Package ‘h2o4gpu’

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Type Package

Title Interface to 'H2O4GPU'

Version 0.3.3

Description Interface to 'H2O4GPU' <https://github.com/h2oai/h2o4gpu>, a collection of 'GPU' solvers for machine learning algorithms.

License Apache License 2.0

URL https://github.com/h2oai/h2o4gpu

BugReports https://github.com/h2oai/h2o4gpu/issues

SystemRequirements Python (>= 3.6) with header files and shared library; H2O4GPU (https://github.com/h2oai/h2o4gpu)

Encoding UTF-8

Depends R (>= 3.1)

Imports utils, magrittr, reticulate (>= 1.4)

RoxygenNote 6.0.1

Suggests testthat, knitr, rmarkdown, Matrix

VignetteBuilder knitr

NeedsCompilation no

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### fit

**Generic Method to Train an H2O4GPU Estimator**

**Description**

Generic Method to Train an H2O4GPU Estimator

Generic Method to Transform a Dataset using Trained H2O4GPU Estimator

**Usage**

```r
fit(object, ...)
transform(object, ...)
```

**Arguments**

- `object` The h2o4gpu model object
- `...` Additional arguments (unused for now).
fit.h2o4gpu_model  

Train an H2O4GPU Estimator

Description
This function builds the model using the training data specified.

Usage
## S3 method for class 'h2o4gpu_model'
fit(object, x, y = NULL, ...)

Arguments

object  The h2o4gpu model object
x  The training data where each column represents a different predictor variable to be used in building the model.
y  A vector of numeric values to be used as response variable in building the model.
Note that if the vector is character or factor, it will be converted to numeric column (e.g. 0, 1, 2, ...) implicitly. For unsupervised models, this argument can be ignored or specified as NULL.
...
Additional arguments (unused for now).

Examples
## Not run:
library(h2o4gpu)

# Setup dataset
x <- iris[1:4]
y <- as.integer(iris$Species) - 1

# Train the classifier
h2o4gpu.random_forest_classifier() %>% fit(x, y)

## End(Not run)

h2o4gpu  
h2o4gpu in R

Description
h2o4gpu in R
Examples

```r
## Not run:
library(h2o4gpu)

# Setup dataset
x <- iris[,1:4]
y <- as.integer(iris$Species) - 1

# Initialize and train the classifier
model <- h2o4gpu.random_forest_classifier() %>% fit(x, y)

# Make predictions
predictions <- model %>% predict(x)

## End(Not run)
```

---

### h2o4gpu.elastic_net_classifier

### Elastic Net Classifier

#### Description

Elastic Net Classifier

#### Usage

```r
h2o4gpu.elastic_net_classifier(alpha = 1, l1_ratio = 0.5,
fit_intercept = TRUE, normalize = FALSE, precompute = FALSE,
max_iter = 5000L, copy_X = TRUE, tol = 0.01, warm_start = FALSE,
positive = FALSE, random_state = NULL, selection = "cyclic",
n_gpus = -1L, lambda_stop_early = TRUE, glm_stop_early = TRUE,
glm_stop_early_error_fraction = 1, verbose = FALSE, n_threads = NULL,
gpu_id = 0L, lambda_min_ratio = 1e-07, n_lambdas = 100L, n_folds = 5L,
tol_seek_factor = 0.1, store_full_path = 0L, lambda_max = NULL,
lambdas = NULL, double_precision = NULL, order = NULL,
backend = "h2o4gpu")
```

