Package 'cuda.ml'

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Description

This package provides a R interface for the RAPIDS cuML library.

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Description

Recursively merge the pair of clusters that minimally increases a given linkage distance.

Usage

```
cuda_ml_agglomerative_clustering(
    x,
    n_clusters = 2L,
    metric = c("euclidean", "l1", "l2", "manhattan", "cosine"),
    connectivity = c("pairwise", "knn"),
    n_neighbors = 15L
)
```

Arguments

x	The input matrix or dataframe. Each data point should be a row and should consist of numeric values only.
n_clusters	The number of clusters to find. Default: 2L.
metric	Metric used for linkage computation. Must be one of "euclidean", "l1", "l2", "manhattan", "cosine". If connectivity is "knn" then only "euclidean" is accepted. Default: "euclidean".
connectivity	The type of connectivity matrix to compute. Must be one of "pairwise", "knn". Default: "pairwise" 'pairwise' will compute the entire fully-connected graph of pairwise distances between each set of points. This is the fastest to compute and can be very fast for smaller datasets but requires $O(n^2)$ space 'knn' will sparsify the fully-connected connectivity matrix to save memory and enable much larger inputs. "n_neighbors" will control the amount of memory used and the graph will be connected automatically in the event "n_neighbors" was not large enough to connect it.
n_neighbors	The number of neighbors to compute when connectivity is "knn". Default: 15L.

Value

A clustering object with the following attributes: "n_clusters": The number of clusters found by the algorithm. "children": The children of each non-leaf node. Values less than nrow(x) correspond to leaves of the tree which are the original samples. children[i + 1][1] and children[i + 1][2] were merged to form node (nrow(x) + i) in the i-th iteration. "labels": cluster label of each data point.

Examples

```
library(cuda.ml)
library(MASS)
library(magrittr)
library(purrr)
set.seed(0L)
gen_pts <- function() {</pre>
  centers <- list(c(1000, 1000), c(-1000, -1000), c(-1000, 1000))
  pts <- centers %>%
    map(~ mvrnorm(50, mu = .x, Sigma = diag(2)))
  rlang::exec(rbind, !!!pts) %>% as.matrix()
}
clust <- cuda_ml_agglomerative_clustering(</pre>
  x = gen_pts(),
  metric = "euclidean",
  n_{clusters} = 3L
)
print(clust$labels)
```

cuda_ml_can_predict_class_probabilities Determine whether a CuML model can predict class probabilities.

Description

Given a trained CuML model, return TRUE if the model is a classifier and is capable of outputting class probabilities as prediction results (e.g., if the model is a KNN or an ensemble classifier), otherwise return FALSE.

Usage

cuda_ml_can_predict_class_probabilities(model)

Arguments

model A trained CuML model.

Value

A logical value indicating whether the model supports outputting class probabilities.

cuda_ml_dbscan Run the DBSCAN clustering algorithm.

Description

Run the DBSCAN (Density-based spatial clustering of applications with noise) clustering algorithm.

Usage

```
cuda_ml_dbscan(
    x,
    min_pts,
    eps,
    cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace")
)
```

Arguments

Х	The input matrix or dataframe. Each data point should be a row and should consist of numeric values only.
min_pts,eps	A point 'p' is a core point if at least 'min_pts' are within distance 'eps' from it.
cuML_log_level	Log level within cuML library functions. Must be one of "off", "critical", "er-
	ror", "warn", "info", "debug", "trace". Default: off.

Value

A list containing the cluster assignments of all data points. A data point not belonging to any cluster (i.e., "noise") will have NA its cluster assignment.

Examples

```
library(cuda.ml)
library(magrittr)
gen_pts <- function() {
   centroids <- list(c(1000, 1000), c(-1000, -1000), c(-1000, 1000))
   pts <- centroids %>%
     purrr::map(~ MASS::mvrnorm(10, mu = .x, Sigma = diag(2)))
   rlang::exec(rbind, !!!pts)
}
```

```
m <- gen_pts()
clusters <- cuda_ml_dbscan(m, min_pts = 5, eps = 3)
print(clusters)</pre>
```

cuda_ml_elastic_net Train a linear model using elastic regression.

Description

Train a linear model with combined L1 and L2 priors as the regularizer.

Usage

```
cuda_ml_elastic_net(x, ...)
## Default S3 method:
cuda_ml_elastic_net(x, ...)
## S3 method for class 'data.frame'
cuda_ml_elastic_net(
 х,
 у,
  alpha = 1,
  11_{ratio} = 0.5,
 max_iter = 1000L,
  tol = 0.001,
  fit_intercept = TRUE,
  normalize_input = FALSE,
  selection = c("cyclic", "random"),
  . . .
)
## S3 method for class 'matrix'
cuda_ml_elastic_net(
 х,
  у,
  alpha = 1,
  l1_ratio = 0.5,
 max_iter = 1000L,
  tol = 0.001,
  fit_intercept = TRUE,
  normalize_input = FALSE,
  selection = c("cyclic", "random"),
  . . .
)
```

```
## S3 method for class 'formula'
cuda_ml_elastic_net(
  formula,
  data,
  alpha = 1,
 l1_ratio = 0.5,
 max_iter = 1000L,
  tol = 0.001,
  fit_intercept = TRUE,
 normalize_input = FALSE,
  selection = c("cyclic", "random"),
  . . .
)
## S3 method for class 'recipe'
cuda_ml_elastic_net(
 х,
  data,
  alpha = 1,
 11_{ratio} = 0.5,
 max_iter = 1000L,
 tol = 0.001,
  fit_intercept = TRUE,
 normalize_input = FALSE,
 selection = c("cyclic", "random"),
  . . .
)
```

х	Depending on the context:
	* Adata frame of predictors. * Amatrix of predictors. * Arecipe specifying a set of preprocessing steps * created from [recipes::recipe()]. * A formula specifying the predictors and the outcome.
	Optional arguments; currently unused.
У	A numeric vector (for regression) or factor (for classification) of desired re- sponses.
alpha	Multiplier of the penalty term (i.e., the result would become and Ordinary Least Square model if alpha were set to 0). Default: 1. For numerical reasons, running elastic regression with alpha set to 0 is not advised. For the alpha-equalsto-0 scenario, one should use cuda_ml_ols to train an OLS model instead. Default: 1.
l1_ratio	The ElasticNet mixing parameter, with $0 \le 11_{ratio} \le 1$. For $11_{ratio} = 0$ the penalty is an L2 penalty. For $11_{ratio} = 1$ it is an L1 penalty. For $0 < 11_{ratio} < 1$, the penalty is a combination of L1 and L2. The penalty term is computed using the following formula: penalty = alpha * $11_{ratio} * w _1 + 0.5 *$ alpha * $(1 - 11_{ratio}) * w ^2_2$ where $ w _1$ is the L1 norm of the coefficients, and $ w _2$ is the L2 norm of the coefficients.

max_iter	The maximum number of coordinate descent iterations. Default: 1000L.	
tol	Stop the coordinate descent when the duality gap is below this threshold. Default: 1e-3.	
fit_intercept	If TRUE, then the model tries to correct for the global mean of the response variable. If FALSE, then the model expects data to be centered. Default: TRUE.	
normalize_input		
	Ignored when fit_intercept is FALSE. If TRUE, then the predictors will be normalized to have a L2 norm of 1. Default: FALSE.	
selection	If "random", then instead of updating coefficients in cyclic order, a random co- efficient is updated in each iteration. Default: "cyclic".	
formula	A formula specifying the outcome terms on the left-hand side, and the predictor terms on the right-hand side.	
data	When arecipe orformula is used, data is specified as adata frame containing the predictors and (if applicable) the outcome.	

Value

An elastic net regressor that can be used with the 'predict' S3 generic to make predictions on new data points.

Examples

```
library(cuda.ml)
```

```
model <- cuda_ml_elastic_net(</pre>
  formula = mpg ~ ., data = mtcars, alpha = 1e-3, l1_ratio = 0.6
)
cuda_ml_predictions <- predict(model, mtcars)</pre>
# predictions will be comparable to those from a `glmnet` model with `lambda`
# set to 1e-3 and `alpha` set to 0.6
# (in `glmnet`, `lambda` is the weight of the penalty term, and `alpha` is
# the elastic mixing parameter between L1 and L2 penalties.
library(glmnet)
glmnet_model <- glmnet(</pre>
  x = as.matrix(mtcars[names(mtcars) != "mpg"]), y = mtcars$mpg,
  alpha = 0.6, lambda = 1e-3, nlambda = 1, standardize = FALSE
)
glm_predictions <- predict(</pre>
  glmnet_model, as.matrix(mtcars[names(mtcars) != "mpg"]),
  s = 0
)
print(
  all.equal(
    as.numeric(glm_predictions),
```

```
cuda_ml_predictions$.pred,
tolerance = 1e-2
)
)
```

cuda_ml_fil_enabled Determine whether Forest Inference Library (FIL) functionalities are enabled in the current installation of cuda.ml.

Description

CuML Forest Inference Library (FIL) functionalities (see https://github.com/rapidsai/cuml/tree/main/python/cuml/fil#readme will require Treelite C API. If you need FIL to run tree-based model ensemble on GPU, and fil_enabled() returns FALSE, then please consider installing Treelite and then re-installing cuda.ml.

