 3.3.0) **Imports** Matrix (>= 1.1-0), methods, data.table (>= 1.9.6), magrittr (>= 1.5), stringi (>= 0.5.2)RoxygenNote 7.0.2 SystemRequirements GNU make, C++11 **Author** Tiangi Chen [aut], Tong He [aut, cre], Michael Benesty [aut], Vadim Khotilovich [aut],

Description Extreme Gradient Boosting, which is an efficient implementation

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agaricus.test

Test part from Mushroom Data Set

Description

This data set is originally from the Mushroom data set, UCI Machine Learning Repository.

Usage

data(agaricus.test)

Format

A list containing a label vector, and a dgCMatrix object with 1611 rows and 126 variables

Details

This data set includes the following fields:

- label the label for each record
- data a sparse Matrix of dgCMatrix class, with 126 columns.

References

https://archive.ics.uci.edu/ml/datasets/Mushroom

Bache, K. & Lichman, M. (2013). UCI Machine Learning Repository [http://archive.ics.uci.edu/ml]. Irvine, CA: University of California, School of Information and Computer Science.

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agaricus.train

Training part from Mushroom Data Set

Description

This data set is originally from the Mushroom data set, UCI Machine Learning Repository.

Usage

```
data(agaricus.train)
```

Format

A list containing a label vector, and a dgCMatrix object with 6513 rows and 127 variables

Details

This data set includes the following fields:

- label the label for each record
- data a sparse Matrix of dgCMatrix class, with 126 columns.

References

https://archive.ics.uci.edu/ml/datasets/Mushroom

Bache, K. & Lichman, M. (2013). UCI Machine Learning Repository [http://archive.ics.uci.edu/ml]. Irvine, CA: University of California, School of Information and Computer Science.

callbacks

Callback closures for booster training.

Description

These are used to perform various service tasks either during boosting iterations or at the end. This approach helps to modularize many of such tasks without bloating the main training methods, and it offers .

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Details

By default, a callback function is run after each boosting iteration. An R-attribute is_pre_iteration could be set for a callback to define a pre-iteration function.

When a callback function has finalize parameter, its finalizer part will also be run after the boosting is completed.

WARNING: side-effects!!! Be aware that these callback functions access and modify things in the environment from which they are called from, which is a fairly uncommon thing to do in R.

To write a custom callback closure, make sure you first understand the main concepts about R environments. Check either R documentation on environment or the Environments chapter from the "Advanced R" book by Hadley Wickham. Further, the best option is to read the code of some of the existing callbacks - choose ones that do something similar to what you want to achieve. Also, you would need to get familiar with the objects available inside of the xgb.train and xgb.cv internal environments.

See Also

cb.print.evaluation, cb.evaluation.log, cb.reset.parameters, cb.early.stop, cb.save.model, cb.cv.predict, xgb.train, xgb.cv

cb.cv.predict

Callback closure for returning cross-validation based predictions.

Description

Callback closure for returning cross-validation based predictions.

Usage

```
cb.cv.predict(save_models = FALSE)
```

Arguments

save_models a flag for whether to save the folds' models.

Details

This callback function saves predictions for all of the test folds, and also allows to save the folds' models.

It is a "finalizer" callback and it uses early stopping information whenever it is available, thus it must be run after the early stopping callback if the early stopping is used.

Callback function expects the following values to be set in its calling frame: bst_folds, basket, data, end_iteration, params, num_parallel_tree, num_class.

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Value

Predictions are returned inside of the pred element, which is either a vector or a matrix, depending on the number of prediction outputs per data row. The order of predictions corresponds to the order of rows in the original dataset. Note that when a custom folds list is provided in xgb.cv, the predictions would only be returned properly when this list is a non-overlapping list of k sets of indices, as in a standard k-fold CV. The predictions would not be meaningful when user-provided folds have overlapping indices as in, e.g., random sampling splits. When some of the indices in the training dataset are not included into user-provided folds, their prediction value would be NA.

See Also

callbacks

cb.early.stop

Callback closure to activate the early stopping.

Description

Callback closure to activate the early stopping.

Usage

```
cb.early.stop(
  stopping_rounds,
  maximize = FALSE,
  metric_name = NULL,
  verbose = TRUE
)
```

Arguments

stopping_rounds

The number of rounds with no improvement in the evaluation metric in order to

stop the training.

maximize whether to maximize the evaluation metric

metric_name the name of an evaluation column to use as a criteria for early stopping. If not

set, the last column would be used. Let's say the test data in watchlist was labelled as dtest, and one wants to use the AUC in test data for early stopping regardless of where it is in the watchlist, then one of the following would need to be set: metric_name='dtest-auc' or metric_name='dtest_auc'. All dash

'-' characters in metric names are considered equivalent to '_'.

verbose whether to print the early stopping information.

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Details

This callback function determines the condition for early stopping by setting the stop_condition = TRUE flag in its calling frame.

The following additional fields are assigned to the model's R object:

- best_score the evaluation score at the best iteration
- best_iteration at which boosting iteration the best score has occurred (1-based index)
- best_ntreelimit to use with the ntreelimit parameter in predict. It differs from best_iteration in multiclass or random forest settings.

The Same values are also stored as xgb-attributes:

- best_iteration is stored as a 0-based iteration index (for interoperability of binary models)
- best_msg message string is also stored.

At least one data element is required in the evaluation watchlist for early stopping to work.

Callback function expects the following values to be set in its calling frame: stop_condition, bst_evaluation, rank, bst (or bst_folds and basket), iteration, begin_iteration, end_iteration, num_parallel_tree.

See Also

```
callbacks, xgb.attr
```

cb.evaluation.log

Callback closure for logging the evaluation history

Description

Callback closure for logging the evaluation history

Usage

```
cb.evaluation.log()
```

Details

This callback function appends the current iteration evaluation results bst_evaluation available in the calling parent frame to the evaluation_log list in a calling frame.

The finalizer callback (called with finalize = TURE in the end) converts the evaluation_log list into a final data.table.

The iteration evaluation result bst_evaluation must be a named numeric vector.

Note: in the column names of the final data.table, the dash '-' character is replaced with the underscore '_' in order to make the column names more like regular R identifiers.

Callback function expects the following values to be set in its calling frame: evaluation_log, bst_evaluation, iteration.

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See Also

callbacks

cb.gblinear.history

Callback closure for collecting the model coefficients history of a gblinear booster during its training.

Description

Callback closure for collecting the model coefficients history of a gblinear booster during its training.

Usage

```
cb.gblinear.history(sparse = FALSE)
```

Arguments

sparse

when set to FALSE/TURE, a dense/sparse matrix is used to store the result. Sparse format is useful when one expects only a subset of coefficients to be non-zero, when using the "thrifty" feature selector with fairly small number of top features selected per iteration.

Details

To keep things fast and simple, gblinear booster does not internally store the history of linear model coefficients at each boosting iteration. This callback provides a workaround for storing the coefficients' path, by extracting them after each training iteration.

Callback function expects the following values to be set in its calling frame: bst (or bst_folds).

Value

Results are stored in the coefs element of the closure. The xgb.gblinear.history convenience function provides an easy way to access it. With xgb.train, it is either a dense of a sparse matrix. While with xgb.cv, it is a list (an element per each fold) of such matrices.

See Also

```
callbacks, xgb.gblinear.history.
```

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```
#### Binary classification:
# In the iris dataset, it is hard to linearly separate Versicolor class from the rest
# without considering the 2nd order interactions:
require(magrittr)
x <- model.matrix(Species ~ .^2, iris)[,-1]</pre>
colnames(x)
dtrain <- xgb.DMatrix(scale(x), label = 1*(iris$Species == "versicolor"))</pre>
param <- list(booster = "gblinear", objective = "reg:logistic", eval_metric = "auc",</pre>
              lambda = 0.0003, alpha = 0.0003, nthread = 2)
# For 'shotgun', which is a default linear updater, using high eta values may result in
# unstable behaviour in some datasets. With this simple dataset, however, the high learning
# rate does not break the convergence, but allows us to illustrate the typical pattern of
# "stochastic explosion" behaviour of this lock-free algorithm at early boosting iterations.
bst <- xgb.train(param, dtrain, list(tr=dtrain), nrounds = 200, eta = 1.,
                 callbacks = list(cb.gblinear.history()))
# Extract the coefficients' path and plot them vs boosting iteration number:
coef_path <- xgb.gblinear.history(bst)</pre>
matplot(coef_path, type = '1')
# With the deterministic coordinate descent updater, it is safer to use higher learning rates.
# Will try the classical componentwise boosting which selects a single best feature per round:
bst <- xgb.train(param, dtrain, list(tr=dtrain), nrounds = 200, eta = 0.8,
                 updater = 'coord_descent', feature_selector = 'thrifty', top_k = 1,
                 callbacks = list(cb.gblinear.history()))
xgb.gblinear.history(bst) %>% matplot(type = 'l')
# Componentwise boosting is known to have similar effect to Lasso regularization.
# Try experimenting with various values of top_k, eta, nrounds,
# as well as different feature_selectors.
# For xgb.cv:
bst <- xgb.cv(param, dtrain, nfold = 5, nrounds = 100, eta = 0.8,
             callbacks = list(cb.gblinear.history()))
# coefficients in the CV fold #3
xgb.gblinear.history(bst)[[3]] %>% matplot(type = 'l')
#### Multiclass classification:
dtrain <- xgb.DMatrix(scale(x), label = as.numeric(iris$Species) - 1)</pre>
param <- list(booster = "gblinear", objective = "multi:softprob", num_class = 3,</pre>
              lambda = 0.0003, alpha = 0.0003, nthread = 2)
# For the default linear updater 'shotgun' it sometimes is helpful
# to use smaller eta to reduce instability
bst <- xgb.train(param, dtrain, list(tr=dtrain), nrounds = 70, eta = 0.5,
                 callbacks = list(cb.gblinear.history()))
# Will plot the coefficient paths separately for each class:
xgb.gblinear.history(bst, class_index = 0) %>% matplot(type = 'l')
xgb.gblinear.history(bst, class_index = 1) %>% matplot(type = 'l')
xgb.gblinear.history(bst, class_index = 2) %>% matplot(type = '1')
```

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cb.print.evaluation

Callback closure for printing the result of evaluation

Description

Callback closure for printing the result of evaluation

Usage