#### Arguments

- **alpha**: Constant that multiplies the penalty terms. Defaults to 1.0. See the notes for the exact mathematical meaning of this parameter. `alpha = 0` is equivalent to an ordinary least square, solved by the `class:LinearRegressionSklearn` object. For numerical reasons, using `alpha = 0` with the `LassoSklearn` object is not advised. Given this, you should use the `class:LinearRegressionSklearn` object.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>l1_ratio</strong></td>
<td>The ElasticNetSklearn mixing parameter, with 0 (\leq l1_ratio \leq 1). For (l1_ratio = 0) the penalty is an L2 penalty. For (l1_ratio = 1) it is an L1 penalty. For (0 &lt; l1_ratio &lt; 1), the penalty is a combination of L1 and L2.</td>
</tr>
<tr>
<td><strong>fit_intercept</strong></td>
<td>Whether the intercept should be estimated or not. If FALSE, the data is assumed to be already centered.</td>
</tr>
<tr>
<td><strong>normalize</strong></td>
<td>This parameter is ignored when fit_intercept is set to FALSE. If TRUE, the regressors X will be normalized before regression by subtracting the mean and dividing by the l2-norm. If you wish to standardize, please use :class:<code>h2o4gpu.preprocessing.StandardScaler</code> before calling fit on an estimator with normalize=FALSE.</td>
</tr>
<tr>
<td><strong>precompute</strong></td>
<td>Whether to use a precomputed Gram matrix to speed up calculations. The Gram matrix can also be passed as argument. For sparse input this option is always TRUE to preserve sparsity.</td>
</tr>
<tr>
<td><strong>max_iter</strong></td>
<td>The maximum number of iterations</td>
</tr>
<tr>
<td><strong>copy_X</strong></td>
<td>If TRUE, X will be copied; else, it may be overwritten.</td>
</tr>
<tr>
<td><strong>tol</strong></td>
<td>The tolerance for the optimization: if the updates are smaller than tol, the optimization code checks the dual gap for optimality and continues until it is smaller than tol.</td>
</tr>
<tr>
<td><strong>warm_start</strong></td>
<td>When set to TRUE, reuse the solution of the previous call to fit as initialization, otherwise, just erase the previous solution.</td>
</tr>
<tr>
<td><strong>positive</strong></td>
<td>When set to TRUE, forces the coefficients to be positive.</td>
</tr>
<tr>
<td><strong>random_state</strong></td>
<td>The seed of the pseudo random number generator that selects a random feature to update. If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If NULL, the random number generator is the RandomState instance used by np.random. Used when selection == 'random'.</td>
</tr>
<tr>
<td><strong>selection</strong></td>
<td>If set to 'random', a random coefficient is updated every iteration rather than looping over features sequentially by default. This (setting to 'random') often leads to significantly faster convergence especially when tol is higher than 1e-4.</td>
</tr>
<tr>
<td><strong>n_gpus</strong></td>
<td>Number of gpu's to use in GLM solver.</td>
</tr>
<tr>
<td><strong>lambda_stop_early</strong></td>
<td>Stop early when there is no more relative improvement on train or validation.</td>
</tr>
<tr>
<td><strong>glm_stop_early</strong></td>
<td>Stop early when there is no more relative improvement in the primary and dual residuals for ADMM.</td>
</tr>
<tr>
<td><strong>glm_stop_early_error_fraction</strong></td>
<td>Relative tolerance for metric-based stopping criterion (stop if relative improvement is not at least this much).</td>
</tr>
<tr>
<td><strong>verbose</strong></td>
<td>Print verbose information to the console if set to &gt; 0.</td>
</tr>
<tr>
<td><strong>n_threads</strong></td>
<td>Number of threads to use in the gpu. Each thread is an independent model builder.</td>
</tr>
<tr>
<td><strong>gpu_id</strong></td>
<td>ID of the GPU on which the algorithm should run.</td>
</tr>
<tr>
<td><strong>lambda_min_ratio</strong></td>
<td>Minimum lambda ratio to maximum lambda, used in lambda search.</td>
</tr>
<tr>
<td><strong>n_lambdas</strong></td>
<td>Number of lambdas to be used in a search.</td>
</tr>
</tbody>
</table>
n_folds

Number of cross validation folds.

tol_seek_factor

Factor of tolerance to seek once below null model accuracy. Default is 1E-1, so
seeks tolerance of 1E-3 once below null model accuracy for tol=1E-2.

store_full_path

Whether to store full solution for all alphas and lambdas. If 1, then during
predict will compute best and full predictions.

lambda_max

Maximum Lambda value to use. Default is NULL, and then internally compute
standard maximum

lambdas

overrides n_lambdas, lambda_max, and lambda_min_ratio.

double_precision

Internally set unless using _ptr methods. Value can either be 0 (float32) or
1(float64)

order

Order of data. Default is NULL, and internally determined (unless using _ptr
methods) whether row 'r' or column 'c' major order.

backend

Which backend to use. Options are 'auto', 'sklearn', 'h2o4gpu'. Saves as at-
ttribute for actual backend used.

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h2o4gpu.elastic_net_regressor

Elastic Net Regressor

Description

Elastic Net Regressor

Usage

h2o4gpu.elastic_net_regressor(alpha = 1, l1_ratio = 0.5,
fit_intercept = TRUE, normalize = FALSE, precompute = FALSE,
max_iter = 5000L, copy_X = TRUE, tol = 0.01, warm_start = FALSE,
positive = FALSE, random_state = NULL, selection = "cyclic",
n_gpus = -1L, lambda_stop_early = TRUE, glm_stop_early = TRUE,
glm_stop_early_error_fraction = 1, verbose = FALSE, n_threads = NULL,
gpu_id = 0L, lambda_min_ratio = 1e-07, n_lambdas = 100L, n_folds = 5L,
tol_seek_factor = 0.1, store_full_path = 0L, lambda_max = NULL,
lambdas = NULL, double_precision = NULL, order = NULL,
backend = "h2o4gpu")

Arguments

alpha

Constant that multiplies the penalty terms. Defaults to 1.0. See the notes for
the exact mathematical meaning of this parameter. alpha = 0 is equivalent to an
ordinary least square, solved by the :class:`LinearRegressionSklearn` object.
For numerical reasons, using alpha = 0 with the LassoSklearn object is not ad-
vised. Given this, you should use the :class:`LinearRegressionSklearn` object.
The ElasticNetSklearn mixing parameter, with $0 \leq l1\_ratio \leq 1$. For $l1\_ratio = 0$ the penalty is an L2 penalty. For $l1\_ratio = 1$ it is an L1 penalty. For $0 < l1\_ratio < 1$, the penalty is a combination of L1 and L2.