Usage

```
cuda_ml_fil_enabled()
```

Value

A logical value indicating whether the Forest Inference Library (FIL) functionalities are enabled.

Examples

```
if (cuda_ml_fil_enabled()) {
    # run GPU-accelerated Forest Inference Library (FIL) functionalities
} else {
    message(
        "FIL functionalities are disabled in the current installation of ",
        "{cuda.ml}. Please reinstall Treelite C library first, and then re-install",
        " {cuda.ml} to enable FIL."
    )
}
```

cuda_ml_fil_load_model

Load a XGBoost or LightGBM model file.

Description

Load a XGBoost or LightGBM model file using Treelite. The resulting model object can be used to perform high-throughput batch inference on new data points using the GPU acceleration functionality from the CuML Forest Inference Library (FIL).

Usage

```
cuda_ml_fil_load_model(
  filename,
  mode = c("classification", "regression"),
  model_type = c("xgboost", "lightgbm"),
  algo = c("auto", "naive", "tree_reorg", "batch_tree_reorg"),
  threshold = 0.5,
  storage_type = c("auto", "dense", "sparse"),
  threads_per_tree = 1L,
  n_items = 0L,
  blocks_per_sm = 0L
)
```

Arguments

filename	Path to the saved model file.	
mode	Type of task to be performed by the model. Must be one of "classification", "regression".	
model_type	Format of the saved model file. Notice if filename ends with ".json" and model_type is "xgboost", then cuda.ml will assume the model file is in XG-Boost JSON (instead of binary) format. Default: "xgboost".	
algo	Type of the algorithm for inference, must be one of the following "auto": Choose the algorithm automatically. Currently 'batch_tree_reorg' is used for dense storage, and 'naive' for sparse storage "naive": Simple inference using shared memory "tree_reorg": Similar to naive but with trees rearranged to be more coalescing- friendly "batch_tree_reorg": Similar to 'tree_reorg' but predicting multiple rows per thread block. Default: "auto".	
threshold	Class probability threshold for classification. Ignored for regression tasks. Default: 0.5.	
storage_type	In-memory storage format of the FIL model. Must be one of the following "auto": Choose the storage type automatically, - "dense": Create a dense forest, - "sparse": Create a sparse forest. Requires algo to be 'naive' or 'auto'.	
threads_per_tree		
	If >1, then have multiple (neighboring) threads infer on the same tree within a block, which will improve memory bandwith near tree root (but consuming more shared memory). Default: 1L.	
n_items	Number of input samples each thread processes. If 0, then choose (up to 4) that fit into shared memory. Default: 0L.	
blocks_per_sm	Indicates how CuML should determine the number of thread blocks to lauch for the inference kernel 0: Launches the number of blocks proportional to the number of data points>= 1: Attempts to lauch blocks_per_sm blocks for each streaming multiprocessor. This will fail if blocks_per_sm blocks result in more threads than the maximum supported number of threads per GPU. Even if successful, it is not guaranteed that blocks_per_sm blocks will run on an SM concurrently.	

Value

A GPU-accelerated FIL model that can be used with the 'predict' S3 generic to make predictions on new data points.

Examples

```
library(cuda.ml)
library(xgboost)
model_path <- file.path(tempdir(), "xgboost.model")</pre>
model <- xgboost(</pre>
  data = as.matrix(mtcars[names(mtcars) != "mpg"]),
  label = as.matrix(mtcars["mpg"]),
  max.depth = 6,
  eta = 1,
  nthread = 2,
  nrounds = 20,
  objective = "reg:squarederror"
)
xgb.save(model, model_path)
model <- cuda_ml_fil_load_model(</pre>
  model_path,
 mode = "regression",
  model_type = "xgboost"
)
preds <- predict(model, mtcars[names(mtcars) != "mpg"])</pre>
print(preds)
```

 ${\tt cuda_ml_inverse_transform}$

Apply the inverse transformation defined by a trained cuML model.

Description

Given a trained cuML model, apply the inverse transformation defined by that model to an input dataset.

```
cuda_ml_inverse_transform(model, x, ...)
```

model	A model object.
х	The dataset to be transformed.
	Additional model-specific parameters (if any).

Value

The transformed data points.

cuda_ml_is_classifier Determine whether a CuML model is a classifier.

Description

Given a trained CuML model, return TRUE if the model is a classifier, otherwise FALSE (e.g., if the model is a regressor).

Usage

cuda_ml_is_classifier(model)

Arguments

model

A trained CuML model.

Value

A logical value indicating whether the model is a classifier.

cuda_ml_kmeans Run the K means clustering algorithm.

Description

Run the K means clustering algorithm.

```
cuda_ml_kmeans(
    x,
    k,
    max_iters = 300,
    tol = 0,
    init_method = c("kmeans++", "random"),
    seed = 0L,
    cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace")
)
```

cuda_ml_knn

Arguments

x	The input matrix or dataframe. Each data point should be a row and should consist of numeric values only.
k	The number of clusters.
<pre>max_iters</pre>	Maximum number of iterations. Default: 300.
tol	Relative tolerance with regards to inertia to declare convergence. Default: 0 (i.e., do not use inertia-based stopping criterion).
init_method	Method for initializing the centroids. Valid methods include "kmeans++", "ran- dom", or a matrix of k rows, each row specifying the initial value of a centroid. Default: "kmeans++".
seed	Seed to the random number generator. Default: 0.
cuML_log_level	Log level within cuML library functions. Must be one of "off", "critical", "error", "warn", "info", "debug", "trace". Default: off.

Value

A list containing the cluster assignments and the centroid of each cluster. Each centroid will be a column within the 'centroids' matrix.

Examples

```
library(cuda.ml)
kclust <- cuda_ml_kmeans(
    iris[names(iris) != "Species"],
    k = 3, max_iters = 100
)
print(kclust)</pre>
```

cuda_ml_knn Build a KNN model.

Description

Build a k-nearest-model for classification or regression tasks.

```
cuda_ml_knn(x, ...)
## Default S3 method:
cuda_ml_knn(x, ...)
## S3 method for class 'data.frame'
```

```
cuda_ml_knn(
  х,
  у,
  algo = c("brute", "ivfflat", "ivfpq", "ivfsq"),
 metric = c("euclidean", "12", "11", "cityblock", "taxicab", "manhattan",
  "braycurtis", "canberra", "minkowski", "chebyshev", "jensenshannon", "cosine",
    "correlation"),
  p = 2,
 neighbors = 5L,
  . . .
)
## S3 method for class 'matrix'
cuda_ml_knn(
 х,
 у,
  algo = c("brute", "ivfflat", "ivfpq", "ivfsq"),
  metric = c("euclidean", "l2", "l1", "cityblock", "taxicab", "manhattan",
  "braycurtis", "canberra", "minkowski", "chebyshev", "jensenshannon", "cosine",
    "correlation"),
  p = 2,
  neighbors = 5L,
  . . .
)
## S3 method for class 'formula'
cuda_ml_knn(
  formula,
  data,
  algo = c("brute", "ivfflat", "ivfpq", "ivfsq"),
  metric = c("euclidean", "12", "11", "cityblock", "taxicab", "manhattan",
  "braycurtis", "canberra", "minkowski", "chebyshev", "jensenshannon", "cosine",
    "correlation"),
  p = 2,
  neighbors = 5L,
  . . .
)
## S3 method for class 'recipe'
cuda_ml_knn(
  х,
  data,
  algo = c("brute", "ivfflat", "ivfpq", "ivfsq"),
  metric = c("euclidean", "l2", "l1", "cityblock", "taxicab", "manhattan",
  "braycurtis", "canberra", "minkowski", "chebyshev", "jensenshannon", "cosine",
    "correlation"),
  p = 2,
  neighbors = 5L,
```

) ...

Arguments

x	Depending on the context: * Adata frame of predictors. * Amatrix of predictors. * Arecipe specifying a set of preprocessing steps * created from [recipes::recipe()]. * A formula specifying the predictors and the outcome.
	Optional arguments; currently unused.
у	A numeric vector (for regression) or factor (for classification) of desired responses.
algo	The query algorithm to use. Must be one of "brute", "ivfflat", "ivfpq", "ivfsq" or a KNN algorithm specification constructed using the cuda_ml_knn_algo_* family of functions. If the algorithm is specified by one of the cuda_ml_knn_algo_* functions, then values of all required parameters of the algorithm will need to be specified explicitly. If the algorithm is specified by a character vector, then parameters for the algorithm are generated automatically. Descriptions of supported algorithms: - "brute": for brute-force, slow but pro- duces exact results "ivfflat": for inverted file, divide the dataset in partitions and perform search on relevant partitions only "ivfpq": for inverted file and product quantization (vectors are divided into sub-vectors, and each sub-vector is encoded using intermediary k-means clusterings to provide partial informa- tion) "ivfsq": for inverted file and scalar quantization (vectors components are quantized into reduced binary representation allowing faster distances calcula- tions). Default: "brute".
metric	Distance metric to use. Must be one of "euclidean", "12", "11", "cityblock", "taxi- cab", "manhattan", "braycurtis", "canberra", "minkowski", "lp", "chebyshev", "linf", "jensenshannon", "cosine", "correlation". Default: "euclidean".
р	Parameter for the Minkowski metric. If $p = 1$, then the metric is equivalent to manhattan distance (11). If $p = 2$, the metric is equivalent to euclidean distance (12).
neighbors	Number of nearest neighbors to query. Default: 5L.
formula	A formula specifying the outcome terms on the left-hand side, and the predictor terms on the right-hand side.
data	When a <u></u> recipe or <u></u> formula is used, data is specified as a <u></u> data frame containing the predictors and (if applicable) the outcome.