```
cb.print.evaluation(period = 1, showsd = TRUE)
```

Arguments

period results would be printed every number of periods

showsd whether standard deviations should be printed (when available)

Details

The callback function prints the result of evaluation at every period iterations. The initial and the last iteration's evaluations are always printed.

Callback function expects the following values to be set in its calling frame: bst_evaluation (also bst_evaluation_err when available), iteration, begin_iteration, end_iteration.

See Also

callbacks

cb.reset.parameters Callback closure for resetting the booster's parameters at each iteration.

Description

Callback closure for resetting the booster's parameters at each iteration.

Usage

```
cb.reset.parameters(new_params)
```

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Arguments

new_params

a list where each element corresponds to a parameter that needs to be reset. Each element's value must be either a vector of values of length nrounds to be set at each iteration, or a function of two parameters learning_rates(iteration, nrounds) which returns a new parameter value by using the current iteration number and the total number of boosting rounds.

Details

This is a "pre-iteration" callback function used to reset booster's parameters at the beginning of each iteration.

Note that when training is resumed from some previous model, and a function is used to reset a parameter value, the nrounds argument in this function would be the number of boosting rounds in the current training.

Callback function expects the following values to be set in its calling frame: bst or bst_folds, iteration, begin_iteration, end_iteration.

See Also

callbacks

cb.save.model

Callback closure for saving a model file.

Description

Callback closure for saving a model file.

Usage

```
cb.save.model(save_period = 0, save_name = "xgboost.model")
```

Arguments

save_period

save the model to disk after every save_period iterations; 0 means save the

model at the end.

save_name

the name or path for the saved model file. It can contain a sprintf formatting specifier to include the integer iteration number in the file name. E.g., with save_name = 'xgboost_ the file saved at iteration 50 would be named "xg-boost_ 0050 model"

 $boost_0050.model".$

Details

This callback function allows to save an xgb-model file, either periodically after each save_period's or at the end.

Callback function expects the following values to be set in its calling frame: bst, iteration, begin_iteration, end_iteration.

See Also

callbacks

dim.xgb.DMatrix

Dimensions of xgb.DMatrix

Description

Returns a vector of numbers of rows and of columns in an xgb.DMatrix.

Usage

```
## S3 method for class 'xgb.DMatrix'
dim(x)
```

Arguments

Χ

Object of class xgb.DMatrix

Details

Note: since nrow and ncol internally use dim, they can also be directly used with an xgb.DMatrix object.

Examples

```
data(agaricus.train, package='xgboost')
train <- agaricus.train
dtrain <- xgb.DMatrix(train$data, label=train$label)
stopifnot(nrow(dtrain) == nrow(train$data))
stopifnot(ncol(dtrain) == ncol(train$data))
stopifnot(all(dim(dtrain) == dim(train$data)))</pre>
```

Description

Only column names are supported for xgb.DMatrix, thus setting of row names would have no effect and returned row names would be NULL.

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Usage

```
## S3 method for class 'xgb.DMatrix'
dimnames(x)

## S3 replacement method for class 'xgb.DMatrix'
dimnames(x) <- value</pre>
```

Arguments

x object of class xgb.DMatrix

value a list of two elements: the first one is ignored and the second one is column

names

Details

Generic dimnames methods are used by colnames. Since row names are irrelevant, it is recommended to use colnames directly.

Examples

```
data(agaricus.train, package='xgboost')
train <- agaricus.train
dtrain <- xgb.DMatrix(train$data, label=train$label)
dimnames(dtrain)
colnames(dtrain)
colnames(dtrain) <- make.names(1:ncol(train$data))
print(dtrain, verbose=TRUE)</pre>
```

getinfo

Get information of an xgb.DMatrix object

Description

Get information of an xgb.DMatrix object

Usage

```
getinfo(object, ...)
## S3 method for class 'xgb.DMatrix'
getinfo(object, name, ...)
```

Arguments

object Object of class xgb.DMatrix

... other parameters

name the name of the information field to get (see details)

Details

The name field can be one of the following:

- label: label Xgboost learn from ;
- weight: to do a weight rescale;
- base_margin: base margin is the base prediction Xgboost will boost from;
- nrow: number of rows of the xgb.DMatrix.

group can be setup by setinfo but can't be retrieved by getinfo.

Examples

```
data(agaricus.train, package='xgboost')
train <- agaricus.train
dtrain <- xgb.DMatrix(train$data, label=train$label)
labels <- getinfo(dtrain, 'label')
setinfo(dtrain, 'label', 1-labels)
labels2 <- getinfo(dtrain, 'label')
stopifnot(all(labels2 == 1-labels))</pre>
```

predict.xgb.Booster

Predict method for eXtreme Gradient Boosting model

Description

Predicted values based on either xgboost model or model handle object.

Usage

```
## S3 method for class 'xgb.Booster'
predict(
  object,
  newdata,
 missing = NA,
  outputmargin = FALSE,
  ntreelimit = NULL,
  predleaf = FALSE,
  predcontrib = FALSE,
  approxcontrib = FALSE,
  predinteraction = FALSE,
  reshape = FALSE,
  training = FALSE,
)
## S3 method for class 'xgb.Booster.handle'
predict(object, ...)
```

Arguments

object Object of class xgb.Booster or xgb.Booster.handle newdata takes matrix, dgCMatrix, local data file or xgb.DMatrix.

missing Missing is only used when input is dense matrix. Pick a float value that repre-

sents missing values in data (e.g., sometimes 0 or some other extreme value is

used).

outputmargin whether the prediction should be returned in the for of original untransformed

sum of predictions from boosting iterations' results. E.g., setting outputmargin=TRUE for logistic regression would result in predictions for log-odds instead of proba-

bilities.

ntreelimit limit the number of model's trees or boosting iterations used in prediction (see

Details). It will use all the trees by default (NULL value).

predleaf whether predict leaf index.

predcontrib whether to return feature contributions to individual predictions (see Details). approxcontrib whether to use a fast approximation for feature contributions (see Details).

predinteraction

whether to return contributions of feature interactions to individual predictions

(see Details).

reshape whether to reshape the vector of predictions to a matrix form when there are

several prediction outputs per case. This option has no effect when either of

predleaf, predcontrib, or predinteraction flags is TRUE.

training whether is the prediction result used for training. For dart booster, training pre-

dicting will perform dropout.

... Parameters passed to predict.xgb.Booster

Details

Note that ntreelimit is not necessarily equal to the number of boosting iterations and it is not necessarily equal to the number of trees in a model. E.g., in a random forest-like model, ntreelimit would limit the number of trees. But for multiclass classification, while there are multiple trees per iteration, ntreelimit limits the number of boosting iterations.

Also note that ntreelimit would currently do nothing for predictions from gblinear, since gblinear doesn't keep its boosting history.

One possible practical applications of the predleaf option is to use the model as a generator of new features which capture non-linearity and interactions, e.g., as implemented in xgb.create.features.

Setting predcontrib = TRUE allows to calculate contributions of each feature to individual predictions. For "gblinear" booster, feature contributions are simply linear terms (feature_beta * feature_value). For "gbtree" booster, feature contributions are SHAP values (Lundberg 2017) that sum to the difference between the expected output of the model and the current prediction (where the hessian weights are used to compute the expectations). Setting approxcontrib = TRUE approximates these values following the idea explained in http://blog.datadive.net/interpreting-random-forests/.

With predinteraction = TRUE, SHAP values of contributions of interaction of each pair of features are computed. Note that this operation might be rather expensive in terms of compute and memory. Since it quadratically depends on the number of features, it is recommended to perform selection of the most important features first. See below about the format of the returned results.

Value

For regression or binary classification, it returns a vector of length nrows (newdata). For multiclass classification, either a num_class * nrows (newdata) vector or a (nrows (newdata), num_class) dimension matrix is returned, depending on the reshape value.

When predleaf = TRUE, the output is a matrix object with the number of columns corresponding to the number of trees.

When predcontrib = TRUE and it is not a multiclass setting, the output is a matrix object with num_features + 1 columns. The last "+ 1" column in a matrix corresponds to bias. For a multiclass case, a list of num_class elements is returned, where each element is such a matrix. The contribution values are on the scale of untransformed margin (e.g., for binary classification would mean that the contributions are log-odds deviations from bias).

When predinteraction = TRUE and it is not a multiclass setting, the output is a 3d array with dimensions c(nrow, num_features + 1, num_features + 1). The off-diagonal (in the last two dimensions) elements represent different features interaction contributions. The array is symmetric WRT the last two dimensions. The "+ 1" columns corresponds to bias. Summing this array along the last dimension should produce practically the same result as predict with predcontrib = TRUE. For a multiclass case, a list of num_class elements is returned, where each element is such an array.

References

Scott M. Lundberg, Su-In Lee, "A Unified Approach to Interpreting Model Predictions", NIPS Proceedings 2017, https://arxiv.org/abs/1705.07874

Scott M. Lundberg, Su-In Lee, "Consistent feature attribution for tree ensembles", https://arxiv.org/abs/1706.06060

See Also