Whether the intercept should be estimated or not. If FALSE, the data is assumed to be already centered.

This parameter is ignored when fit_intercept is set to FALSE. If TRUE, the regressors X will be normalized before regression by subtracting the mean and dividing by the l2-norm. If you wish to standardize, please use :class:h2o4gpu.preprocessing.StandardScaler before calling fit on an estimator with normalize=FALSE.

Whether to use a precomputed Gram matrix to speed up calculations. The Gram matrix can also be passed as argument. For sparse input this option is always TRUE to preserve sparsity.

The maximum number of iterations.

If TRUE, X will be copied; else, it may be overwritten.

The tolerance for the optimization: if the updates are smaller than tol, the optimization code checks the dual gap for optimality and continues until it is smaller than tol.

When set to TRUE, reuse the solution of the previous call to fit as initialization, otherwise, just erase the previous solution.

When set to TRUE, forces the coefficients to be positive.

The seed of the pseudo random number generator that selects a random feature to update. If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If NULL, the random number generator is the RandomState instance used by np.random. Used when selection == 'random'.

If set to 'random', a random coefficient is updated every iteration rather than looping over features sequentially by default. This (setting to 'random') often leads to significantly faster convergence especially when tol is higher than 1e-4.

Number of gpu's to use in GLM solver.

Stop early when there is no more relative improvement on train or validation.

Stop early when there is no more relative improvement in the primary and dual residuals for ADMM.

Relative tolerance for metric-based stopping criterion (stop if relative improvement is not at least this much).

Print verbose information to the console if set to > 0.

Number of threads to use in the gpu. Each thread is an independent model builder.

ID of the GPU on which the algorithm should run.

Minimum lambda ratio to maximum lambda, used in lambda search.

Number of lambdas to be used in a search.
n_folds

tol_seek_factor

store_full_path

lambda_max

lambda_min_ratio

double_precision

order

backend

Description

Gradient Boosting Classifier

Usage

h2o4gpu.gradient_boosting_classifier(loss = "deviance", learning_rate = 0.1, n_estimators = 100L, subsample = 1, criterion = "friedman_mse", min_samples_split = 2L, min_samples_leaf = 1L, min_weight_fraction_leaf = 0, max_depth = 3L, min_impurity_decrease = 0, min_impurity_split = NULL, init = NULL, random_state = NULL, max_features = "auto", verbose = 0L, max_leaf_nodes = NULL, warm_start = FALSE, presort = "auto", colsample_bytree = 1, num_parallel_tree = 1L, tree_method = "gpu_hist", n_gpus = -1L, predictor = "gpu_predictor", objective = "binary:logistic", booster = "gbtree", n_jobs = 1L, gamma = 0L, min_child_weight = 1L, max_delta_step = 0L, colsample_bylevel = 1L, reg_alpha = 0L, reg_lambda = 1L, scale_pos_weight = 1L, base_score = 0.5, missing = NULL, backend = "h2o4gpu", ...)
Arguments

**loss**
loss function to be optimized. 'deviance' refers to deviance (= logisitic regression) for classification with probabilistic outputs. For loss 'exponential' gradient boosting recovers the AdaBoost algorithm.

**learning_rate**
learning rate shrinks the contribution of each tree by learning_rate. There is a trade-off between learning_rate and n_estimators.

**n_estimators**
The number of boosting stages to perform. Gradient boosting is fairly robust to over-fitting so a large number usually results in better performance.

**subsample**
The fraction of samples to be used for fitting the individual base learners. If smaller than 1.0 this results in Stochastic Gradient Boosting. subsample interacts with the parameter n_estimators. Choosing subsample < 1.0 leads to a reduction of variance and an increase in bias.

**criterion**
The function to measure the quality of a split. Supported criteria are "friedman_mse" for the mean squared error with improvement score by Friedman, "mse" for mean squared error, and "mae" for the mean absolute error. The default value of "friedman_mse" is generally the best as it can provide a better approximation in some cases.

**min_samples_split**
The minimum number of samples required to split an internal node:

**min_samples_leaf**
The minimum number of samples required to be at a leaf node:

**min_weight_fraction_leaf**
The minimum weighted fraction of the sum total of weights (of all the input samples) required to be at a leaf node. Samples have equal weight when sample_weight is not provided.

**max_depth**
maximum depth of the individual regression estimators. The maximum depth limits the number of nodes in the tree. Tune this parameter for best performance; the best value depends on the interaction of the input variables.

**min_impurity_decrease**
A node will be split if this split induces a decrease of the impurity greater than or equal to this value.

**min_impurity_split**
Threshold for early stopping in tree growth. A node will split if its impurity is above the threshold, otherwise it is a leaf.

**init**
An estimator object that is used to compute the initial predictions. init has to provide fit and predict. If NULL it uses loss.init_estimator.

**random_state**
If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If NULL, the random number generator is the RandomState instance used by np.random.