Value

A KNN model that can be used with the 'predict' S3 generic to make predictions on new data points. The model object contains the following: - "knn_index": a GPU pointer to the KNN index. - "algo": enum value of the algorithm being used for the KNN query. - "metric": enum value of the distance metric used in KNN computations. - "p": parameter for the Minkowski metric. - "n_samples": number of input data points. - "n_dims": dimension of each input data point.

Examples

```
library(cuda.ml)
library(MASS)
library(magrittr)
library(purrr)
set.seed(0L)
centers <- list(c(3, 3), c(-3, -3), c(-3, 3))
gen_pts <- function(cluster_sz) {</pre>
  pts <- centers %>%
    map(~ mvrnorm(cluster_sz, mu = .x, Sigma = diag(2)))
  rlang::exec(rbind, !!!pts) %>% as.matrix()
}
gen_labels <- function(cluster_sz) {</pre>
  seq_along(centers) %>%
    sapply(function(x) rep(x, cluster_sz)) %>%
    factor()
}
sample_cluster_sz <- 1000</pre>
sample_pts <- cbind(</pre>
  gen_pts(sample_cluster_sz) %>% as.data.frame(),
  label = gen_labels(sample_cluster_sz)
)
model <- cuda_ml_knn(label ~ ., sample_pts, algo = "ivfflat", metric = "euclidean")</pre>
test_cluster_sz <- 10</pre>
test_pts <- gen_pts(test_cluster_sz) %>% as.data.frame()
predictions <- predict(model, test_pts)</pre>
print(predictions, n = 30)
```

cuda_ml_knn_algo_ivfflat

Build a specification for the "ivfflat" KNN query algorithm.

Description

Build a specification of the flat-inverted-file KNN query algorithm, with all required parameters specified explicitly.

Usage

cuda_ml_knn_algo_ivfflat(nlist, nprobe)

nlist	Number of cells to partition dataset into.
nprobe	At query time, the number of cells used for approximate nearest neighbor search.

Value

An object encapsulating all required parameters of the "ivfflat" KNN query algorithm.

cuda_ml_knn_algo_ivfpq

Build a specification for the "ivfpq" KNN query algorithm.

Description

Build a specification of the inverted-file-product-quantization KNN query algorithm, with all required parameters specified explicitly.

Usage

```
cuda_ml_knn_algo_ivfpq(
   nlist,
   nprobe,
   m,
   n_bits,
   use_precomputed_tables = FALSE
)
```

Arguments

nlist	Number of cells to partition dataset into.	
nprobe	At query time, the number of cells used for approximate nearest neighbor search.	
m	Number of subquantizers.	
n_bits	Bits allocated per subquantizer.	
use_precomputed_tables		
	Whether to use precomputed tables.	

Value

An object encapsulating all required parameters of the "ivfpq" KNN query algorithm.

```
cuda_ml_knn_algo_ivfsq
```

Build a specification for the "ivfsq" KNN query algorithm.

Description

Build a specification of the inverted-file-scalar-quantization KNN query algorithm, with all required parameters specified explicitly.

Usage

```
cuda_ml_knn_algo_ivfsq(
    nlist,
    nprobe,
    qtype = c("QT_8bit", "QT_4bit", "QT_8bit_uniform", "QT_4bit_uniform", "QT_fp16",
        "QT_8bit_direct", "QT_6bit"),
    encode_residual = FALSE
)
```

Arguments

nlist	Number of cells to partition dataset into.	
nprobe	At query time, the number of cells used for approximate nearest neighbor search.	
qtype	Quantizer type. Must be one of "QT_8bit", "QT_4bit", "QT_8bit_uniform", "QT_4bit_uniform", "QT_fp16", "QT_8bit_direct", "QT_6bit".	
encode_residual		
	Whether to encode residuals.	

Value

An object encapsulating all required parameters of the "ivfsq" KNN query algorithm.

cuda_ml_lasso

Train a linear model using LASSO regression.

Description

Train a linear model using LASSO (Least Absolute Shrinkage and Selection Operator) regression.

```
cuda_ml_lasso
```

```
cuda_ml_lasso(x, ...)
## Default S3 method:
cuda_ml_lasso(x, ...)
## S3 method for class 'data.frame'
cuda_ml_lasso(
 х,
 у,
  alpha = 1,
 max_iter = 1000L,
  tol = 0.001,
  fit_intercept = TRUE,
  normalize_input = FALSE,
  selection = c("cyclic", "random"),
  . . .
)
## S3 method for class 'matrix'
cuda_ml_lasso(
 х,
 у,
  alpha = 1,
 max_iter = 1000L,
  tol = 0.001,
  fit_intercept = TRUE,
  normalize_input = FALSE,
  selection = c("cyclic", "random"),
  . . .
)
## S3 method for class 'formula'
cuda_ml_lasso(
  formula,
  data,
  alpha = 1,
 max_iter = 1000L,
  tol = 0.001,
  fit_intercept = TRUE,
  normalize_input = FALSE,
  selection = c("cyclic", "random"),
  . . .
)
## S3 method for class 'recipe'
cuda_ml_lasso(
 х,
```

```
data,
  alpha = 1,
  max_iter = 1000L,
  tol = 0.001,
  fit_intercept = TRUE,
  normalize_input = FALSE,
  selection = c("cyclic", "random"),
  ...
)
```

x	Depending on the context:
	* Adata frame of predictors. * Amatrix of predictors. * Arecipe specifying a set of preprocessing steps * created from [recipes::recipe()]. * A
	formula specifying the predictors and the outcome.
	Optional arguments; currently unused.
У	A numeric vector (for regression) or factor (for classification) of desired re- sponses.
alpha	Multiplier of the L1 penalty term (i.e., the result would become and Ordinary Least Square model if alpha were set to 0). Default: 1.
max_iter	The maximum number of coordinate descent iterations. Default: 1000L.
tol	Stop the coordinate descent when the duality gap is below this threshold. Default: 1e-3.
fit_intercept	If TRUE, then the model tries to correct for the global mean of the response variable. If FALSE, then the model expects data to be centered. Default: TRUE.
normalize_inpu	t
	Ignored when fit_intercept is FALSE. If TRUE, then the predictors will be normalized to have a L2 norm of 1. Default: FALSE.
selection	If "random", then instead of updating coefficients in cyclic order, a random co- efficient is updated in each iteration. Default: "cyclic".
formula	A formula specifying the outcome terms on the left-hand side, and the predictor terms on the right-hand side.
data	When arecipe orformula is used, data is specified as adata frame containing the predictors and (if applicable) the outcome.

Value

A LASSO regressor that can be used with the 'predict' S3 generic to make predictions on new data points.

Examples

library(cuda.ml)

```
model <- cuda_ml_lasso(formula = mpg ~ ., data = mtcars, alpha = 1e-3)</pre>
cuda_ml_predictions <- predict(model, mtcars)</pre>
# predictions will be comparable to those from a `glmnet` model with `lambda`
# set to 1e-3 and `alpha` set to 1
# (in `glmnet`, `lambda` is the weight of the penalty term, and `alpha` is
# the elastic mixing parameter between L1 and L2 penalties.
library(glmnet)
glmnet_model <- glmnet(</pre>
  x = as.matrix(mtcars[names(mtcars) != "mpg"]), y = mtcars$mpg,
  alpha = 1, lambda = 1e-3, nlambda = 1, standardize = FALSE
)
glm_predictions <- predict(</pre>
  glmnet_model, as.matrix(mtcars[names(mtcars) != "mpg"]),
  s = 0
)
print(
  all.equal(
    as.numeric(glm_predictions),
    cuda_ml_predictions$.pred,
    tolerance = 1e-2
  )
)
```

cuda_ml_logistic_reg Train a logistic regression model.