```
xgb.train.
```

```
# Predicting feature contributions to predictions:
# the result is an nsamples X (nfeatures + 1) matrix
pred_contr <- predict(bst, test$data, predcontrib = TRUE)</pre>
str(pred_contr)
# verify that contributions' sums are equal to log-odds of predictions (up to float precision):
summary(rowSums(pred_contr) - qlogis(pred))
# for the 1st record, let's inspect its features that had non-zero contribution to prediction:
contr1 <- pred_contr[1,]</pre>
contr1 <- contr1[-length(contr1)]</pre>
                                      # drop BIAS
contr1 <- contr1[contr1 != 0]</pre>
                                      # drop non-contributing features
contr1 <- contr1[order(abs(contr1))] # order by contribution magnitude</pre>
old_mar <- par("mar")</pre>
par(mar = old_mar + c(0,7,0,0))
barplot(contr1, horiz = TRUE, las = 2, xlab = "contribution to prediction in log-odds")
par(mar = old_mar)
## multiclass classification in iris dataset:
lb <- as.numeric(iris$Species) - 1</pre>
num_class <- 3
set.seed(11)
bst <- xgboost(data = as.matrix(iris[, -5]), label = lb,</pre>
               max_depth = 4, eta = 0.5, nthread = 2, nrounds = 10, subsample = 0.5,
               objective = "multi:softprob", num_class = num_class)
# predict for softmax returns num_class probability numbers per case:
pred <- predict(bst, as.matrix(iris[, -5]))</pre>
str(pred)
# reshape it to a num_class-columns matrix
pred <- matrix(pred, ncol=num_class, byrow=TRUE)</pre>
# convert the probabilities to softmax labels
pred_labels <- max.col(pred) - 1</pre>
# the following should result in the same error as seen in the last iteration
sum(pred_labels != lb)/length(lb)
# compare that to the predictions from softmax:
set.seed(11)
bst <- xgboost(data = as.matrix(iris[, -5]), label = lb,</pre>
               max_depth = 4, eta = 0.5, nthread = 2, nrounds = 10, subsample = 0.5,
               objective = "multi:softmax", num_class = num_class)
pred <- predict(bst, as.matrix(iris[, -5]))</pre>
str(pred)
all.equal(pred, pred_labels)
# prediction from using only 5 iterations should result
# in the same error as seen in iteration 5:
pred5 <- predict(bst, as.matrix(iris[, -5]), ntreelimit=5)</pre>
sum(pred5 != lb)/length(lb)
## random forest-like model of 25 trees for binary classification:
set.seed(11)
```

print.xgb.Booster

print.xgb.Booster

Print xgb.Booster

Description

Print information about xgb.Booster.

Usage

```
## S3 method for class 'xgb.Booster'
print(x, verbose = FALSE, ...)
```

Arguments

```
x an xgb.Booster objectverbose whether to print detailed data (e.g., attribute values)... not currently used
```

print.xgb.cv.synchronous

```
print.xgb.cv.synchronous
```

Print xgb.cv result

Description

Prints formatted results of xgb.cv.

Usage

```
## S3 method for class 'xgb.cv.synchronous'
print(x, verbose = FALSE, ...)
```

Arguments

```
x an xgb.cv.synchronous objectverbose whether to print detailed data... passed to data.table.print
```

Details

When not verbose, it would only print the evaluation results, including the best iteration (when available).

Examples

print.xgb.DMatrix

Print xgb.DMatrix

Description

Print information about xgb.DMatrix. Currently it displays dimensions and presence of info-fields and colnames.

Usage

```
## S3 method for class 'xgb.DMatrix'
print(x, verbose = FALSE, ...)
```

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Arguments

```
x an xgb.DMatrix objectverbose whether to print colnames (when present)... not currently used
```

Examples

```
data(agaricus.train, package='xgboost')
train <- agaricus.train
dtrain <- xgb.DMatrix(train$data, label=train$label)
dtrain
print(dtrain, verbose=TRUE)</pre>
```

setinfo

Set information of an xgb.DMatrix object

Description

Set information of an xgb.DMatrix object

Usage

```
setinfo(object, ...)
## S3 method for class 'xgb.DMatrix'
setinfo(object, name, info, ...)
```

Arguments

object Object of class "xgb.DMatrix"
... other parameters
name the name of the field to get
info the specific field of information to set

Details

The name field can be one of the following:

- label: label Xgboost learn from;
- weight: to do a weight rescale;
- base_margin: base margin is the base prediction Xgboost will boost from;
- group: number of rows in each group (to use with rank: pairwise objective).

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Examples

```
data(agaricus.train, package='xgboost')
train <- agaricus.train
dtrain <- xgb.DMatrix(train$data, label=train$label)

labels <- getinfo(dtrain, 'label')
setinfo(dtrain, 'label', 1-labels)
labels2 <- getinfo(dtrain, 'label')
stopifnot(all.equal(labels2, 1-labels))</pre>
```

slice

Get a new DMatrix containing the specified rows of original xgb.DMatrix object

Description

Get a new DMatrix containing the specified rows of original xgb.DMatrix object

Usage

```
slice(object, ...)
## S3 method for class 'xgb.DMatrix'
slice(object, idxset, ...)
## S3 method for class 'xgb.DMatrix'
object[idxset, colset = NULL]
```

Arguments

object	Object of class "xgb.DMatrix"
	other parameters (currently not used)
idxset	a integer vector of indices of rows needed
colset	currently not used (columns subsetting is not available)

```
data(agaricus.train, package='xgboost')
train <- agaricus.train
dtrain <- xgb.DMatrix(train$data, label=train$label)

dsub <- slice(dtrain, 1:42)
labels1 <- getinfo(dsub, 'label')
dsub <- dtrain[1:42, ]
labels2 <- getinfo(dsub, 'label')
all.equal(labels1, labels2)</pre>
```

22 xgb.attr

xgb.attr

Accessors for serializable attributes of a model.

Description

These methods allow to manipulate the key-value attribute strings of an xgboost model.

Usage

```
xgb.attr(object, name)
xgb.attr(object, name) <- value
xgb.attributes(object)
xgb.attributes(object) <- value</pre>
```

Arguments

object Object of class xgb.Booster or xgb.Booster.handle.

name a non-empty character string specifying which attribute is to be accessed.

value a value of an attribute for xgb.attr<-; for xgb.attributes<- it's a list (or an

object coercible to a list) with the names of attributes to set and the elements corresponding to attribute values. Non-character values are converted to character. When attribute value is not a scalar, only the first index is used. Use NULL to

remove an attribute.

Details

The primary purpose of xgboost model attributes is to store some meta-data about the model. Note that they are a separate concept from the object attributes in R. Specifically, they refer to key-value strings that can be attached to an xgboost model, stored together with the model's binary representation, and accessed later (from R or any other interface). In contrast, any R-attribute assigned to an R-object of xgb.Booster class would not be saved by xgb.save because an xgboost model is an external memory object and its serialization is handled externally. Also, setting an attribute that has the same name as one of xgboost's parameters wouldn't change the value of that parameter for a model. Use xgb.parameters<— to set or change model parameters.

The attribute setters would usually work more efficiently for xgb.Booster.handle than for xgb.Booster, since only just a handle (pointer) would need to be copied. That would only matter if attributes need to be set many times. Note, however, that when feeding a handle of an xgb.Booster object to the attribute setters, the raw model cache of an xgb.Booster object would not be automatically updated, and it would be user's responsibility to call xgb.save.raw to update it.

The xgb.attributes<- setter either updates the existing or adds one or several attributes, but it doesn't delete the other existing attributes.

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Value

xgb.attr returns either a string value of an attribute or NULL if an attribute wasn't stored in a model. xgb.attributes returns a list of all attribute stored in a model or NULL if a model has no stored attributes.

Examples

```
data(agaricus.train, package='xgboost')
train <- agaricus.train
bst <- xgboost(data = train$data, label = train$label, max_depth = 2,</pre>
               eta = 1, nthread = 2, nrounds = 2, objective = "binary:logistic")
xgb.attr(bst, "my_attribute") <- "my attribute value"
print(xgb.attr(bst, "my_attribute"))
xgb.attributes(bst) <- list(a = 123, b = "abc")</pre>
xgb.save(bst, 'xgb.model')
bst1 <- xgb.load('xgb.model')</pre>
if (file.exists('xgb.model')) file.remove('xgb.model')
print(xgb.attr(bst1, "my_attribute"))
print(xgb.attributes(bst1))
# deletion:
xgb.attr(bst1, "my_attribute") <- NULL</pre>
print(xgb.attributes(bst1))
xgb.attributes(bst1) <- list(a = NULL, b = NULL)</pre>
print(xgb.attributes(bst1))
```

xgb.Booster.complete Restore missing parts of an incomplete xgb.Booster object.

Description

It attempts to complete an xgb.Booster object by restoring either its missing raw model memory dump (when it has no raw data but its xgb.Booster.handle is valid) or its missing internal handle (when its xgb.Booster.handle is not valid but it has a raw Booster memory dump).

Usage