**max_features**
The number of features to consider when looking for the best split:

**verbose**
Enable verbose output. If 1 then it prints progress and performance once in a while (the more trees the lower the frequency). If greater than 1 then it prints progress and performance for every tree.
max_leaf_nodes  Grow trees with max_leaf_nodes in best-first fashion. Best nodes are defined as relative reduction in impurity. If NULL then unlimited number of leaf nodes.

warm_start  When set to TRUE, reuse the solution of the previous call to fit and add more estimators to the ensemble, otherwise, just erase the previous solution.

presort  Whether to presort the data to speed up the finding of best splits in fitting. Auto mode by default will use presorting on dense data and default to normal sorting on sparse data. Setting presort to true on sparse data will raise an error.

colsample_bytree  Subsample ratio of columns when constructing each tree.

num_parallel_tree  Number of trees to grow per round

tree_method  The tree construction algorithm used in XGBoost Distributed and external memory version only support approximate algorithm. Choices: ‘auto’, ‘exact’, ‘approx’, ‘hist’, ‘gpu_exact’, ‘gpu_hist’ ‘auto’: Use heuristic to choose faster one. - For small to medium dataset, exact greedy will be used. - For very large dataset, approximate algorithm will be chosen. - Because old behavior is always use exact greedy in single machine, - user will get a message when approximate algorithm is chosen to notify this choice. ‘exact’: Exact greedy algorithm. ‘approx’: Approximate greedy algorithm using sketching and histogram. ‘hist’: Fast histogram optimized approximate greedy algorithm. It uses some performance improvements such as bins caching. ‘gpu_exact’: GPU implementation of exact algorithm. ‘gpu_hist’: GPU implementation of hist algorithm.

n_gpus  Number of gpu’s to use in GradientBoostingClassifier solver. Default is -1.

predictor  The type of predictor algorithm to use. Provides the same results but allows the use of GPU or CPU. - ‘cpu_predictor’: Multicore CPU prediction algorithm. - ‘gpu_predictor’: Prediction using GPU. Default for ‘gpu_exact’ and ‘gpu_hist’ tree method.

objective  Specify the learning task and the corresponding learning objective or a custom objective function to be used Note: A custom objective function can be provided for the objective parameter. In this case, it should have the signature objective(y_true, y_pred) -> grad, hess:

booster  Specify which booster to use: gtree, glinear or dart.

n_jobs  Number of parallel threads used to run xgboost.

gamma  Minimum loss reduction required to make a further partition on a leaf node of the tree.

min_child_weight  Minimum sum of instance weight(hessian) needed in a child.

max_delta_step  Maximum delta step we allow each tree’s weight estimation to be.

colsample_bylevel  Subsample ratio of columns for each split, in each level.

reg_alpha  L1 regularization term on weights

reg_lambda  L2 regularization term on weights

scale_pos_weight  Balancing of positive and negative weights.
Gradient Boosting Regressor

Description

Gradient Boosting Regressor

Usage

```r
h2o4gpu.gradient_boosting_regressor(loss = "ls", learning_rate = 0.1,
  n_estimators = 100L, subsample = 1, criterion = "friedman_mse",
  min_samples_split = 2L, min_samples_leaf = 1L,
  min_weight_fraction_leaf = 0, max_depth = 3L, min_impurity_decrease = 0,
  min_impurity_split = NULL, init = NULL, random_state = NULL,
  max_features = "auto", alpha = 0.9, verbose = 0L,
  max_leaf_nodes = NULL, warm_start = FALSE, presort = "auto",
  colsample_bytree = 1, num_parallel_tree = 1L, tree_method = "gpu_hist",
  n_gpus = -1L, predictor = "gpu_predictor", objective = "reg:linear",
  booster = "gbtree", n_jobs = 1L, gamma = 0L, min_child_weight = 1L,
  max_delta_step = 0L, colsample_bylevel = 1L, reg_alpha = 0L,
  reg_lambda = 1L, scale_pos_weight = 1L, base_score = 0.5,
  missing = NULL, backend = "h2o4gpu", ...)
```

Arguments

- **loss**: loss function to be optimized. 'ls' refers to least squares regression. 'lad' (least absolute deviation) is a highly robust loss function solely based on order information of the input variables. 'huber' is a combination of the two. 'quantile' allows quantile regression (use alpha to specify the quantile).

- **learning_rate**: learning rate shrinks the contribution of each tree by learning_rate. There is a trade-off between learning_rate and n_estimators.

- **n_estimators**: The number of boosting stages to perform. Gradient boosting is fairly robust to over-fitting so a large number usually results in better performance.