Description

Train a logistic regression model using Quasi-Newton (QN) algorithms (i.e., Orthant-Wise Limited Memory Quasi-Newton (OWL-QN) if there is L1 regularization, Limited Memory BFGS (L-BFGS) otherwise).

```
cuda_ml_logistic_reg(x, ...)
## Default S3 method:
cuda_ml_logistic_reg(x, ...)
## S3 method for class 'data.frame'
cuda_ml_logistic_reg(
    x,
    y,
    fit_intercept = TRUE,
```

```
penalty = c("l2", "l1", "elasticnet", "none"),
  tol = 1e-04,
  C = 1,
  class_weight = NULL,
  sample_weight = NULL,
 max_iters = 1000L,
 linesearch_max_iters = 50L,
 l1_ratio = NULL,
  . . .
)
## S3 method for class 'matrix'
cuda_ml_logistic_reg(
  х,
  у,
  fit_intercept = TRUE,
  penalty = c("12", "11", "elasticnet", "none"),
  tol = 1e-04,
 C = 1,
  class_weight = NULL,
  sample_weight = NULL,
 max_iters = 1000L,
  linesearch_max_iters = 50L,
 l1_ratio = NULL,
  . . .
)
## S3 method for class 'formula'
cuda_ml_logistic_reg(
  formula,
  data,
  fit_intercept = TRUE,
  penalty = c("12", "11", "elasticnet", "none"),
  tol = 1e-04,
  C = 1,
  class_weight = NULL,
  sample_weight = NULL,
 max_iters = 1000L,
  linesearch_max_iters = 50L,
  l1_ratio = NULL,
  . . .
)
## S3 method for class 'recipe'
cuda_ml_logistic_reg(
  х,
  data,
  fit_intercept = TRUE,
```

```
penalty = c("l2", "l1", "elasticnet", "none"),
tol = 1e-04,
C = 1,
class_weight = NULL,
sample_weight = NULL,
max_iters = 1000L,
linesearch_max_iters = 50L,
l1_ratio = NULL,
...
```

x	Depending on the context: * Adata frame of predictors. * Amatrix of predictors. * Arecipe specifying a set of preprocessing steps * created from [recipes::recipe()]. * A formula specifying the predictors and the outcome.
	Optional arguments; currently unused.
У	A numeric vector (for regression) or factor (for classification) of desired re- sponses.
fit_intercept	If TRUE, then the model tries to correct for the global mean of the response variable. If FALSE, then the model expects data to be centered. Default: TRUE.
penalty	The penalty type, must be one of "none", "11", "12", "elasticnet". If "none" or "12" is selected, then L-BFGS solver will be used. If "11" is selected, solver OWL-QN will be used. If "elasticnet" is selected, OWL-QN will be used if 11_ratio > 0, otherwise L-BFGS will be used. Default: "12".
tol	Tolerance for stopping criteria. Default: 1e-4.
С	Inverse of regularization strength; must be a positive float. Default: 1.0.
class_weight	If NULL, then each class has equal weight of 1. If class_weight is set to "balanced", then weights will be inversely proportional to class frequencies in the input data. If otherwise, then class_weight must be a named numeric vector of weight values, with names being class labels. If class_weight is not NULL, then each entry in sample_weight will be adjusted by multiplying its original value with the class weight of the corresponding sample's class. Default: NULL.
sample_weight	Array of weights assigned to individual samples. If NULL, then each sample has an equal weight of 1. Default: NULL.
<pre>max_iters linesearch_max</pre>	Maximum number of solver iterations. Default: 1000L. _iters
	Max number of linesearch iterations per outer iteration used in the LBFGS- and OWL- QN solvers. Default: 50L.
l1_ratio	The Elastic-Net mixing parameter, must NULL or be within the range of [0, 1]. Default: NULL.
formula	A formula specifying the outcome terms on the left-hand side, and the predictor terms on the right-hand side.
data	When arecipe orformula is used, data is specified as adata frame containing the predictors and (if applicable) the outcome.

Examples

```
library(cuda.ml)
X <- scale(as.matrix(iris[names(iris) != "Species"]))</pre>
y <- iris$Species</pre>
model <- cuda_ml_logistic_reg(X, y, max_iters = 100)</pre>
predictions <- predict(model, X)</pre>
# NOTE: if we were only performing binary classifications (e.g., by having
# `iris_data <- iris %>% mutate(Species = (Species == "setosa"))`), then the
# above would be conceptually equivalent to the following:
#
# iris_data <- iris %>% mutate(Species = (Species == "setosa"))
# model <- glm(</pre>
   Species ~ ., data = iris_data, family = binomial(link = "logit"),
#
#
    control = glm.control(epsilon = 1e-8, maxit = 100)
#)
#
# predict(model, iris_data, type = "response")
```

cuda_ml_ols Train a OLS model.

Description

Train an Ordinary Least Square (OLS) model for regression tasks.

Usage

```
cuda_ml_ols(x, ...)
## Default S3 method:
cuda_ml_ols(x, ...)
## S3 method for class 'data.frame'
cuda_ml_ols(
    x,
    y,
    method = c("svd", "eig", "qr"),
    fit_intercept = TRUE,
    normalize_input = FALSE,
    ...
)
## S3 method for class 'matrix'
cuda_ml_ols(
    x,
```

```
у,
 method = c("svd", "eig", "qr"),
 fit_intercept = TRUE,
 normalize_input = FALSE,
  • • •
)
## S3 method for class 'formula'
cuda_ml_ols(
 formula,
 data,
 method = c("svd", "eig", "qr"),
 fit_intercept = TRUE,
 normalize_input = FALSE,
  . . .
)
## S3 method for class 'recipe'
cuda_ml_ols(
 х,
 data,
 method = c("svd", "eig", "qr"),
 fit_intercept = TRUE,
 normalize_input = FALSE,
  . . .
)
```

х	Depending on the context:
	* Adata frame of predictors. * Amatrix of predictors. * Arecipe specifying a set of preprocessing steps * created from [recipes::recipe()]. * A formula specifying the predictors and the outcome.
	Optional arguments; currently unused.
У	A numeric vector (for regression) or factor (for classification) of desired responses.
method	Must be one of "svd", "eig", "qr".
	- "svd": compute SVD decomposition using Jacobi iterations "eig": use an eigendecomposition of the covariance matrix "qr": use the QR decomposition algorithm and solve ' $Rx = Q^T y$ '.
	If the number of features is larger than the sample size, then the "svd" algorithm will be force-selected because it is the only algorithm that can support this type of scenario.
	Default: "svd".
fit_intercept	If TRUE, then the model tries to correct for the global mean of the response variable. If FALSE, then the model expects data to be centered. Default: TRUE.

normalize_input	
	Ignored when fit_intercept is FALSE. If TRUE, then the predictors will be normalized to have a L2 norm of 1. Default: FALSE.
	A formula specifying the outcome terms on the left-hand side, and the predictor terms on the right-hand side.
data	When arecipe orformula is used, data is specified as adata frame containing the predictors and (if applicable) the outcome.

Value

A OLS regressor that can be used with the 'predict' S3 generic to make predictions on new data points.

Examples

```
library(cuda.ml)
```

```
model <- cuda_ml_ols(formula = mpg ~ ., data = mtcars, method = "qr")
predictions <- predict(model, mtcars[names(mtcars) != "mpg"])</pre>
```

```
# predictions will be comparable to those from a `stats::lm` model
lm_model <- stats::lm(formula = mpg ~ ., data = mtcars, method = "qr")
lm_predictions <- predict(lm_model, mtcars[names(mtcars) != "mpg"])</pre>
```

```
print(
   all.equal(
      as.numeric(lm_predictions),
      predictions$.pred,
      tolerance = 1e-3
   )
)
```

cuda_ml_pca

Perform principal component analysis.

Description

Compute principal component(s) of the input data. Each feature from the input will be meancentered (but not scaled) before the SVD computation takes place.

```
cuda_ml_pca(
    x,
    n_components = NULL,
    eig_algo = c("dq", "jacobi"),
    tol = 1e-07,
```

```
n_iters = 15L,
whiten = FALSE,
transform_input = TRUE,
cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace")
)
```

x	The input matrix or dataframe. Each data point should be a row and should consist of numeric values only.
n_components	Number of principal component(s) to keep. Default: min(nrow(x), ncol(x)).
eig_algo	Eigen decomposition algorithm to be applied to the covariance matrix. Valid choices are "dq" (divid-and-conquer method for symmetric matrices) and "ja-cobi" (the Jacobi method for symmetric matrices). Default: "dq".
tol	Tolerance for singular values computed by the Jacobi method. Default: 1e-7.
n_iters	Maximum number of iterations for the Jacobi method. Default: 15.
whiten	If TRUE, then de-correlate all components, making each component have unit variance and removing multi-collinearity. Default: FALSE.
transform_input	
	If TRUE, then compute an approximate representation of the input data. Default: TRUE.
<pre>cuML_log_level</pre>	Log level within cuML library functions. Must be one of "off", "critical", "error", "warn", "info", "debug", "trace". Default: off.

Value

A PCA model object with the following attributes: - "components": a matrix of n_components rows containing the top principal components. - "explained_variance": amount of variance within the input data explained by each component. - "explained_variance_ratio": fraction of variance within the input data explained by each component. - "singular_values": singular values (non-negative) corresponding to the top principal components. - "mean": the column wise mean of x which was used to mean-center x first. - "transformed_data": (only present if "transform_input" is set to TRUE) an approximate representation of input data based on principal components. - "pca_params": opaque pointer to PCA parameters which will be used for performing inverse transforms.

The model object can be used as input to the inverse_transform() function to map a representation based on principal components back to the original feature space.

Examples

```
library(cuda.ml)
```

```
iris.pca <- cuda_ml_pca(iris[1:4], n_components = 3)
print(iris.pca)</pre>
```

cuda_ml_rand_forest Train a random forest model.