```
xgb.Booster.complete(object, saveraw = TRUE)
```

Arguments

object of class xgb.Booster

saveraw a flag indicating whether to append raw Booster memory dump data when it

doesn't already exist.

24 xgb.create.features

Details

While this method is primarily for internal use, it might be useful in some practical situations.

E.g., when an xgb.Booster model is saved as an R object and then is loaded as an R object, its handle (pointer) to an internal xgboost model would be invalid. The majority of xgboost methods should still work for such a model object since those methods would be using xgb.Booster.complete internally. However, one might find it to be more efficient to call the xgb.Booster.complete function explicitly once after loading a model as an R-object. That would prevent further repeated implicit reconstruction of an internal booster model.

Value

An object of xgb. Booster class.

Examples

Description

May improve the learning by adding new features to the training data based on the decision trees from a previously learned model.

Usage

```
xgb.create.features(model, data, ...)
```

Arguments

```
model decision tree boosting model learned on the original data data original data (usually provided as a dgCMatrix matrix) ... currently not used
```

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Details

This is the function inspired from the paragraph 3.1 of the paper:

Practical Lessons from Predicting Clicks on Ads at Facebook

(Xinran He, Junfeng Pan, Ou Jin, Tianbing Xu, Bo Liu, Tao Xu, Yan, xin Shi, Antoine Atallah, Ralf Herbrich, Stuart Bowers, Joaquin Quinonero Candela)

International Workshop on Data Mining for Online Advertising (ADKDD) - August 24, 2014

https://research.fb.com/publications/practical-lessons-from-predicting-clicks-on-ads-at-facebook/.

Extract explaining the method:

"We found that boosted decision trees are a powerful and very convenient way to implement nonlinear and tuple transformations of the kind we just described. We treat each individual tree as a categorical feature that takes as value the index of the leaf an instance ends up falling in. We use 1-of-K coding of this type of features.

For example, consider the boosted tree model in Figure 1 with 2 subtrees, where the first subtree has 3 leafs and the second 2 leafs. If an instance ends up in leaf 2 in the first subtree and leaf 1 in second subtree, the overall input to the linear classifier will be the binary vector [0,1,0,1,0], where the first 3 entries correspond to the leaves of the first subtree and last 2 to those of the second subtree.

[...]

We can understand boosted decision tree based transformation as a supervised feature encoding that converts a real-valued vector into a compact binary-valued vector. A traversal from root node to a leaf node represents a rule on certain features."

Value

dgCMatrix matrix including both the original data and the new features.

26 xgb.cv

xgb.cv

Cross Validation

Description

The cross validation function of xgboost

Usage

```
xgb.cv(
  params = list(),
  data,
 nrounds,
 nfold,
 label = NULL,
 missing = NA,
 prediction = FALSE,
  showsd = TRUE,
 metrics = list(),
 obj = NULL,
  feval = NULL,
  stratified = TRUE,
  folds = NULL,
  train_folds = NULL,
  verbose = TRUE,
  print_every_n = 1L,
  early_stopping_rounds = NULL,
 maximize = NULL,
 callbacks = list(),
)
```

xgb.cv 27

Arguments

params the list of parameters. Commonly used ones are:

• objective objective function, common ones are

- reg: squarederror Regression with squared loss
- binary: logistic logistic regression for classification
- eta step size of each boosting step
- max_depth maximum depth of the tree
- nthread number of thread used in training, if not set, all threads are used

See xgb.train for further details. See also demo/ for walkthrough example in R.

data takes an xgb. DMatrix, matrix, or dgCMatrix as the input.

nrounds the max number of iterations

nfold the original dataset is randomly partitioned into nfold equal size subsamples.

label vector of response values. Should be provided only when data is an R-matrix.

missing is only used when input is a dense matrix. By default is set to NA, which means

that NA values should be considered as 'missing' by the algorithm. Sometimes, 0 or other extreme value might be used to represent missing values.

prediction A logical value indicating whether to return the test fold predictions from each

CV model. This parameter engages the cb.cv.predict callback.

showsd boolean, whether to show standard deviation of cross validation

metrics, list of evaluation metrics to be used in cross validation, when it is not specified, the evaluation metric is chosen according to objective function. Possible options

are:

• error binary classification error rate

- rmse Rooted mean square error
- logloss negative log-likelihood function
- auc Area under curve
- aucpr Area under PR curve
- merror Exact matching error, used to evaluate multi-class classification

obj customized objective function. Returns gradient and second order gradient with

given prediction and dtrain.

feval customized evaluation function. Returns list(metric='metric-name',value='metric-value')

with given prediction and dtrain.

stratified a boolean indicating whether sampling of folds should be stratified by the val-

ues of outcome labels.

folds list provides a possibility to use a list of pre-defined CV folds (each element

must be a vector of test fold's indices). When folds are supplied, the nfold and

stratified parameters are ignored.

train_folds list list specifying which indicies to use for training. If NULL (the default) all

indices not specified in folds will be used for training.

verbose boolean, print the statistics during the process

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print_every_n Print each n-th iteration evaluation messages when verbose>0. Default is 1

which means all messages are printed. This parameter is passed to the cb.print.evaluation

callback.

early_stopping_rounds

If NULL, the early stopping function is not triggered. If set to an integer k, training with a validation set will stop if the performance doesn't improve for k

rounds. Setting this parameter engages the cb.early.stop callback.

maximize If feval and early_stopping_rounds are set, then this parameter must be set

as well. When it is TRUE, it means the larger the evaluation score the better. This

parameter is passed to the cb.early.stop callback.

callbacks a list of callback functions to perform various task during boosting. See callbacks.

Some of the callbacks are automatically created depending on the parameters' values. User can provide either existing or their own callback methods in order

to customize the training process.

... other parameters to pass to params.

Details

The original sample is randomly partitioned into nfold equal size subsamples.

Of the nfold subsamples, a single subsample is retained as the validation data for testing the model, and the remaining nfold -1 subsamples are used as training data.

The cross-validation process is then repeated nrounds times, with each of the nfold subsamples used exactly once as the validation data.

All observations are used for both training and validation.

Adapted from http://en.wikipedia.org/wiki/Cross-validation_%28statistics%29#k-fold_cross-validation

Value

An object of class xgb.cv.synchronous with the following elements:

- call a function call.
- params parameters that were passed to the xgboost library. Note that it does not capture parameters changed by the cb.reset.parameters callback.
- callbacks callback functions that were either automatically assigned or explicitly passed.
- evaluation_log evaluation history stored as a data.table with the first column corresponding to iteration number and the rest corresponding to the CV-based evaluation means and standard deviations for the training and test CV-sets. It is created by the cb.evaluation.log callback.
- niter number of boosting iterations.
- nfeatures number of features in training data.
- folds the list of CV folds' indices either those passed through the folds parameter or randomly generated.
- best_iteration iteration number with the best evaluation metric value (only available with early stopping).

xgb.DMatrix 29

• best_ntreelimit the ntreelimit value corresponding to the best iteration, which could further be used in predict method (only available with early stopping).

- pred CV prediction values available when prediction is set. It is either vector or matrix (see cb.cv.predict).
- models a liost of the CV folds' models. It is only available with the explicit setting of the cb.cv.predict(save_models = TRUE) callback.

Examples

xgb.DMatrix

Construct xgb.DMatrix object

Description

Construct xgb.DMatrix object from either a dense matrix, a sparse matrix, or a local file. Supported input file formats are either a libsym text file or a binary file that was created previously by xgb.DMatrix.save).

Usage

```
xgb.DMatrix(data, info = list(), missing = NA, silent = FALSE, ...)
```

Arguments

data	a matrix object (either numeric or integer), a $dgCMatrix$ object, or a character string representing a filename.
info	a named list of additional information to store in the xgb.DMatrix object. See setinfo for the specific allowed kinds of
missing	a float value to represents missing values in data (used only when input is a dense matrix). It is useful when a 0 or some other extreme value represents missing values in data.
silent	whether to suppress printing an informational message after loading from a file.
•••	the info data could be passed directly as parameters, without creating an info list.

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Examples

```
data(agaricus.train, package='xgboost')
train <- agaricus.train
dtrain <- xgb.DMatrix(train$data, label=train$label)
xgb.DMatrix.save(dtrain, 'xgb.DMatrix.data')
dtrain <- xgb.DMatrix('xgb.DMatrix.data')
if (file.exists('xgb.DMatrix.data')) file.remove('xgb.DMatrix.data')</pre>
```

xgb.DMatrix.save

Save xgb.DMatrix object to binary file

Description

Save xgb.DMatrix object to binary file

Usage

```
xgb.DMatrix.save(dmatrix, fname)
```

Arguments

dmatrix the xgb.DMatrix object fname the name of the file to write.

Examples