- **subsample**: The fraction of samples to be used for fitting the individual base learners. If smaller than 1.0 this results in Stochastic Gradient Boosting. subsample interacts with the parameter n_estimators. Choosing subsample < 1.0 leads to a reduction of variance and an increase in bias.
criterion

The function to measure the quality of a split. Supported criteria are "friedman_mse" for the mean squared error with improvement score by Friedman, "mse" for mean squared error, and "mae" for the mean absolute error. The default value of "friedman_mse" is generally the best as it can provide a better approximation in some cases.

min_samples_split

The minimum number of samples required to split an internal node:

min_samples_leaf

The minimum number of samples required to be at a leaf node:

min_weight_fraction_leaf

The minimum weighted fraction of the sum total of weights (of all the input samples) required to be at a leaf node. Samples have equal weight when sample_weight is not provided.

max_depth

Maximum depth of the individual regression estimators. The maximum depth limits the number of nodes in the tree. Tune this parameter for best performance; the best value depends on the interaction of the input variables.

min_impurity_decrease

A node will be split if this split induces a decrease of the impurity greater than or equal to this value.

min_impurity_split

Threshold for early stopping in tree growth. A node will split if its impurity is above the threshold, otherwise it is a leaf.

init

An estimator object that is used to compute the initial predictions. init has to provide fit and predict. If NULL it uses loss.init_estimator.

random_state

If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If NULL, the random number generator is the RandomState instance used by np.random.

max_features

The number of features to consider when looking for the best split:

alpha

The alpha-quantile of the huber loss function and the quantile loss function. Only if loss='huber' or loss='quantile'.

verbose

Enable verbose output. If 1 then it prints progress and performance once in a while (the more trees the lower the frequency). If greater than 1 then it prints progress and performance for every tree.

max_leaf_nodes

Grow trees with max_leaf_nodes in best-first fashion. Best nodes are defined as relative reduction in impurity. If NULL then unlimited number of leaf nodes.

warm_start

When set to TRUE, reuse the solution of the previous call to fit and add more estimators to the ensemble, otherwise, just erase the previous solution.

presort

Whether to presort the data to speed up the finding of best splits in fitting. Auto mode by default will use presorting on dense data and default to normal sorting on sparse data. Setting presort to true on sparse data will raise an error.

colsample_bytree

Subsample ratio of columns when constructing each tree.

num_parallel_tree

Number of trees to grow per round
**tree_method**  The tree construction algorithm used in XGBoost Distributed and external memory version only support approximate algorithm. Choices: ‘auto’, ‘exact’, ‘approx’, ‘hist’, ‘gpu_exact’, ‘gpu_hist’ ‘auto’: Use heuristic to choose faster one. - For small to medium dataset, exact greedy will be used. - For very large dataset, approximate algorithm will be chosen. - Because old behavior is always use exact greedy in single machine, - user will get a message when approximate algorithm is chosen to notify this choice. ‘exact’: Exact greedy algorithm. ‘approx’: Approximate greedy algorithm using sketching and histogram. ‘hist’: Fast histogram optimized approximate greedy algorithm. It uses some performance improvements such as bins caching. ‘gpu_exact’: GPU implementation of exact algorithm. ‘gpu_hist’: GPU implementation of hist algorithm.

**n_gpus**  Number of gpu’s to use in GradientBoostingRegressor solver. Default is -1.

**predictor**  The type of predictor algorithm to use. Provides the same results but allows the use of GPU or CPU. - `cpu_predictor`: Multicore CPU prediction algorithm. - `gpu_predictor`: Prediction using GPU. Default for `gpu_exact` and `gpu_hist` tree method.

**objective**  Specify the learning task and the corresponding learning objective or a custom objective function to be used. Note: A custom objective function can be provided for the objective parameter. In this case, it should have the signature `objective(y_true, y_pred) -> grad, hess`:

**booster**  Specify which booster to use: gbtree, gblinear or dart.

**n_jobs**  Number of parallel threads used to run xgboost.

**gamma**  Minimum loss reduction required to make a further partition on a leaf node of the tree.

**min_child_weight**  Minimum sum of instance weight(hessian) needed in a child.

**max_delta_step**  Maximum delta step we allow each tree’s weight estimation to be.

**colsample_bylevel**  Subsample ratio of columns for each split, in each level.

**reg_alpha**  L1 regularization term on weights

**reg_lambda**  L2 regularization term on weights

**scale_pos_weight**  Balancing of positive and negative weights.

**base_score**  The initial prediction score of all instances, global bias.

**missing**  Value in the data which needs to be present as a missing value. If NULL, defaults to np.nan.

**backend**  Which backend to use. Options are ’auto’, ’sklearn’, ’h2o4gpu’. Saves as attribute for actual backend used.

...  Other parameters for XGBoost object. Full documentation of parameters can be found here: https://github.com/dmlc/xgboost/blob/master/doc/parameter.md
h2o4gpu.kmeans  

K-means Clustering

Description

K-means Clustering

Usage

h2o4gpu.kmeans(n_clusters = 8L, init = "k-means++", n_init = 1L, max_iter = 300L, tol = 1e-04, precompute_distances = "auto", verbose = 0L, random_state = NULL, copy_x = TRUE, n_jobs = 1L, algorithm = "auto", gpu_id = 0L, n_gpus = -1L, do_checks = 1L, backend = "h2o4gpu")

Arguments

n_clusters  The number of clusters to form as well as the number of centroids to generate.