Description

Train a random forest model for classification or regression tasks.

```
cuda_ml_rand_forest(x, ...)
## Default S3 method:
cuda_ml_rand_forest(x, ...)
## S3 method for class 'data.frame'
cuda_ml_rand_forest(
 х,
 у,
 mtry = NULL,
  trees = NULL,
 min_n = 2L,
  bootstrap = TRUE,
  max_depth = 16L,
 max_leaves = Inf,
 max_predictors_per_note_split = NULL,
  n_bins = 128L,
 min_samples_leaf = 1L,
  split_criterion = NULL,
 min_impurity_decrease = 0,
 max_batch_size = 128L,
  n_streams = 8L,
 cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace"),
  . . .
)
## S3 method for class 'matrix'
cuda_ml_rand_forest(
  х,
 у,
  mtry = NULL,
  trees = NULL,
 min_n = 2L,
  bootstrap = TRUE,
 max_depth = 16L,
 max_leaves = Inf,
 max_predictors_per_note_split = NULL,
  n_bins = 128L,
```

```
min_samples_leaf = 1L,
  split_criterion = NULL,
  min_impurity_decrease = 0,
 max_batch_size = 128L,
  n_streams = 8L,
 cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace"),
)
## S3 method for class 'formula'
cuda_ml_rand_forest(
  formula,
  data,
 mtry = NULL,
  trees = NULL,
  min_n = 2L,
  bootstrap = TRUE,
  max_depth = 16L,
 max_leaves = Inf,
 max_predictors_per_note_split = NULL,
  n_bins = 128L,
  min_samples_leaf = 1L,
  split_criterion = NULL,
 min_impurity_decrease = 0,
 max_batch_size = 128L,
  n_streams = 8L,
 cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace"),
)
## S3 method for class 'recipe'
cuda_ml_rand_forest(
  х,
  data,
 mtry = NULL,
  trees = NULL,
  min_n = 2L,
  bootstrap = TRUE,
  max_depth = 16L,
 max_leaves = Inf,
 max_predictors_per_note_split = NULL,
  n_bins = 128L,
 min_samples_leaf = 1L,
  split_criterion = NULL,
 min_impurity_decrease = 0,
 max_batch_size = 128L,
  n_streams = 8L,
 cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace"),
```

) ...

Arguments

guinents	
x	Depending on the context: * Adata frame of predictors. * Amatrix of predictors. * Arecipe specifying a set of preprocessing steps * created from [recipes::recipe()]. * A formula specifying the predictors and the outcome.
	Optional arguments; currently unused.
У	A numeric vector (for regression) or factor (for classification) of desired responses.
mtry	The number of predictors that will be randomly sampled at each split when cre- ating the tree models. Default: the square root of the total number of predictors.
trees	An integer for the number of trees contained in the ensemble. Default: 100L.
min_n	An integer for the minimum number of data points in a node that are required for the node to be split further. Default: 2L.
bootstrap	Whether to perform bootstrap. If TRUE, each tree in the forest is built on a bootstrapped sample with replacement. If FALSE, the whole dataset is used to build each tree.
max_depth	Maximum tree depth. Default: 16L.
<pre>max_leaves</pre>	Maximum leaf nodes per tree. Soft constraint. Default: Inf (unlimited).
<pre>max_predictors_</pre>	_per_note_split Number of predictor to consider per node split. Default: square root of the total number predictors.
n_bins	Number of bins used by the split algorithm. Default: 128L.
<pre>min_samples_lea</pre>	af
	The minimum number of data points in each leaf node. Default: 1L.
split_criterior	
	The criterion used to split nodes, can be "gini" or "entropy" for classifications, and "mse" or "mae" for regressions. Default: "gini" for classification; "mse" for regression.
<pre>min_impurity_de</pre>	
	Minimum decrease in impurity requried for node to be spilt. Default: 0.
<pre>max_batch_size</pre>	Maximum number of nodes that can be processed in a given batch. Default: 128L.
n_streams	Number of CUDA streams to use for building trees. Default: 8L.
cuML_log_level	Log level within cuML library functions. Must be one of "off", "critical", "error", "warn", "info", "debug", "trace". Default: off.
formula	A formula specifying the outcome terms on the left-hand side, and the predictor terms on the right-hand side.
data	When arecipe orformula is used, data is specified as adata frame containing the predictors and (if applicable) the outcome.

Value

A random forest classifier / regressor object that can be used with the 'predict' S3 generic to make predictions on new data points.

Examples

```
library(cuda.ml)
# Classification
model <- cuda_ml_rand_forest(
   formula = Species ~ .,
   data = iris,
   trees = 100
)
predictions <- predict(model, iris[names(iris) != "Species"])
# Regression
model <- cuda_ml_rand_forest(
   formula = mpg ~ .,
   data = mtcars,
   trees = 100
)
predictions <- predict(model, mtcars[names(mtcars) != "mpg"])</pre>
```

cuda_ml_rand_proj Random projection for dimensionality reduction.

Description

Generate a random projection matrix for dimensionality reduction, and optionally transform input data to a projection in a lower dimension space using the generated random matrix.

```
cuda_ml_rand_proj(
    x,
    n_components = NULL,
    eps = 0.1,
    gaussian_method = TRUE,
    density = NULL,
    transform_input = TRUE,
    seed = 0L
)
```

x	The input matrix or dataframe. Each data point should be a row and should consist of numeric values only.
n_components	Dimensionality of the target projection space. If NULL, then the parameter is deducted using the Johnson-Lindenstrauss lemma, taking into consideration the number of samples and the eps parameter. Default: NULL.
eps	Error tolerance during projection. Default: 0.1.
gaussian_metho	d
	If TRUE, then use the Gaussian random projection method. Otherwise, use the sparse random projection method. See https://en.wikipedia.org/wiki/Random_projection for details. Default: TRUE.
density	Ratio of non-zero component in the random projection matrix. If NULL, then the value is set to the minimum density as recommended by Ping Li et al.: 1 / sqrt(n_features). Default: NULL.
transform_input	
	Whether to project input data onto a lower dimension space using the random matrix. Default: TRUE.
seed	Seed for the pseudorandom number generator. Default: 0L.

Value

A context object containing GPU pointer to a random matrix that can be used as input to the cuda_ml_transform() function. If transform_input is set to TRUE, then the context object will also contain a "transformed_data" attribute containing the lower dimensional projection of the input data.

Examples

```
library(cuda.ml)
library(mlbench)

data(Vehicle)
vehicle_data <- Vehicle[order(Vehicle$Class), which(names(Vehicle) != "Class")]
model <- cuda_ml_rand_proj(vehicle_data, n_components = 4)
set.seed(0L)
print(kmeans(model$transformed_data, centers = 4, iter.max = 1000))</pre>
```

cuda_ml_ridge Train a linear model using ridge regression.

Description

Train a linear model with L2 regularization.

```
cuda_ml_ridge(x, ...)
## Default S3 method:
cuda_ml_ridge(x, ...)
## S3 method for class 'data.frame'
cuda_ml_ridge(
  х,
  у,
  alpha = 1,
  fit_intercept = TRUE,
  normalize_input = FALSE,
  . . .
)
## S3 method for class 'matrix'
cuda_ml_ridge(
  х,
  у,
  alpha = 1,
  fit_intercept = TRUE,
  normalize_input = FALSE,
  . . .
)
## S3 method for class 'formula'
cuda_ml_ridge(
  formula,
  data,
  alpha = 1,
  fit_intercept = TRUE,
  normalize_input = FALSE,
  . . .
)
## S3 method for class 'recipe'
cuda_ml_ridge(
  х,
  data,
  alpha = 1,
  fit_intercept = TRUE,
  normalize_input = FALSE,
  . . .
)
```

х	Depending on the context:
	* Adata frame of predictors. * Amatrix of predictors. * Arecipe specifying a set of preprocessing steps * created from [recipes::recipe()]. * A formula specifying the predictors and the outcome.
	Optional arguments; currently unused.
У	A numeric vector (for regression) or factor (for classification) of desired re- sponses.
alpha	Multiplier of the L2 penalty term (i.e., the result would become and Ordinary Least Square model if alpha were set to 0). Default: 1.
fit_intercept	If TRUE, then the model tries to correct for the global mean of the response variable. If FALSE, then the model expects data to be centered. Default: TRUE.
normalize_input	
	Ignored when fit_intercept is FALSE. If TRUE, then the predictors will be normalized to have a L2 norm of 1. Default: FALSE.
formula	A formula specifying the outcome terms on the left-hand side, and the predictor terms on the right-hand side.
data	When arecipe orformula is used, data is specified as adata frame containing the predictors and (if applicable) the outcome.

Value

A ridge regressor that can be used with the 'predict' S3 generic to make predictions on new data points.

Examples

```
library(cuda.ml)
```

```
model <- cuda_ml_ridge(formula = mpg ~ ., data = mtcars, alpha = 1e-3)
cuda_ml_predictions <- predict(model, mtcars[names(mtcars) != "mpg"])
# predictions will be comparable to those from a `glmnet` model with `lambda`
# set to 2e-3 and `alpha` set to 0
# (in `glmnet`, `lambda` is the weight of the penalty term, and `alpha` is
# the elastic mixing parameter between L1 and L2 penalties.
library(glmnet)
glmnet_model <- glmnet(
    x = as.matrix(mtcars[names(mtcars) != "mpg"]), y = mtcars$mpg,
    alpha = 0, lambda = 2e-3, nlambda = 1, standardize = FALSE
)
glmnet_predictions <- predict(
    glmnet_model, as.matrix(mtcars[names(mtcars) != "mpg"]),
    s = 0</pre>
```

cuda_ml_serialize

```
)
print(
   all.equal(
    as.numeric(glmnet_predictions),
    cuda_ml_predictions$.pred,
    tolerance = 1e-3
   )
)
```

cuda_ml_serialize Serialize a CuML model

Description

Given a CuML model, serialize its state into a connection.