```
data(agaricus.train, package='xgboost')
train <- agaricus.train
dtrain <- xgb.DMatrix(train$data, label=train$label)
xgb.DMatrix.save(dtrain, 'xgb.DMatrix.data')
dtrain <- xgb.DMatrix('xgb.DMatrix.data')
if (file.exists('xgb.DMatrix.data')) file.remove('xgb.DMatrix.data')</pre>
```

xgb.dump

Dump an xgboost model in text format.

Description

Dump an xgboost model in text format.

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Usage

```
xgb.dump(
  model,
  fname = NULL,
  fmap = "",
  with_stats = FALSE,
  dump_format = c("text", "json"),
   ...
)
```

Arguments

model the model object.

fname the name of the text file where to save the model text dump. If not provided or

set to NULL, the model is returned as a character vector.

fmap feature map file representing feature types. Detailed description could be found

athttps://github.com/dmlc/xgboost/wiki/Binary-Classification#dump-model.

See demo/ for walkthrough example in R, and https://github.com/dmlc/xgboost/blob/master/demo/data/featmap.txt for example Format.

with_stats whether to dump some additional statistics about the splits. When this option is

on, the model dump contains two additional values: gain is the approximate loss function gain we get in each split; cover is the sum of second order gradient in

each node.

dump_format either 'text' or 'json' format could be specified.

... currently not used

Value

If fname is not provided or set to NULL the function will return the model as a character vector. Otherwise it will return TRUE.

32 xgb.ggplot.deepness

```
xgb.gblinear.history Extract gblinear coefficients history.
```

Description

A helper function to extract the matrix of linear coefficients' history from a gblinear model created while using the cb.gblinear.history() callback.

Usage

```
xgb.gblinear.history(model, class_index = NULL)
```

Arguments

model either an xgb.Booster or a result of xgb.cv(), trained using the cb.gblinear.history()

callback.

class_index zero-based class index to extract the coefficients for only that specific class in

a multinomial multiclass model. When it is NULL, all the coefficients are re-

turned. Has no effect in non-multiclass models.

Value

For an xgb.train result, a matrix (either dense or sparse) with the columns corresponding to iteration's coefficients (in the order as xgb.dump() would return) and the rows corresponding to boosting iterations.

For an xgb.cv result, a list of such matrices is returned with the elements corresponding to CV folds.

Description

Visualizes distributions related to depth of tree leafs. xgb.plot.deepness uses base R graphics, while xgb.ggplot.deepness uses the ggplot backend.

Usage

```
xgb.ggplot.deepness(
  model = NULL,
  which = c("2x1", "max.depth", "med.depth", "med.weight")
)
xgb.plot.deepness(
  model = NULL,
```

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```
which = c("2x1", "max.depth", "med.depth", "med.weight"),
plot = TRUE,
...
)
```

Arguments

model	either an xgb.Booster model generated by the xgb.train function or a data.table result of the xgb.model.dt.tree function.
which	which distribution to plot (see details).
plot	(base R barplot) whether a barplot should be produced. If FALSE, only a data.table is returned.
	other parameters passed to barplot or plot.

Details

When which="2x1", two distributions with respect to the leaf depth are plotted on top of each other:

- the distribution of the number of leafs in a tree model at a certain depth;
- the distribution of average weighted number of observations ("cover") ending up in leafs at certain depth.

Those could be helpful in determining sensible ranges of the max_depth and min_child_weight parameters.

When which="max.depth" or which="med.depth", plots of either maximum or median depth per tree with respect to tree number are created. And which="med.weight" allows to see how a tree's median absolute leaf weight changes through the iterations.

This function was inspired by the blog post https://github.com/aysent/random-forest-leaf-visualization.

Value

Other than producing plots (when plot=TRUE), the xgb.plot.deepness function silently returns a processed data.table where each row corresponds to a terminal leaf in a tree model, and contains information about leaf's depth, cover, and weight (which is used in calculating predictions).

The xgb.ggplot.deepness silently returns either a list of two ggplot graphs when which="2x1" or a single ggplot graph for the other which options.

See Also

```
xgb.train, xgb.model.dt.tree.
```

```
subsample = 0.5, min_child_weight = 2)

xgb.plot.deepness(bst)

xgb.ggplot.deepness(bst)

xgb.plot.deepness(bst, which='max.depth', pch=16, col=rgb(0,0,1,0.3), cex=2)

xgb.plot.deepness(bst, which='med.weight', pch=16, col=rgb(0,0,1,0.3), cex=2)
```

xgb.ggplot.importance Plot feature importance as a bar graph

Description

Represents previously calculated feature importance as a bar graph. xgb.plot.importance uses base R graphics, while xgb.ggplot.importance uses the ggplot backend.

Usage

```
xgb.ggplot.importance(
  importance_matrix = NULL,
  top_n = NULL,
 measure = NULL,
  rel_to_first = FALSE,
  n_{clusters} = c(1:10),
)
xgb.plot.importance(
  importance_matrix = NULL,
  top_n = NULL,
 measure = NULL,
  rel_to_first = FALSE,
  left_margin = 10,
  cex = NULL,
 plot = TRUE,
)
```

Arguments

importance_matrix

a data.table returned by xgb.importance.

top_n maximal number of top features to include into the plot.

measure the name of importance measure to plot. When NULL, 'Gain' would be used for

trees and 'Weight' would be used for gblinear.

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rel_to_first	whether importance values should be represented as relative to the highest ranked feature. See Details.
n_clusters	(ggplot only) a numeric vector containing the min and the max range of the possible number of clusters of bars.
• • •	other parameters passed to barplot (except horiz, border, cex.names, names.arg, and las).
left_margin	(base R barplot) allows to adjust the left margin size to fit feature names. When it is NULL, the existing par('mar') is used.
cex	(base R barplot) passed as cex.names parameter to barplot.
plot	(base R barplot) whether a barplot should be produced. If FALSE, only a data.table is returned.

Details

The graph represents each feature as a horizontal bar of length proportional to the importance of a feature. Features are shown ranked in a decreasing importance order. It works for importances from both gblinear and gbtree models.

When rel_to_first = FALSE, the values would be plotted as they were in importance_matrix. For gbtree model, that would mean being normalized to the total of 1 ("what is feature's importance contribution relative to the whole model?"). For linear models, rel_to_first = FALSE would show actual values of the coefficients. Setting rel_to_first = TRUE allows to see the picture from the perspective of "what is feature's importance contribution relative to the most important feature?"

The ggplot-backend method also performs 1-D clustering of the importance values, with bar colors corresponding to different clusters that have somewhat similar importance values.

Value

The xgb.plot.importance function creates a barplot (when plot=TRUE) and silently returns a processed data.table with n_top features sorted by importance.

The xgb.ggplot.importance function returns a ggplot graph which could be customized afterwards. E.g., to change the title of the graph, add + ggtitle("A GRAPH NAME") to the result.

See Also

barplot.

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```
gg + ggplot2::ylab("Frequency")
```

xgb.importance

Importance of features in a model.

Description

Creates a data. table of feature importances in a model.

Usage

```
xgb.importance(
  feature_names = NULL,
  model = NULL,
  trees = NULL,
  data = NULL,
  label = NULL,
  target = NULL
```

Arguments

feature_names character vector of feature names. If the model already contains feature names,

those would be used when feature_names=NULL (default value). Non-null

feature_names could be provided to override those in the model.

model object of class xgb.Booster.

trees (only for the gbtree booster) an integer vector of tree indices that should be

included into the importance calculation. If set to NULL, all trees of the model are parsed. It could be useful, e.g., in multiclass classification to get feature importances for each class separately. IMPORTANT: the tree index in xgboost

models is zero-based (e.g., use trees = 0:4 for first 5 trees).

data deprecated.
label deprecated.
target deprecated.

Details

This function works for both linear and tree models.

For linear models, the importance is the absolute magnitude of linear coefficients. For that reason, in order to obtain a meaningful ranking by importance for a linear model, the features need to be on the same scale (which you also would want to do when using either L1 or L2 regularization).

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Value

For a tree model, a data. table with the following columns:

- Features names of the features used in the model;
- Gain represents fractional contribution of each feature to the model based on the total gain of this feature's splits. Higher percentage means a more important predictive feature.
- Cover metric of the number of observation related to this feature;
- Frequency percentage representing the relative number of times a feature have been used in trees.

A linear model's importance data. table has the following columns:

- Features names of the features used in the model;
- Weight the linear coefficient of this feature;
- Class (only for multiclass models) class label.

If feature_names is not provided and model doesn't have feature_names, index of the features will be used instead. Because the index is extracted from the model dump (based on C++ code), it starts at 0 (as in C/C++ or Python) instead of 1 (usual in R).