init  Method for initialization, defaults to 'random': 'k-means++': selects initial cluster centers for k-mean clustering in a smart way to speed up convergence. Not supported yet - if chosen we will use SKLearn’s methods. 'random': choose k observations (rows) at random from data for the initial centroids. If an ndarray is passed, it should be of shape (n_clusters, n_features) and gives the initial centers. Not supported yet - if chosen we will use SKLearn’s methods.

n_init  Number of time the k-means algorithm will be run with different centroid seeds. The final results will be the best output of n_init consecutive runs in terms of inertia. Not supported yet - always runs 1.

max_iter  Maximum number of iterations of the algorithm.

tol  Relative tolerance to declare convergence.

precompute_distances  Precompute distances (faster but takes more memory). 'auto': do not precompute distances if n_samples * n_clusters > 12 million. This corresponds to about 100MB overhead per job using double precision. TRUE: always precompute distances FALSE: never precompute distances Not supported yet - always uses auto if running h2o4gpu version.

verbose  Logger verbosity level.

random_state  random_state for RandomState. Must be convertible to 32 bit unsigned integers.

copy_x  When pre-computing distances it is more numerically accurate to center the data first. If copy_x is TRUE, then the original data is not modified. If FALSE, the original data is modified, and put back before the function returns, but small numerical differences may be introduced by subtracting and then adding the data mean. Not supported yet - always uses TRUE if running h2o4gpu version.
The number of jobs to use for the computation. This works by computing each of the n_init runs in parallel. If -1 all CPUs are used. If 1 is given, no parallel computing code is used at all, which is useful for debugging. For n_jobs below -1, (n_cpus + 1 + n_jobs) are used. Thus for n_jobs = -2, all CPUs but one are used. Not supported yet - CPU backend not yet implemented.

K-means algorithm to use. The classical EM-style algorithm is "full". The "elkan" variation is more efficient by using the triangle inequality, but currently doesn’t support sparse data. "auto" chooses "elkan" for dense data and "full" for sparse data. Not supported yet - always uses full if running h2o4gpu version.

ID of the GPU on which the algorithm should run.

Number of GPUs on which the algorithm should run. < 0 means all possible GPUs on the machine. 0 means no GPUs, run on CPU.

If set to 0 GPU error check will not be performed.

Which backend to use. Options are 'auto', 'sklearn', 'h2o4gpu'. Saves as attribute for actual backend used.

Principal Component Analysis (PCA)

**Arguments**

- `n_components`: Desired dimensionality of output data
- `copy`: If FALSE, data passed to fit are overwritten and running fit(X).transform(X) will not yield the expected results, use fit_transform(X) instead.
- `whiten`: When TRUE (FALSE by default) the components_ vectors are multiplied by the square root of (n_samples) and divided by the singular values to ensure uncorrelated outputs with unit component-wise variances.
- `svd_solver`: 'auto' is selected by a default policy based on X.shape and n_components: if the input data is larger than 500x500 and the number of components to extract is lower than 80 percent of the smallest dimension of the data, then the more efficient 'randomized' method is enabled. Otherwise the exact full SVD is computed and optionally truncated afterwards. 'full' runs exact full SVD calling the standard LAPACK solver via scipy.linalg.svd and select the components by postprocessing 'arpack' runs SVD truncated to n_components calling ARPACK solver via scipy.sparse.linalg.svds. It requires strictly 0 < n_components < columns. 'randomized' runs randomized SVD by the method of Halko et al.
tol

Tolerance for singular values computed by svd_solver == 'arpack'.

iterated_power

Number of iterations for the power method computed by svd_solver == 'randomized'.

random_state

If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If NULL, the random number generator is the RandomState instance used by np.random. Used when svd_solver == 'arpack' or 'randomized'.

verbose

Verbose or not

backend

Which backend to use. Options are 'auto', 'sklearn', 'h2o4gpu'. Saves as attribute for actual backend used.

gpu_id

ID of the GPU on which the algorithm should run. Only used by h2o4gpu backend.

h2o4gpu.random_forest_classifier

Random Forest Classifier

Description

Random Forest Classifier

Usage

```r
h2o4gpu.random_forest_classifier(n_estimators = 100L, criterion = "gini",
max_depth = 3L, min_samples_split = 2L, min_samples_leaf = 1L,
min_weight_fraction_leaf = 0, max_features = "auto",
max_leaf_nodes = NULL, min_impurity_decrease = 0,
min_impurity_split = NULL, bootstrap = TRUE, oob_score = FALSE,
n_jobs = 1L, random_state = NULL, verbose = 0L, warm_start = FALSE,
class_weight = NULL, subsample = 1, colsample_bytree = 1,
num_parallel_tree = 1L, tree_method = "gpu_hist", n_gpus = -1L,
predictor = "gpu_predictor", backend = "h2o4gpu")
```

Arguments

- **n_estimators**: The number of trees in the forest.
- **criterion**: The function to measure the quality of a split. Supported criteria are "gini" for the Gini impurity and "entropy" for the information gain. Note: this parameter is tree-specific.
- **max_depth**: The maximum depth of the tree. If NULL, then nodes are expanded until all leaves are pure or until all leaves contain less than min_samples_split samples.
- **min_samples_split**: The minimum number of samples required to split an internal node:
- **min_samples_leaf**: The minimum number of samples required to be at a leaf node:
min_weight_fraction_leaf
The minimum weighted fraction of the sum total of weights (of all the input samples) required to be at a leaf node. Samples have equal weight when sample_weight is not provided.