Usage

```
cuda_ml_serialize(model, connection = NULL, ...)
cuda_ml_serialise(model, connection = NULL, ...)
```

Arguments

model	The model object.
connection	An open connection or NULL. If NULL, then the model state is serialized to a raw vector. Default: NULL.
	Additional arguments to base::serialize().

Value

NULL unless connection is NULL, in which case the serialized model state is returned as a raw vector.

See Also

serialize

cuda_ml_sgd

Description

Train a linear model using mini-batch stochastic gradient descent.

```
cuda_ml_sgd(x, ...)
## Default S3 method:
cuda_ml_sgd(x, ...)
## S3 method for class 'data.frame'
cuda_ml_sgd(
 х,
  у,
  fit_intercept = TRUE,
  loss = c("squared_loss", "log", "hinge"),
  penalty = c("none", "l1", "l2", "elasticnet"),
  alpha = 1e-04,
  11_{ratio} = 0.5,
  epochs = 1000L,
  tol = 0.001,
  shuffle = TRUE,
  learning_rate = c("constant", "invscaling", "adaptive"),
  eta0 = 0.001,
  power_t = 0.5,
  batch_size = 32L,
  n_iters_no_change = 5L,
  . . .
)
## S3 method for class 'matrix'
cuda_ml_sgd(
 х,
  у,
  fit_intercept = TRUE,
  loss = c("squared_loss", "log", "hinge"),
  penalty = c("none", "l1", "l2", "elasticnet"),
  alpha = 1e-04,
  l1_ratio = 0.5,
  epochs = 1000L,
  tol = 0.001,
  shuffle = TRUE,
  learning_rate = c("constant", "invscaling", "adaptive"),
```
```
eta0 = 0.001,
  power_t = 0.5,
  batch_size = 32L,
  n_iters_no_change = 5L,
  . . .
)
## S3 method for class 'formula'
cuda_ml_sgd(
  formula,
  data,
  fit_intercept = TRUE,
  loss = c("squared_loss", "log", "hinge"),
  penalty = c("none", "l1", "l2", "elasticnet"),
  alpha = 1e-04,
  11_ratio = 0.5,
  epochs = 1000L,
  tol = 0.001,
  shuffle = TRUE,
  learning_rate = c("constant", "invscaling", "adaptive"),
  eta0 = 0.001,
  power_t = 0.5,
 batch_size = 32L,
  n_iters_no_change = 5L,
  . . .
)
## S3 method for class 'recipe'
cuda_ml_sgd(
  х,
  data,
  fit_intercept = TRUE,
  loss = c("squared_loss", "log", "hinge"),
  penalty = c("none", "l1", "l2", "elasticnet"),
  alpha = 1e-04,
  11_ratio = 0.5,
  epochs = 1000L,
  tol = 0.001,
  shuffle = TRUE,
  learning_rate = c("constant", "invscaling", "adaptive"),
  eta0 = 0.001,
  power_t = 0.5,
  batch_size = 32L,
  n_iters_no_change = 5L,
  . . .
)
```

x	Depending on the context:
	* Adata frame of predictors. * Amatrix of predictors. * Arecipe specifying a set of preprocessing steps * created from [recipes::recipe()]. * A formula specifying the predictors and the outcome.
	Optional arguments; currently unused.
У	A numeric vector (for regression) or factor (for classification) of desired re- sponses.
fit_intercept	If TRUE, then the model tries to correct for the global mean of the response variable. If FALSE, then the model expects data to be centered. Default: TRUE.
loss	Loss function, must be one of "squared_loss", "log", "hinge".
penalty	Type of regularization to perform, must be one of "none", "11", "12", "elasticnet". - "none": no regularization "11": perform regularization based on the L1-norm (LASSO) which tries to minimize the sum of the absolute values of the coeffi- cients "12": perform regularization based on the L2 norm (Ridge) which tries to minimize the sum of the square of the coefficients "elasticnet": perform the Elastic Net regularization which is based on the weighted averable of L1 and L2 norms. Default: "none".
alpha	Multiplier of the penalty term. Default: 1e-4.
l1_ratio	The ElasticNet mixing parameter, with $0 \le 11$ _ratio ≤ 1 . For 11 _ratio $= 0$ the penalty is an L2 penalty. For 11 _ratio $= 1$ it is an L1 penalty. For $0 < 11$ _ratio < 1 , the penalty is a combination of L1 and L2. The penalty term is computed using the following formula: penalty $=$ alpha $* 11$ _ratio $* w _1 + 0.5 *$ alpha $* (1 - 11$ _ratio) $* w ^2_2$ where $ w _1$ is the L1 norm of the coefficients, and $ w _2$ is the L2 norm of the coefficients.
epochs	The number of times the model should iterate through the entire dataset during training. Default: 1000L.
tol	Threshold for stopping training. Training will stop if (loss in current epoch) > (loss in previous epoch) - tol. Default: 1e-3.
shuffle	Whether to shuffles the training data after each epoch. Default: True.
learning_rate	Must be one of "constant", "invscaling", "adaptive".
	- "constant": the learning rate will be kept constant "invscaling": (learning rate) = (initial learning rate) / pow(t, power_t) where t is the number of epochs and power_t is a tunable parameter of this model "adaptive": (learning rate) = (initial learning rate) as long as the training loss keeps decreasing. Each time the last n_iter_no_change consecutive epochs fail to decrease the training loss by tol, the current learning rate is divided by 5. Default: "constant".
eta0	The initial learning rate. Default: 1e-3.
power_t	The exponent used in the invscaling learning rate calculations.
batch_size	The number of samples that will be included in each batch. Default: 32L.
n_iters_no_cha	nge The maximum number of epochs to train if there is no imporvement in the model. Default: 5.

formula	A formula specifying the outcome terms on the left-hand side, and the predictor terms on the right-hand side.
data	When arecipe orformula is used, data is specified as adata frame containing the predictors and (if applicable) the outcome.

Value

A linear model that can be used with the 'predict' S3 generic to make predictions on new data points.

Examples

```
library(cuda.ml)
model <- cuda_ml_sgd(
  mpg ~ ., mtcars,
  batch_size = 4L, epochs = 50000L,
  learning_rate = "adaptive", eta0 = 1e-5,
  penalty = "12", alpha = 1e-5, tol = 1e-6,
  n_iters_no_change = 10L
)
preds <- predict(model, mtcars[names(mtcars) != "mpg"])
print(all.equal(preds$.pred, mtcars$mpg, tolerance = 0.09))</pre>
```

cuda_ml_svm Train a SVM model.

Description

Train a Support Vector Machine model for classification or regression tasks.

```
cuda_ml_svm(x, ...)
## Default S3 method:
cuda_ml_svm(x, ...)
## S3 method for class 'data.frame'
cuda_ml_svm(
    x,
    y,
    cost = 1,
    kernel = c("rbf", "tanh", "polynomial", "linear"),
    gamma = NULL,
    coef0 = 0,
```

```
degree = 3L,
  tol = 0.001,
  max_iter = NULL,
  nochange_steps = 1000L,
  cache_size = 1024,
  epsilon = 0.1,
  sample_weights = NULL,
 cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace"),
)
## S3 method for class 'matrix'
cuda_ml_svm(
  х,
 у,
  cost = 1,
  kernel = c("rbf", "tanh", "polynomial", "linear"),
  gamma = NULL,
  coef0 = 0,
  degree = 3L,
  tol = 0.001,
 max_iter = NULL,
 nochange_steps = 1000L,
  cache_size = 1024,
 epsilon = 0.1,
  sample_weights = NULL,
 cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace"),
  . . .
)
## S3 method for class 'formula'
cuda_ml_svm(
  formula,
  data,
  cost = 1,
  kernel = c("rbf", "tanh", "polynomial", "linear"),
  gamma = NULL,
  coef0 = 0,
  degree = 3L,
  tol = 0.001,
 max_iter = NULL,
 nochange_steps = 1000L,
  cache_size = 1024,
  epsilon = 0.1,
  sample_weights = NULL,
 cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace"),
  . . .
)
```