```
# binomial classification using gbtree:
data(agaricus.train, package='xgboost')
bst <- xgboost(data = agaricus.train$data, label = agaricus.train$label, max_depth = 2,
               eta = 1, nthread = 2, nrounds = 2, objective = "binary:logistic")
xgb.importance(model = bst)
# binomial classification using gblinear:
bst <- xgboost(data = agaricus.train$data, label = agaricus.train$label, booster = "gblinear",</pre>
               eta = 0.3, nthread = 1, nrounds = 20, objective = "binary:logistic")
xgb.importance(model = bst)
# multiclass classification using gbtree:
nclass <- 3
nrounds <- 10
mbst <- xgboost(data = as.matrix(iris[, -5]), label = as.numeric(iris$Species) - 1,</pre>
               max_depth = 3, eta = 0.2, nthread = 2, nrounds = nrounds,
               objective = "multi:softprob", num_class = nclass)
# all classes clumped together:
xgb.importance(model = mbst)
# inspect importances separately for each class:
xgb.importance(model = mbst, trees = seq(from=0, by=nclass, length.out=nrounds))
xgb.importance(model = mbst, trees = seq(from=1, by=nclass, length.out=nrounds))
xgb.importance(model = mbst, trees = seq(from=2, by=nclass, length.out=nrounds))
# multiclass classification using gblinear:
mbst <- xgboost(data = scale(as.matrix(iris[, -5])), label = as.numeric(iris$Species) - 1,</pre>
               booster = "gblinear", eta = 0.2, nthread = 1, nrounds = 15,
```

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```
objective = "multi:softprob", num_class = nclass)
xgb.importance(model = mbst)
```

xgb.load

Load xgboost model from binary file

Description

Load xgboost model from the binary model file.

Usage

```
xgb.load(modelfile)
```

Arguments

modelfile

the name of the binary input file.

Details

The input file is expected to contain a model saved in an xgboost-internal binary format using either xgb.save or cb.save.model in R, or using some appropriate methods from other xgboost interfaces. E.g., a model trained in Python and saved from there in xgboost format, could be loaded from R.

Note: a model saved as an R-object, has to be loaded using corresponding R-methods, not xgb.load.

Value

An object of xgb. Booster class.

See Also

```
xgb.save, xgb.Booster.complete.
```

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xgb.model.dt.tree

Parse a boosted tree model text dump

Description

Parse a boosted tree model text dump into a data. table structure.

Usage

```
xgb.model.dt.tree(
  feature_names = NULL,
  model = NULL,
  text = NULL,
  trees = NULL,
  use_int_id = FALSE,
  ...
)
```

Arguments

feature_names	character vector of feature names. If the model already contains feature names, those would be used when feature_names=NULL (default value). Non-null feature_names could be provided to override those in the model.
model	object of class xgb.Booster
text	character vector previously generated by the xgb.dump function (where parameter with_stats = TRUE should have been set). text takes precedence over model.
trees	an integer vector of tree indices that should be parsed. If set to NULL, all trees of the model are parsed. It could be useful, e.g., in multiclass classification to get only the trees of one certain class. IMPORTANT: the tree index in xgboost models is zero-based (e.g., use trees = 0:4 for first 5 trees).
use_int_id	a logical flag indicating whether nodes in columns "Yes", "No", "Missing" should be represented as integers (when FALSE) or as "Tree-Node" character strings

Value

. . .

A data. table with detailed information about model trees' nodes.

(when FALSE). currently not used.

The columns of the data. table are:

- Tree: integer ID of a tree in a model (zero-based index)
- Node: integer ID of a node in a tree (zero-based index)
- ID: character identifier of a node in a model (only when use_int_id=FALSE)

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• Feature: for a branch node, it's a feature id or name (when available); for a leaf note, it simply labels it as 'Leaf'

- Split: location of the split for a branch node (split condition is always "less than")
- Yes: ID of the next node when the split condition is met
- No: ID of the next node when the split condition is not met
- Missing: ID of the next node when branch value is missing
- Quality: either the split gain (change in loss) or the leaf value
- Cover: metric related to the number of observation either seen by a split or collected by a leaf during training.

When use_int_id=FALSE, columns "Yes", "No", and "Missing" point to model-wide node identifiers in the "ID" column. When use_int_id=TRUE, those columns point to node identifiers from the corresponding trees in the "Node" column.

Examples

xgb.parameters<-

Accessors for model parameters.

Description

Only the setter for xgboost parameters is currently implemented.

Usage

```
xgb.parameters(object) <- value</pre>
```

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Arguments

object Object of class xgb.Booster or xgb.Booster.handle.

value a list (or an object coercible to a list) with the names of parameters to set and the

elements corresponding to parameter values.

Details

Note that the setter would usually work more efficiently for xgb.Booster.handle than for xgb.Booster, since only just a handle would need to be copied.

Examples

xgb.plot.multi.trees Project all trees on one tree and plot it

Description

Visualization of the ensemble of trees as a single collective unit.

Usage

```
xgb.plot.multi.trees(
  model,
  feature_names = NULL,
  features_keep = 5,
  plot_width = NULL,
  plot_height = NULL,
  render = TRUE,
  ...
)
```

Arguments

model produced by the xgb.train function.

feature_names names of each feature as a character vector.

features_keep number of features to keep in each position of the multi trees.

plot_width width in pixels of the graph to produce

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```
plot_height height in pixels of the graph to produce
render a logical flag for whether the graph should be rendered (see Value).
... currently not used
```

Details

This function tries to capture the complexity of a gradient boosted tree model in a cohesive way by compressing an ensemble of trees into a single tree-graph representation. The goal is to improve the interpretability of a model generally seen as black box.

Note: this function is applicable to tree booster-based models only.

It takes advantage of the fact that the shape of a binary tree is only defined by its depth (therefore, in a boosting model, all trees have similar shape).

Moreover, the trees tend to reuse the same features.

The function projects each tree onto one, and keeps for each position the features_keep first features (based on the Gain per feature measure).

This function is inspired by this blog post: https://wellecks.wordpress.com/2015/02/21/peering-into-the-black-box-visualizing-lambdamart/

Value

When render = TRUE: returns a rendered graph object which is an htmlwidget of class grViz. Similar to ggplot objects, it needs to be printed to see it when not running from command line.

When render = FALSE: silently returns a graph object which is of DiagrammeR's class dgr_graph. This could be useful if one wants to modify some of the graph attributes before rendering the graph with render_graph.

xgb.plot.shap 43

xgb.plot.shap

SHAP contribution dependency plots

Description

Visualizing the SHAP feature contribution to prediction dependencies on feature value.

Usage

```
xgb.plot.shap(
  data,
  shap_contrib = NULL,
  features = NULL,
  top_n = 1,
 model = NULL,
  trees = NULL,
  target_class = NULL,
  approxcontrib = FALSE,
  subsample = NULL,
  n_{col} = 1,
  col = rgb(0, 0, 1, 0.2),
  pch = ".",
  discrete_n_uniq = 5,
  discrete_jitter = 0.01,
 ylab = "SHAP",
 plot_NA = TRUE,
  col_NA = rgb(0.7, 0, 1, 0.6),
  pch_NA = ".",
  pos_NA = 1.07,
 plot_loess = TRUE,
  col_loess = 2,
  span_loess = 0.5,
 which = c("1d", "2d"),
 plot = TRUE,
)
```

Arguments

data	data as a matrix or dgCMatrix.
shap_contrib	a matrix of SHAP contributions that was computed earlier for the above data. When it is NULL, it is computed internally using model and data.
features	a vector of either column indices or of feature names to plot. When it is NULL, feature importance is calculated, and top_n high ranked features are taken.
top_n	when features is NULL, top_n [1, 100] most important features in a model are taken.

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model an xgb.Booster model. It has to be provided when either shap_contrib or

features is missing.

trees passed to xgb.importance when features = NULL.

target_class is only relevant for multiclass models. When it is set to a 0-based class index,

only SHAP contributions for that specific class are used. If it is not set, SHAP

importances are averaged over all classes.

approxcontrib passed to predict.xgb.Booster when shap_contrib = NULL.

subsample a random fraction of data points to use for plotting. When it is NULL, it is set

so that up to 100K data points are used.

n_col a number of columns in a grid of plots.

col color of the scatterplot markers.

pch scatterplot marker.

discrete_n_uniq

a maximal number of unique values in a feature to consider it as discrete.

discrete_jitter

an amount parameter of jitter added to discrete features' positions.

ylab a y-axis label in 1D plots.

plot_NA whether the contributions of cases with missing values should also be plotted.

col_NA a color of marker for missing value contributions.

pch_NA a marker type for NA values.

pos_NA a relative position of the x-location where NA values are shown: min(x) +

 $(\max(x) - \min(x)) * pos_NA.$

plot_loess whether to plot loess-smoothed curves. The smoothing is only done for features

with more than 5 distinct values.

col_loess a color to use for the loess curves.
span_loess the span parameter in loess's call.

which whether to do univariate or bivariate plotting. NOTE: only 1D is implemented

so far.

plot whether a plot should be drawn. If FALSE, only a lits of matrices is returned.

... other parameters passed to plot.

Details

These scatterplots represent how SHAP feature contributions depend of feature values. The similarity to partial dependency plots is that they also give an idea for how feature values affect predictions. However, in partial dependency plots, we usually see marginal dependencies of model prediction on feature value, while SHAP contribution dependency plots display the estimated contributions of a feature to model prediction for each individual case.

When plot_loess = TRUE is set, feature values are rounded to 3 significant digits and weighted LOESS is computed and plotted, where weights are the numbers of data points at each rounded value.

Note: SHAP contributions are shown on the scale of model margin. E.g., for a logistic binomial objective, the margin is prediction before a sigmoidal transform into probability-like values. Also,

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since SHAP stands for "SHapley Additive exPlanation" (model prediction = sum of SHAP contributions for all features + bias), depending on the objective used, transforming SHAP contributions for a feature from the marginal to the prediction space is not necessarily a meaningful thing to do.

Value

In addition to producing plots (when plot=TRUE), it silently returns a list of two matrices:

- data the values of selected features:
- shap_contrib the contributions of selected features.

References

Scott M. Lundberg, Su-In Lee, "A Unified Approach to Interpreting Model Predictions", NIPS Proceedings 2017, https://arxiv.org/abs/1705.07874

Scott M. Lundberg, Su-In Lee, "Consistent feature attribution for tree ensembles", https://arxiv.org/abs/1706.06060