max_features
The number of features to consider when looking for the best split:

max_leaf_nodes
Grow trees with max_leaf_nodes in best-first fashion. Best nodes are defined as relative reduction in impurity. If NULL then unlimited number of leaf nodes.

min_impurity_decrease
A node will be split if this split induces a decrease of the impurity greater than or equal to this value.

min_impurity_split
Threshold for early stopping in tree growth. A node will split if its impurity is above the threshold, otherwise it is a leaf.

bootstrap
Whether bootstrap samples are used when building trees.

oob_score
whether to use out-of-bag samples to estimate the R^2 on unseen data.

n_jobs
The number of jobs to run in parallel for both fit and predict. If -1, then the number of jobs is set to the number of cores.

random_state
If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If NULL, the random number generator is the RandomState instance used by np.random.

verbose
Controls the verbosity of the tree building process.

warm_start
When set to TRUE, reuse the solution of the previous call to fit and add more estimators to the ensemble, otherwise, just fit a whole new forest.

class_weight
"balanced_subsample" or NULL, optional (default=NULL) Weights associated with classes in the form {class_label: weight}. If not given, all classes are supposed to have weight one. For multi-output problems, a list of dicts can be provided in the same order as the columns of y.

subsample
Subsample ratio of the training instance.

colsample_bytree
Subsample ratio of columns when constructing each tree.

num_parallel_tree
Number of trees to grow per round

tree_method
The tree construction algorithm used in XGBoost Distributed and external memory version only support approximate algorithm. Choices: ‘auto’, ‘exact’, ‘approx’, ‘hist’, ‘gpu_exact’, ‘gpu_hist’ ‘auto’: Use heuristic to choose faster one. - For small to medium dataset, exact greedy will be used. - For very large dataset, approximate algorithm will be chosen. - Because old behavior is always use exact greedy in single machine, - user will get a message when approximate algorithm is chosen to notify this choice. ‘exact’: Exact greedy algorithm. ‘approx’: Approximate greedy algorithm using sketching and histogram. ‘hist’: Fast histogram optimized approximate greedy algorithm. It uses some performance improvements such as bins caching. ‘gpu_exact’: GPU implementation of exact algorithm. ‘gpu_hist’: GPU implementation of hist algorithm.

n_gpus
Number of gpu’s to use in RandomForestClassifier solver. Default is -1.
h2o4gpu.random_forest_regressor

Random Forest Regressor

Description

Random Forest Regressor

Usage

```r
h2o4gpu.random_forest_regressor(n_estimators = 100L, criterion = "mse",
max_depth = 3L, min_samples_split = 2L, min_samples_leaf = 1L,
min_weight_fraction_leaf = 0, max_features = "auto",
max_leaf_nodes = NULL, min_impurity_decrease = 0,
min_impurity_split = NULL, bootstrap = TRUE, oob_score = FALSE,
n_jobs = 1L, random_state = NULL, verbose = 0L, warm_start = FALSE,
subsample = 1, colsample_bytree = 1, num_parallel_tree = 1L,
tree_method = "gpu_hist", n_gpus = -1L, predictor = "gpu_predictor",
backend = "h2o4gpu")
```

Arguments

- `n_estimators`: The number of trees in the forest.
- `criterion`: The function to measure the quality of a split. Supported criteria are "mse" for the mean squared error, which is equal to variance reduction as feature selection criterion, and "mae" for the mean absolute error.
- `max_depth`: The maximum depth of the tree. If NULL, then nodes are expanded until all leaves are pure or until all leaves contain less than `min_samples_split` samples.
- `min_samples_split`: The minimum number of samples required to split an internal node:
- `min_samples_leaf`: The minimum number of samples required to be at a leaf node:
- `min_weight_fraction_leaf`: The minimum weighted fraction of the sum total of weights (of all the input samples) required to be at a leaf node. Samples have equal weight when `sample_weight` is not provided.
- `max_features`: The number of features to consider when looking for the best split:
max_leaf_nodes  Grow trees with max_leaf_nodes in best-first fashion. Best nodes are defined as relative reduction in impurity. If NULL, then unlimited number of leaf nodes.

min_impurity_decrease  A node will be split if this split induces a decrease of the impurity greater than or equal to this value.

min_impurity_split  Threshold for early stopping in tree growth. A node will split if its impurity is above the threshold, otherwise it is a leaf.

bootstrap  Whether bootstrap samples are used when building trees.

oob_score  Whether to use out-of-bag samples to estimate the $R^2$ on unseen data.

n_jobs  The number of jobs to run in parallel for both fit and predict. If -1, then the number of jobs is set to the number of cores.

random_state  If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If NULL, the random number generator is the RandomState instance used by np.random.

verbose  Controls the verbosity of the tree building process.