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```
## S3 method for class 'recipe'
cuda_ml_svm(
 х,
 data,
 cost = 1,
 kernel = c("rbf", "tanh", "polynomial", "linear"),
 gamma = NULL,
 coef0 = 0,
 degree = 3L,
  tol = 0.001,
 max_iter = NULL,
 nochange_steps = 1000L,
 cache_size = 1024,
 epsilon = 0.1,
  sample_weights = NULL,
 cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace"),
  . . .
)
```

х	Depending on the context:
	* Adata frame of predictors. * Amatrix of predictors. * Arecipe specifying a set of preprocessing steps * created from [recipes::recipe()]. * A formula specifying the predictors and the outcome.
	Optional arguments; currently unused.
У	A numeric vector (for regression) or factor (for classification) of desired responses.
cost	A positive number for the cost of predicting a sample within or on the wrong side of the margin. Default: 1.
kernel	Type of the SVM kernel function (must be one of "rbf", "tanh", "polynomial", or "linear"). Default: "rbf".
gamma	The gamma coefficient (only relevant to polynomial, RBF, and tanh kernel func- tions, see explanations below). Default: 1 / (num features).
	The following kernels are implemented: - RBF K(x_1, x_2) = exp(-gamma x_1-x_2 ^2) - TANH K(x_1, x_2) = tanh(gamma <x_1,x_2> + coef0) - POLYNO-MIAL K(x_1, x_2) = (gamma <x_1,x_2> + coef0)^degree - LINEAR K(x_1,x_2) = <x_1,x_2>, where <, > denotes the dot product.</x_1,x_2></x_1,x_2></x_1,x_2>
coef0	The 0th coefficient (only applicable to polynomial and tanh kernel functions, see explanations below). Default: 0.
	The following kernels are implemented: - RBF K(x_1, x_2) = exp(-gamma x_1-x_2 ^2) - TANH K(x_1, x_2) = tanh(gamma <x_1,x_2> + coef0) - POLYNO-MIAL K(x_1, x_2) = (gamma <x_1,x_2> + coef0)^degree - LINEAR K(x_1,x_2) = <x_1,x_2>, where <, > denotes the dot product.</x_1,x_2></x_1,x_2></x_1,x_2>

Degree of the polynomial kernel function (note: not applicable to other kernel types, see explanations below). Default: 3.	
The following kernels are implemented: - RBF K(x_1, x_2) = exp(-gamma x_1-x_2 ^2) - TANH K(x_1, x_2) = tanh(gamma <x_1,x_2> + coef0) - POLYNO-MIAL K(x_1, x_2) = (gamma <x_1,x_2> + coef0)^degree - LINEAR K(x_1,x_2) = <x_1,x_2>, where <, > denotes the dot product.</x_1,x_2></x_1,x_2></x_1,x_2>	
Tolerance to stop fitting. Default: 1e-3.	
Maximum number of outer iterations in SmoSolver. Default: 100 * (num samples).	
Number of steps with no change w.r.t convergence. Default: 1000.	
Size of kernel cache (MiB) in device memory. Default: 1024.	
Espsilon parameter of the epsilon-SVR model. There is no penalty for points that are predicted within the epsilon-tube around the target values. Please note this parameter is only relevant for regression tasks. Default: 0.1.	
Optional weight assigned to each input data point.	
Log level within cuML library functions. Must be one of "off", "critical", "error", "warn", "info", "debug", "trace". Default: off.	
A formula specifying the outcome terms on the left-hand side, and the predictor terms on the right-hand side.	
When arecipe orformula is used, data is specified as adata frame containing the predictors and (if applicable) the outcome.	

Value

A SVM classifier / regressor object that can be used with the 'predict' S3 generic to make predictions on new data points.

Examples

```
library(cuda.ml)
# Classification
model <- cuda_ml_svm(
  formula = Species ~ .,
  data = iris,
   kernel = "rbf"
)
predictions <- predict(model, iris[names(iris) != "Species"])
# Regression
model <- cuda_ml_svm(
  formula = mpg ~ .,
  data = mtcars,
   kernel = "rbf"</pre>
```

```
)
predictions <- predict(model, mtcars)</pre>
```

cuda_ml_transform *Transform data using a trained cuML model.*

Description

Given a trained cuML model, transform an input dataset using that model.

Usage

```
cuda_ml_transform(model, x, ...)
```

Arguments

model	A model object.
x	The dataset to be transformed.
	Additional model-specific parameters (if any).

Value

The transformed data points.

	cuda_ml_tsne	t-distributed Stochastic Neighbor Embedding.
--	--------------	--

Description

t-distributed Stochastic Neighbor Embedding (TSNE) for visualizing high- dimensional data.

```
cuda_ml_tsne(
    x,
    n_components = 2L,
    n_neighbors = ceiling(3 * perplexity),
    method = c("barnes_hut", "fft", "exact"),
    angle = 0.5,
    n_iter = 1000L,
    learning_rate = 200,
    learning_rate_method = c("adaptive", "none"),
    perplexity = 30,
    perplexity_max_iter = 100L,
```

```
perplexity_tol = 1e-05,
early_exaggeration = 12,
late_exaggeration_iter = 250L,
min_grad_norm = 1e-07,
pre_momentum = 0.5,
post_momentum = 0.8,
square_distances = TRUE,
seed = NULL,
cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace")
)
```

x	The input matrix or dataframe. Each data point should be a row and should consist of numeric values only.	
n_components	Dimension of the embedded space.	
n_neighbors	The number of datapoints to use in the attractive forces. Default: ceiling(3 * perplexity).	
method	T-SNE method, must be one of "barnes_hut", "fft", "exact". The "exact" method will be more accurate but slower. Both "barnes_hut" and "fft" methods are fast approximations.	
angle	Valid values are between 0.0 and 1.0, which trade off speed and accuracy, respectively. Generally, these values are set between 0.2 and 0.8. (Barnes-Hut only.)	
n_iter	Maximum number of iterations for the optimization. Should be at least 250. Default: 1000L.	
learning_rate	Learning rate of the t-SNE algorithm, usually between (10, 1000). If the learning rate is too high, then t-SNE result could look like a cloud / ball of points.	
learning_rate_method		
	Must be one of "adaptive", "none". If "adaptive", then learning rate, early exaggeration, and perplexity are automatically tuned based on input size. Default: "adaptive".	
perplexity	The target value of the conditional distribution's perplexity (see https://en.wikipedia.org/wiki/T-distributed_stochastic_neighbor_embedding for details).	
perplexity_max_iter		
	The number of epochs the best Gaussian bands are found for. Default: 100L.	
perplexity_tol	Stop optimizing the Gaussian bands when the conditional distribution's perplex- ity is within this desired tolerance compared to its taget value. Default: 1e-5.	
early_exaggeration		
	Controls the space between clusters. Not critical to tune this. Default: 12.0.	
late_exaggeration		
	Controls the space between clusters. It may be beneficial to increase this slightly to improve cluster separation. This will be applied after 'exaggeration_iter' iterations (FFT only).	

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cuda_ml_tsvd

exaggeration_iter	
	Number of exaggeration iterations. Default: 250L.
min_grad_norm	If the gradient norm is below this threshold, the optimization will be stopped. Default: 1e-7.
pre_momentum	During the exaggeration iteration, more forcefully apply gradients. Default: 0.5.
post_momentum	During the late phases, less forcefully apply gradients. Default: 0.8.
square_distances	
	Whether TSNE should square the distance values.
seed	Seed to the psuedorandom number generator. Setting this can make repeated runs look more similar. Note, however, that this highly parallelized t-SNE implementation is not completely deterministic between runs, even with the same seed being used for each run. Default: NULL.
cuML_log_level	Log level within cuML library functions. Must be one of "off", "critical", "error", "warn", "info", "debug", "trace". Default: off.

Value

A matrix containing the embedding of the input data in a low- dimensional space, with each row representing an embedded data point.

Examples

```
library(cuda.ml)
embedding <- cuda_ml_tsne(iris[1:4], method = "exact")
set.seed(0L)
print(kmeans(embedding, centers = 3))</pre>
```

cuda_ml_tsvd Truncated SVD.

Description

Dimensionality reduction using Truncated Singular Value Decomposition.

```
cuda_ml_tsvd(
    x,
    n_components = 2L,
    eig_algo = c("dq", "jacobi"),
    tol = 1e-07,
    n_iters = 15L,
    transform_input = TRUE,
    cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace")
)
```

x	The input matrix or dataframe. Each data point should be a row and should consist of numeric values only.	
n_components	Desired dimensionality of output data. Must be strictly less than $ncol(x)$ (i.e., the number of features in input data). Default: 2.	
eig_algo	Eigen decomposition algorithm to be applied to the covariance matrix. Valid choices are "dq" (divid-and-conquer method for symmetric matrices) and "ja-cobi" (the Jacobi method for symmetric matrices). Default: "dq".	
tol	Tolerance for singular values computed by the Jacobi method. Default: 1e-7.	
n_iters	Maximum number of iterations for the Jacobi method. Default: 15.	
transform_input		
	If TRUE, then compute an approximate representation of the input data. Default: TRUE.	
cuML_log_level	Log level within cuML library functions. Must be one of "off", "critical", "error", "warn", "info", "debug", "trace". Default: off.	

Value

A TSVD model object with the following attributes: - "components": a matrix of n_components rows to be used for dimensionality reduction on new data points. - "explained_variance": (only present if "transform_input" is set to TRUE) amount of variance within the input data explained by each component. - "explained_variance_ratio": (only present if "transform_input" is set to TRUE) fraction of variance within the input data explained by each component. - "singular_values": The singular values corresponding to each component. The singular values are equal to the 2-norms of the n_components variables in the lower-dimensional space. - "tsvd_params": opaque pointer to TSVD parameters which will be used for performing inverse transforms.

Examples

```
library(cuda.ml)
```

```
iris.tsvd <- cuda_ml_tsvd(iris[1:4], n_components = 2)
print(iris.tsvd)</pre>
```

cuda_ml_umap	
--------------	--

Uniform Manifold Approximation and Projection (UMAP) for dimension reduction.

Description

Run the Uniform Manifold Approximation and Projection (UMAP) algorithm to find a low dimensional embedding of the input data that approximates an underlying manifold.

cuda_ml_umap

Usage