```
data(agaricus.train, package='xgboost')
data(agaricus.test, package='xgboost')
bst <- xgboost(agaricus.train$data, agaricus.train$label, nrounds = 50,</pre>
               eta = 0.1, max_depth = 3, subsample = .5,
               method = "hist", objective = "binary:logistic", nthread = 2, verbose = 0)
xgb.plot.shap(agaricus.test$data, model = bst, features = "odor=none")
contr <- predict(bst, agaricus.test$data, predcontrib = TRUE)</pre>
xgb.plot.shap(agaricus.test$data, contr, model = bst, top_n = 12, n_col = 3)
# multiclass example - plots for each class separately:
nclass <- 3
nrounds <- 20
x <- as.matrix(iris[, -5])</pre>
set.seed(123)
is.na(x[sample(nrow(x) * 4, 30)]) \leftarrow TRUE # introduce some missing values
mbst <- xgboost(data = x, label = as.numeric(iris$Species) - 1, nrounds = nrounds,</pre>
                max_depth = 2, eta = 0.3, subsample = .5, nthread = 2,
                objective = "multi:softprob", num_class = nclass, verbose = 0)
trees0 <- seq(from=0, by=nclass, length.out=nrounds)</pre>
col <- rgb(0, 0, 1, 0.5)
xgb.plot.shap(x, model = mbst, trees = trees0, target_class = 0, top_n = 4,
              n_{col} = 2, col = col, pch = 16, pch_{NA} = 17)
xgb.plot.shap(x, model = mbst, trees = trees0 + 1, target_class = 1, top_n = 4,
              n_{col} = 2, col = col, pch = 16, pch_{NA} = 17)
xgb.plot.shap(x, model = mbst, trees = trees0 + 2, target_class = 2, top_n = 4,
              n_{col} = 2, col = col, pch = 16, pch_{NA} = 17)
```

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xgb.plot.tree

Plot a boosted tree model

Description

Read a tree model text dump and plot the model.

Usage

```
xgb.plot.tree(
  feature_names = NULL,
  model = NULL,
  trees = NULL,
  plot_width = NULL,
  plot_height = NULL,
  render = TRUE,
  show_node_id = FALSE,
  ...
)
```

Arguments

feature_names names of each feature as a character vector.

model produced by the xgb.train function.

trees an integer vector of tree indices that should be visualized. If set to NULL, all

trees of the model are included. IMPORTANT: the tree index in xgboost model

is zero-based (e.g., use trees = 0:2 for the first 3 trees in a model).

plot_width the width of the diagram in pixels.
plot_height the height of the diagram in pixels.

render a logical flag for whether the graph should be rendered (see Value).

show_node_id a logical flag for whether to show node id's in the graph.

... currently not used.

Details

The content of each node is organised that way:

- Feature name.
- Cover: The sum of second order gradient of training data classified to the leaf. If it is square loss, this simply corresponds to the number of instances seen by a split or collected by a leaf during training. The deeper in the tree a node is, the lower this metric will be.
- Gain (for split nodes): the information gain metric of a split (corresponds to the importance of the node in the model).
- Value (for leafs): the margin value that the leaf may contribute to prediction.

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The tree root nodes also indicate the Tree index (0-based).

The "Yes" branches are marked by the "< split_value" label. The branches that also used for missing values are marked as bold (as in "carrying extra capacity").

This function uses GraphViz as a backend of DiagrammeR.

Value

When render = TRUE: returns a rendered graph object which is an htmlwidget of class grViz. Similar to ggplot objects, it needs to be printed to see it when not running from command line.

When render = FALSE: silently returns a graph object which is of DiagrammeR's class dgr_graph. This could be useful if one wants to modify some of the graph attributes before rendering the graph with render_graph.

Examples

xgb.save

Save xgboost model to binary file

Description

Save xgboost model to a file in binary format.

Usage

```
xgb.save(model, fname)
```

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Arguments

model model object of xgb. Booster class.

fname name of the file to write.

Details

This methods allows to save a model in an xgboost-internal binary format which is universal among the various xgboost interfaces. In R, the saved model file could be read-in later using either the xgb.load function or the xgb_model parameter of xgb.train.

Note: a model can also be saved as an R-object (e.g., by using readRDS or save). However, it would then only be compatible with R, and corresponding R-methods would need to be used to load it.

See Also

```
xgb.load, xgb.Booster.complete.
```

Examples

xgb.save.raw

Save xgboost model to R's raw vector, user can call xgb.load to load the model back from raw vector

Description

Save xgboost model from xgboost or xgb.train

Usage

```
xgb.save.raw(model)
```

Arguments

model

the model object.

Examples

xgb.train

eXtreme Gradient Boosting Training

Description

xgb.train is an advanced interface for training an xgboost model. The xgboost function is a simpler wrapper for xgb.train.

Usage

```
xgb.train(
  params = list(),
  data,
  nrounds,
  watchlist = list(),
  obj = NULL,
  feval = NULL,
  verbose = 1,
  print_every_n = 1L,
  early_stopping_rounds = NULL,
  maximize = NULL,
  save_period = NULL,
  save_name = "xgboost.model",
  xgb_model = NULL,
  callbacks = list(),
)
xgboost(
  data = NULL,
  label = NULL,
  missing = NA,
 weight = NULL,
  params = list(),
  nrounds,
```