warm_start  When set to TRUE, reuse the solution of the previous call to fit and add more estimators to the ensemble, otherwise, just fit a whole new forest.

subsample  Subsample ratio of the training instance.

colsample_bytree  Subsample ratio of columns when constructing each tree.

num_parallel_tree  Number of trees to grow per round

tree_method  The tree construction algorithm used in XGBoost Distributed and external memory version only support approximate algorithm. Choices: ‘auto’, ‘exact’, ‘approx’, ‘hist’, ‘gpu_exact’, ‘gpu_hist’ ‘auto’: Use heuristic to choose faster one. - For small to medium dataset, exact greedy will be used. - For very large dataset, approximate algorithm will be chosen. - Because old behavior is always use exact greedy in single machine, - user will get a message when approximate algorithm is chosen to notify this choice. ‘exact’: Exact greedy algorithm. ‘approx’: Approximate greedy algorithm using sketching and histogram. ‘hist’: Fast histogram optimized approximate greedy algorithm. It uses some performance improvements such as bins caching. ‘gpu_exact’: GPU implementation of exact algorithm. ‘gpu_hist’: GPU implementation of hist algorithm.

n_gpus  Number of gpu’s to use in RandomForestRegressor solver. Default is -1.

default  The type of predictor algorithm to use. Provides the same results but allows the use of GPU or CPU. - ‘cpu_predictor’: Multicore CPU prediction algorithm. - ‘gpu_predictor’: Prediction using GPU. Default for ‘gpu_exact’ and ‘gpu_hist’ tree method.

backend  Which backend to use. Options are ‘auto’, ‘sklearn’, ‘h2o4gpu’. Saves as attribute for actual backend used.
**h2o4gpu.truncated_svd  Truncated Singular Value Decomposition (TruncatedSVD)**

**Description**

Truncated Singular Value Decomposition (TruncatedSVD)

**Usage**

```r
h2o4gpu.truncated_svd(n_components = 2L, algorithm = "power",
                      n_iter = 100L, random_state = NULL, tol = 1e-05, verbose = FALSE,
                      backend = "h2o4gpu", n_gpus = 1L, gpu_id = 0L)
```

**Arguments**

- `n_components`: Desired dimensionality of output data
- `algorithm`: SVD solver to use. H2O4GPU options: Either "cusolver" (similar to ARPACK) or "power" for the power method. SKlearn options: Either "arpack" for the ARPACK wrapper in SciPy (scipy.sparse.linalg.svds), or "randomized" for the randomized algorithm due to Halko (2009).
- `n_iter`: number of iterations (only relevant for power method) Should be at most 2147483647 due to INT_MAX in C++ backend.
- `random_state`: seed (NULL for auto-generated)
- `tol`: Tolerance for "power" method. Ignored by "cusolver". Should be > 0.0 to ensure convergence. Should be 0.0 to effectively ignore and only base convergence upon n_iter
- `verbose`: Verbose or not
- `backend`: Which backend to use. Options are 'auto', 'sklearn', 'h2o4gpu'. Saves as attribute for actual backend used.
- `n_gpus`: How many gpus to use. If 0, use CPU backup method. Currently SVD only uses 1 GPU, so >1 has no effect compared to 1.
- `gpu_id`: ID of the GPU on which the algorithm should run.

**predict.h2o4gpu_model  Make Predictions using Trained H2O4GPU Estimator**

**Description**

This function makes predictions from new data using a trained H2O4GPU model and returns class predictions for classification and predicted values for regression.
### Usage

```r
## S3 method for class 'h2o4gpu_model'
predict(object, x, type = "raw", ...)
```

### Arguments

- **object**: The h2o4gpu model object
- **x**: The new data where each column represents a different predictor variable to be used in generating predictions.
- **type**: One of "raw" or "prob", indicating the type of output: predicted values or probabilities
- **...**: Additional arguments (unused for now).

### Examples

```r
## Not run:
library(h2o4gpu)

# Setup dataset
x <- iris[1:4]
y <- as.integer(iris$Species) - 1

# Initialize and train the classifier
model <- h2o4gpu.random_forest_classifier() %>% fit(x, y)

# Make predictions
predictions <- model %>% predict(x)

## End(Not run)
```

---

### Description

This function transforms the given new data using a trained H2O4GPU model.

### Usage

```r
## S3 method for class 'h2o4gpu_model'
transform(object, x, ...)
```
Arguments

object The h2o4gpu model object
x The new data where each column represents a different predictor variable to be used in generating predictions.
...
Additional arguments (unused for now).

Examples

## Not run:

```r
library(h2o4gpu)

# Prepare data
iris$Species <- as.integer(iris$Species)  # convert to numeric data

# Randomly sample 80% of the rows for the training set
set.seed(1)
train_idx <- sample(1:nrow(iris), 0.8*nrow(iris))
train <- iris[train_idx, ]
test <- iris[-train_idx, ]

# Train a K-Means model
model_km <- h2o4gpu.kmeans(n_clusters = 3L) %>% fit(train)

# Transform test data
test_dist <- model_km %>% transform(test)

## End(Not run)
```
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