```
cuda_ml_umap(
 х,
 y = NULL,
 n_{components} = 2L,
 n_{neighbors} = 15L,
 n_{epochs} = 500L,
 learning_rate = 1,
  init = c("spectral", "random"),
 min_dist = 0.1,
  spread = 1,
  set_op_mix_ratio = 1,
  local_connectivity = 1L,
  repulsion_strength = 1,
  negative_sample_rate = 5L,
  transform_queue_size = 4,
  a = NULL,
  b = NULL,
  target_n_neighbors = n_neighbors,
  target_metric = c("categorical", "euclidean"),
  target_weight = 0.5,
  transform_input = TRUE,
  seed = NULL,
 cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace")
)
```

Arguments

Х	The input matrix or dataframe. Each data point should be a row and should consist of numeric values only.
У	An optional numeric vector of target values for supervised dimension reduction. Default: NULL.
n_components	The dimension of the space to embed into. Default: 2.
n_neighbors	The size of local neighborhood (in terms of number of neighboring sample points) used for manifold approximation. Default: 15.
n_epochs	The number of training epochs to be used in optimizing the low dimensional embedding. Default: 500.
learning_rate	The initial learning rate for the embedding optimization. Default: 1.0.
init	Initialization mode of the low dimensional embedding. Must be one of "spec- tral", "random". Default: "spectral".
min_dist	The effective minimum distance between embedded points. Default: 0.1.
spread	The effective scale of embedded points. In combination with min_dist this determines how clustered/clumped the embedded points are. Default: 1.0.
<pre>set_op_mix_ratio</pre>	
	Interpolate between (fuzzy) union and intersection as the set operation used to combine local fuzzy simplicial sets to obtain a global fuzzy simplicial sets. Both

fuzzy set operations use the product t-norm. The value of this parameter should be between 0.0 and 1.0; a value of 1.0 will use a pure fuzzy union, while 0.0 will use a pure fuzzy intersection. Default: 1.0.

local_connectivity

The local connectivity required - i.e. the number of nearest neighbors that should be assumed to be connected at a local level. Default: 1.

repulsion_strength

Weighting applied to negative samples in low dimensional embedding optimization. Values higher than one will result in greater weight being given to negative samples. Default: 1.0.

negative_sample_rate

The number of negative samples to select per positive sample in the optimization process. Default: 5.

transform_queue_size

For transform operations (embedding new points using a trained model this will control how aggressively to search for nearest neighbors. Default: 4.0.

a, b More specific parameters controlling the embedding. If not set, then these values are set automatically as determined by min_dist and spread. Default: NULL.

target_n_neighbors

The number of nearest neighbors to use to construct the target simplcial set. Default: n_neighbors.

- target_metric The metric for measuring distance between the actual and and the target values (y) if using supervised dimension reduction. Must be one of "categorical", "euclidean". Default: "categorical".
- target_weight Weighting factor between data topology and target topology. A value of 0.0 weights entirely on data, a value of 1.0 weights entirely on target. The default of 0.5 balances the weighting equally between data and target.

transform_input

If TRUE, then compute an approximate representation of the input data. Default: TRUE.

- seed Optional seed for pseudo random number generator. Default: NULL. Setting a PRNG seed will enable consistency of trained embeddings, allowing for reproducible results to 3 digits of precision, but at the expense of potentially slower training and increased memory usage. If the PRNG seed is not set, then the trained embeddings will not be deterministic.
- cuML_log_level Log level within cuML library functions. Must be one of "off", "critical", "error", "warn", "info", "debug", "trace". Default: off.

Value

A UMAP model object that can be used as input to the cuda_ml_transform() function. If transform_input is set to TRUE, then the model object will contain a "transformed_data" attribute containing the lower dimensional embedding of the input data.

cuda_ml_unserialize

Examples

```
library(cuda.ml)
```

```
model <- cuda_ml_umap(
    x = iris[1:4],
    y = iris[[5]],
    n_components = 2,
    n_epochs = 200,
    transform_input = TRUE
)
set.seed(0L)
print(kmeans(model$transformed, iter.max = 100, centers = 3))</pre>
```

cuda_ml_unserialize Unserialize a CuML model state

Description

Unserialize a CuML model state into a CuML model object.

Usage

```
cuda_ml_unserialize(connection, ...)
```

```
cuda_ml_unserialise(connection, ...)
```

Arguments

connection	An open connection or a raw vector.
	Additional arguments to base::unserialize().

Value

A unserialized CuML model.

See Also

unserialize

cuML_major_version

Description

Get the major version of the RAPIDS cuML shared library cuda.ml was linked to.

Usage

```
cuML_major_version()
```

Value

The major version of the RAPIDS cuML shared library cuda.ml was linked to in a character vector, or NA_character_ if cuda.ml was not linked to any version of RAPIDS cuML.

Examples

library(cuda.ml)

print(cuML_major_version())

cuML_minor_version Get the minor version of the RAPIDS cuML shared library cuda.ml was linked to.

Description

Get the minor version of the RAPIDS cuML shared library cuda.ml was linked to.

Usage

cuML_minor_version()

Value

The minor version of the RAPIDS cuML shared library cuda.ml was linked to in a character vector, or NA_character_ if cuda.ml was not linked to any version of RAPIDS cuML.

Examples

library(cuda.ml)

print(cuML_minor_version())

has_cuML

Determine whether cuda.ml was linked to a valid version of the RAPIDS cuML shared library.

Description

Determine whether cuda.ml was linked to a valid version of the RAPIDS cuML shared library.

Usage

has_cuML()

Value

A logical value indicating whether the current installation cuda.ml was linked to a valid version of the RAPIDS cuML shared library.

Examples

```
library(cuda.ml)
if (!has_cuML()) {
  warning(
    "Please install the RAPIDS cuML shared library first, and then re-",
    "install {cuda.ml}."
  )
}
```

predict.cuda_ml_fil Make predictions on new data points.

Description

Make predictions on new data points using a FIL model.

```
## S3 method for class 'cuda_ml_fil'
predict(object, x, output_class_probabilities = FALSE, ...)
```

object	A trained CuML model.
x	A matrix or dataframe containing new data points.
output_class_pr	obabilities
	Whether to output class probabilities. NOTE: setting output_class_probabilities to TRUE is only valid when the model being applied is a classification model and supports class probabilities output. CuML classification models supporting class probabilities include knn, fil, and rand_forest. A warning message will be emitted if output_class_probabilities is set to TRUE or FALSE but the model being applied does not support class probabilities output.
•••	Additional arguments to predict(). Currently unused.

Value

Predictions on new data points.

predict.cuda_ml_knn Make predictions on new data points.

Description

Make predictions on new data points using a CuML KNN model.

Usage

```
## S3 method for class 'cuda_ml_knn'
predict(object, x, output_class_probabilities = NULL, ...)
```

Arguments

object	A trained CuML model.
x	A matrix or dataframe containing new data points.
output_class_pr	obabilities
	Whether to output class probabilities. NOTE: setting output_class_probabilities to TRUE is only valid when the model being applied is a classification model and supports class probabilities output. CuML classification models supporting class probabilities include knn, fil, and rand_forest. A warning message will be emitted if output_class_probabilities is set to TRUE or FALSE but the model being applied does not support class probabilities output.
	Additional arguments to predict(). Currently unused.

Value

predict.cuda_ml_linear_model

Make predictions on new data points.

Description

Make predictions on new data points using a linear model.

Usage

```
## S3 method for class 'cuda_ml_linear_model'
predict(object, x, ...)
```

Arguments

object	A trained CuML model.
х	A matrix or dataframe containing new data points.
	Additional arguments to predict(). Currently unused.

Value

Predictions on new data points.

Description

Make predictions on new data points using a CuML logistic regression model.

Usage

```
## S3 method for class 'cuda_ml_logistic_reg'
predict(object, x, ...)
```

Arguments

object	A trained CuML model.
х	A matrix or dataframe containing new data points.
	Additional arguments to predict(). Currently unused.

Value

predict.cuda_ml_rand_forest

Make predictions on new data points.

Description

Make predictions on new data points using a CuML random forest model.

Usage

```
## S3 method for class 'cuda_ml_rand_forest'
predict(
    object,
    x,
    output_class_probabilities = NULL,
    cuML_log_level = c("off", "critical", "error", "warn", "info", "debug", "trace"),
    ...
)
```

Arguments

object	A trained CuML model.	
x	A matrix or dataframe containing new data points.	
output_class_probabilities		
	Whether to output class probabilities. NOTE: setting output_class_probabilities to TRUE is only valid when the model being applied is a classification model and supports class probabilities output. CuML classification models supporting class probabilities include knn, fil, and rand_forest. A warning message will be emitted if output_class_probabilities is set to TRUE or FALSE but the model being applied does not support class probabilities output.	
cuML_log_level	Log level within cuML library functions. Must be one of "off", "critical", "error", "warn", "info", "debug", "trace". Default: off.	
	Additional arguments to predict(). Currently unused.	

Value

predict.cuda_ml_svm Make predictions on new data points.

Description

Make predictions on new data points using a CuML SVM model.

Usage

```
## S3 method for class 'cuda_ml_svm'
predict(object, x, ...)
```

Arguments

object	A trained CuML model.
х	A matrix or dataframe containing new data points.
	Additional arguments to predict(). Currently unused.

Value

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