```
verbose = 1,
print_every_n = 1L,
early_stopping_rounds = NULL,
maximize = NULL,
save_period = NULL,
save_name = "xgboost.model",
xgb_model = NULL,
callbacks = list(),
...
)
```

Arguments

params

the list of parameters. The complete list of parameters is available at http://xgboost.readthedocs.io/en/latest/parameter.html. Below is a shorter summary:

- 1. General Parameters
 - booster which booster to use, can be gbtree or gblinear. Default: gbtree.
- 2. Booster Parameters
- 2.1. Parameter for Tree Booster
 - eta control the learning rate: scale the contribution of each tree by a factor of 0 < eta < 1 when it is added to the current approximation. Used to prevent overfitting by making the boosting process more conservative. Lower value for eta implies larger value for nrounds: low eta value means model more robust to overfitting but slower to compute. Default: 0.3
 - gamma minimum loss reduction required to make a further partition on a leaf node of the tree. the larger, the more conservative the algorithm will be
 - max_depth maximum depth of a tree. Default: 6
 - min_child_weight minimum sum of instance weight (hessian) needed in a child. If the tree partition step results in a leaf node with the sum of instance weight less than min_child_weight, then the building process will give up further partitioning. In linear regression mode, this simply corresponds to minimum number of instances needed to be in each node. The larger, the more conservative the algorithm will be. Default: 1
 - subsample subsample ratio of the training instance. Setting it to 0.5 means that xgboost randomly collected half of the data instances to grow trees and this will prevent overfitting. It makes computation shorter (because less data to analyse). It is advised to use this parameter with eta and increase nrounds. Default: 1
 - colsample_bytree subsample ratio of columns when constructing each tree. Default: 1
 - num_parallel_tree Experimental parameter. number of trees to grow per round. Useful to test Random Forest through Xgboost (set colsample_bytree < 1, subsample < 1 and round = 1) accordingly. Default: 1

monotone_constraints A numerical vector consists of 1, 0 and -1 with its length equals to the number of features in the training data. 1 is increasing, -1 is decreasing and 0 is no constraint.

• interaction_constraints A list of vectors specifying feature indices of permitted interactions. Each item of the list represents one permitted interaction where specified features are allowed to interact with each other. Feature index values should start from 0 (0 references the first column). Leave argument unspecified for no interaction constraints.

2.2. Parameter for Linear Booster

- lambda L2 regularization term on weights. Default: 0
- lambda_bias L2 regularization term on bias. Default: 0
- alpha L1 regularization term on weights. (there is no L1 reg on bias because it is not important). Default: 0

3. Task Parameters

- objective specify the learning task and the corresponding learning objective, users can pass a self-defined function to it. The default objective options are below:
 - reg: squarederror Regression with squared loss (Default).
 - reg:logistic logistic regression.
 - binary:logistic logistic regression for binary classification. Output probability.
 - binary:logitraw logistic regression for binary classification, output score before logistic transformation.
 - num_class set the number of classes. To use only with multiclass objectives.
 - multi:softmax set xgboost to do multiclass classification using the softmax objective. Class is represented by a number and should be from 0 to num_class -1.
 - multi:softprob same as softmax, but prediction outputs a vector of ndata * nclass elements, which can be further reshaped to ndata, nclass matrix. The result contains predicted probabilities of each data point belonging to each class.
 - rank:pairwise set xgboost to do ranking task by minimizing the pairwise loss.
- base_score the initial prediction score of all instances, global bias. Default: 0.5
- eval_metric evaluation metrics for validation data. Users can pass a self-defined function to it. Default: metric will be assigned according to objective(rmse for regression, and error for classification, mean average precision for ranking). List is provided in detail section.

data

training dataset. xgb.train accepts only an xgb.DMatrix as the input. xgboost, in addition, also accepts matrix, dgCMatrix, or name of a local data file.

nrounds

max number of boosting iterations.

watchlist named list of xgb.DMatrix datasets to use for evaluating model performance.

Metrics specified in either eval_metric or feval will be computed for each of these datasets during each boosting iteration, and stored in the end as a field named evaluation_log in the resulting object. When either verbose>=1 or cb.print.evaluation callback is engaged, the performance results are contin-

 $uously\ printed\ out\ during\ the\ training.\ E.g.,\ specifying\ watchlist=list(validation 1=mat 1,validation 1=mat 1=mat 1,validation 1=mat 1=mat$

allows to track the performance of each round's model on mat1 and mat2.

customized objective function. Returns gradient and second order gradient with

given prediction and dtrain.

feval customized evaluation function. Returns list(metric='metric-name',value='metric-value')

with given prediction and dtrain.

verbose If 0, xgboost will stay silent. If 1, it will print information about performance. If

2, some additional information will be printed out. Note that setting verbose > 0 automatically engages the cb.print.evaluation(period=1) callback func-

tion.

print_every_n Print each n-th iteration evaluation messages when verbose>0. Default is 1

which means all messages are printed. This parameter is passed to the cb.print.evaluation

callback.

early_stopping_rounds

obj

If NULL, the early stopping function is not triggered. If set to an integer k, training with a validation set will stop if the performance doesn't improve for k

rounds. Setting this parameter engages the cb.early.stop callback.

maximize If feval and early_stopping_rounds are set, then this parameter must be set

as well. When it is TRUE, it means the larger the evaluation score the better. This

parameter is passed to the cb.early.stop callback.

save_period when it is non-NULL, model is saved to disk after every save_period rounds,

0 means save at the end. The saving is handled by the cb.save.model callback.

save_name the name or path for periodically saved model file.

xgb_model a previously built model to continue the training from. Could be either an object

of class xgb.Booster, or its raw data, or the name of a file with a previously

saved model.

callbacks a list of callback functions to perform various task during boosting. See callbacks.

Some of the callbacks are automatically created depending on the parameters' values. User can provide either existing or their own callback methods in order

to customize the training process.

... other parameters to pass to params.

label vector of response values. Should not be provided when data is a local data file

name or an xgb.DMatrix.

missing by default is set to NA, which means that NA values should be considered as

'missing' by the algorithm. Sometimes, 0 or other extreme value might be used to represent missing values. This parameter is only used when input is a dense

matrix.

weight a vector indicating the weight for each row of the input.

Details

These are the training functions for xgboost.

The xgb.train interface supports advanced features such as watchlist, customized objective and evaluation metric functions, therefore it is more flexible than the xgboost interface.

Parallelization is automatically enabled if OpenMP is present. Number of threads can also be manually specified via nthread parameter.

The evaluation metric is chosen automatically by Xgboost (according to the objective) when the eval_metric parameter is not provided. User may set one or several eval_metric parameters. Note that when using a customized metric, only this single metric can be used. The following is the list of built-in metrics for which Xgboost provides optimized implementation:

- rmse root mean square error. http://en.wikipedia.org/wiki/Root_mean_square_error
- logloss negative log-likelihood. http://en.wikipedia.org/wiki/Log-likelihood
- mlogloss multiclass logloss. http://wiki.fast.ai/index.php/Log_Loss
- error Binary classification error rate. It is calculated as (# wrong cases) / (# all cases). By default, it uses the 0.5 threshold for predicted values to define negative and positive instances. Different threshold (e.g., 0.) could be specified as "error@0."
- merror Multiclass classification error rate. It is calculated as (# wrong cases) / (# all cases).
- auc Area under the curve. http://en.wikipedia.org/wiki/Receiver_operating_characteristic# 'Area_under_curve for ranking evaluation.
- aucpr Area under the PR curve. https://en.wikipedia.org/wiki/Precision_and_recall for ranking evaluation.
- ndcg Normalized Discounted Cumulative Gain (for ranking task). http://en.wikipedia. org/wiki/NDCG

The following callbacks are automatically created when certain parameters are set:

- cb.print.evaluation is turned on when verbose > 0; and the print_every_n parameter is passed to it.
- cb.evaluation.log is on when watchlist is present.
- cb.early.stop: when early_stopping_rounds is set.
- cb.save.model: when save_period > 0 is set.

Value

An object of class xgb. Booster with the following elements:

- handle a handle (pointer) to the xgboost model in memory.
- raw a cached memory dump of the xgboost model saved as R's raw type.
- niter number of boosting iterations.
- evaluation_log evaluation history stored as a data.table with the first column corresponding to iteration number and the rest corresponding to evaluation metrics' values. It is created by the cb.evaluation.log callback.

- call a function call.
- params parameters that were passed to the xgboost library. Note that it does not capture parameters changed by the cb.reset.parameters callback.
- callbacks callback functions that were either automatically assigned or explicitly passed.
- best_iteration iteration number with the best evaluation metric value (only available with early stopping).
- best_ntreelimit the ntreelimit value corresponding to the best iteration, which could further be used in predict method (only available with early stopping).
- best_score the best evaluation metric value during early stopping. (only available with early stopping).
- feature_names names of the training dataset features (only when column names were defined in training data).
- nfeatures number of features in training data.

References

Tianqi Chen and Carlos Guestrin, "XGBoost: A Scalable Tree Boosting System", 22nd SIGKDD Conference on Knowledge Discovery and Data Mining, 2016, https://arxiv.org/abs/1603.02754

See Also

```
callbacks, predict.xgb.Booster, xgb.cv
```

```
data(agaricus.train, package='xgboost')
data(agaricus.test, package='xgboost')
dtrain <- xgb.DMatrix(agaricus.train$data, label = agaricus.train$label)</pre>
dtest <- xgb.DMatrix(agaricus.test$data, label = agaricus.test$label)</pre>
watchlist <- list(train = dtrain, eval = dtest)</pre>
## A simple xgb.train example:
param <- list(max_depth = 2, eta = 1, verbose = 0, nthread = 2,</pre>
               objective = "binary:logistic", eval_metric = "auc")
bst <- xgb.train(param, dtrain, nrounds = 2, watchlist)</pre>
## An xgb.train example where custom objective and evaluation metric are used:
logregobj <- function(preds, dtrain) {</pre>
   labels <- getinfo(dtrain, "label")</pre>
   preds <- 1/(1 + exp(-preds))
   grad <- preds - labels</pre>
   hess <- preds * (1 - preds)
   return(list(grad = grad, hess = hess))
}
evalerror <- function(preds, dtrain) {</pre>
  labels <- getinfo(dtrain, "label")</pre>
```

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```
err <- as.numeric(sum(labels != (preds > 0)))/length(labels)
 return(list(metric = "error", value = err))
}
# These functions could be used by passing them either:
# as 'objective' and 'eval_metric' parameters in the params list:
param <- list(max_depth = 2, eta = 1, verbose = 0, nthread = 2,</pre>
              objective = logregobj, eval_metric = evalerror)
bst <- xgb.train(param, dtrain, nrounds = 2, watchlist)</pre>
# or through the ... arguments:
param <- list(max_depth = 2, eta = 1, verbose = 0, nthread = 2)</pre>
bst <- xgb.train(param, dtrain, nrounds = 2, watchlist,</pre>
                 objective = logregobj, eval_metric = evalerror)
# or as dedicated 'obj' and 'feval' parameters of xgb.train:
bst <- xgb.train(param, dtrain, nrounds = 2, watchlist,</pre>
                 obj = logregobj, feval = evalerror)
## An xgb.train example of using variable learning rates at each iteration:
param <- list(max_depth = 2, eta = 1, verbose = 0, nthread = 2,</pre>
              objective = "binary:logistic", eval_metric = "auc")
my_etas \leftarrow list(eta = c(0.5, 0.1))
bst <- xgb.train(param, dtrain, nrounds = 2, watchlist,</pre>
                 callbacks = list(cb.reset.parameters(my_etas)))
## Early stopping:
bst <- xgb.train(param, dtrain, nrounds = 25, watchlist,</pre>
                 early_stopping_rounds = 3)
## An 'xgboost' interface example:
bst <- xgboost(data = agaricus.train$data, label = agaricus.train$label,</pre>
               max_depth = 2, eta = 1, nthread = 2, nrounds = 2,
               objective = "binary:logistic")
pred <- predict(bst, agaricus.test$data)</pre>
```

xgboost-deprecated

Deprecation notices.

Description

At this time, some of the parameter names were changed in order to make the code style more uniform. The deprecated parameters would be removed in the next release.

Details

To see all the current deprecated and new parameters, check the xgboost:::depr_par_lut table.

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A deprecation warning is shown when any of the deprecated parameters is used in a call. An additional warning is shown when there was a partial match to a deprecated parameter (as R is able to partially match parameter names).

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