XGBtk: an XGBoost Tool Kit for Julia

User manual

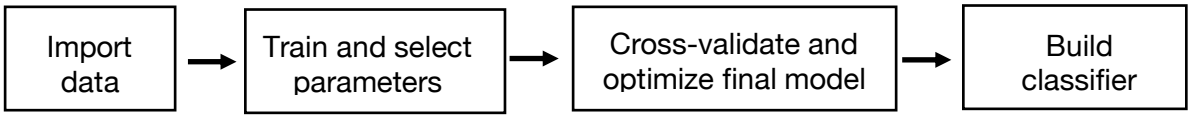
Introduction

XGBoost is a powerful and highly efficient software library for creating gradient boosted trees (1). The library is implemented in C++ with wrappers available for a several high-level computational languages. Driven in large part by high accuracy, speed, and community support, XGBoost is now a leading tool for supervised learning on large heterogeneous data sets.

Implementation of the XGBoost libraries in Python and R are well-developed. The Julia programming language is a fast and flexible language well-suited to machine learning applications. Wrappers implementing XGBoost in the Julia language are available but limited in scope. Simplified, automated analysis for evaluating various boosting models and tuning model parameters is highly desirable. To enable greater use of XGBoost and the XGBoost.jl package, we developed a collection of wrappers and downstream analysis functions and implemented them in the XGB-toolkit (XGBtk). This package builds on the XGBoost.jl package. Currently, XGBtk implements mlogloss for multi-class probabilistic classification. Other classifiers will be added in the future. The current package implements XGB version 1.6 and uses XGBoost.jl version 1.5.2. The package builds on the work of the Julia XGBoost.jl team and the Distributed Deep Machine Learning Community(2, 3).

Overview

The learning method can be described by these simple steps:



Once the binary classifier is created, large datasets with the same variables can be classified very quickly.

XGBtk Functions and Implementation

Setup

Initially, you will need to install the Julia programming language (tested with version 1.7.3) and then add the following registered Julia packages: SparseArrays, DataFrames, CSV, Plots, DelimitedFiles, Printf, LinearAlgebra, StatsBase, Statistics, and Random.

Start the Julia REPL and make sure you do not already have the XGBoost package.

```
] status
```

If XGBoost is listed, then remove it with the command rm(“XGBoost”)

Now add the customized (but not yet registered) XGBtk package.

```
] add https://github.com/ScottWatkins/XGBtk.jl
```

XGBtk contains a slightly modified version of the XGBoost.jl standard library. Add the modified version of the XGBoost package included in the XGBtk package. Add the unregistered modified XGBoost package included in XGBtk.jl

```
] dev /Users/scott/.julia/dev/XGBtk/src/XGBoost/
```

At the Julia prompt, start using the XGBtk package

```
julia> using XGBtk
```

You are now ready perform supervised learning on large datasets. The following tutorial will get you started.

A short tutorial

The mushrooms_train.csv data file in the testdata directory contains 6513 mushroom observations with 125 variables describing each mushroom. The first column contains the known classification: 1 for edible, 0 for non-edible. This data set is also used in the standard XGBoost.jl package for a binary classification example. Instead of the binary classification, we will use a probabilist approach to classify the edibility of the mushrooms. Probabilistic classification can provide granularity needed for accurate data interpretation. For instance, a mushroom classified as 97% edible should be preferable to one classified as 54% edible.

1. **Import the training data**

Data can be imported from csv files. The data should be formatted as a standard table where observations (cases, records) are in rows and variables (features, predictors) are in columns. Each variable should be an ordered set of integers starting at zero or one. The data matrix can contain one or two optional leading columns consisting of the observation ids and the known labels.

The first step is to create a Dmatix variable that contains the data that will be used for training a XGBooster model. The testdata directory contains a training data set of 6513 mushrooms with 126 variables collected on each mushroom. The first column designates whether the mushroom is edible. In this case, there are no sample ids for the mushrooms, and the first column contains the known (truth) labels, 0 for inedible and 1 for edible.

```
dtrain, features = csv2dmat("/path/to/testdata/mushrooms_train.csv",
weight="none", file_has_labels=true, file_has_ids=false);
```

```
Converting mushrooms_train.csv to DMatrix format...
Input features matrix size = (6513, 126)
Input labels are coded as: [0, 1]
```

2. **Obtain XGBoost parameters to accurately classify the data.**

We will now use the data set to build a classifier for edibility. Cross-validation will be used to optimize parameters for the classifier.

First, initialize the following eight (required) parameters with their default values using a dictionary (note: param not params).

```
param = Dict("objective"=>"multi:softprob", "max_depth"=>6,
"eta"=>0.3, "alpha"=>0.0, "gamma"=>0.0, "lambda"=>1.0,
"max_delta_step"=>0, "min_child_weight"=>0)
```

Now, run a simple classifier using the parameters you defined and one round of training

```
predictions, cvdat, cvheader, trainerr, bestcvround =
runCVtrain(dtrain; param=param, num_rounds=1)
```

Look at the summary results. The results show that our classification error was about five percent, too high for classifying our forest bounty.

Change the num_rounds to 10. This action results in a 0.0 error rate, suggesting that these data are very easy to classify using default parameters.

Change the num_rounds to 200. Observe that the training stops at about 140 because there is no improvement in the evaluation metric (mlogloss). This early stopping feature saves computational time when optimizing many parameters.

To illustrate how we might optimize parameters like tree depth (max_depth) and learning rate (eta), add these key word arguments (kwargs) to the command. Specify a range for each parameter in a range array [start, step, stop]. The example below tests three tree depths and two learning rates (eta) for six total runs.

```
predictions, cvdat, cvheader, trainerr, bestcvround =
runCVtrain(dtrain; param=param, num_rounds=200, max_depth=[5,1,7],
eta=[0.2, 0.1, 0.3])
```

Notice that the output summary indicates that the lowest mlogloss occurs at a tree depth of 7 but another run with a 0.0% classification error has a depth of 5. Deeper trees can produce lower evaluation metrics but may over fit the training data.

The predictions for all runs are held in the predictions variable. For example, predictions[1] is a matrix containing the output of the first run and has four columns: the predicted class, the known class, and the probabilities for each class, class zero and class one. The length of the matrix is equal to the number of samples. The width is 2 plus the number of classes.

The bestcvround is a data frame of the parameters and metrics for all runs. Look at the bestcvround to choose the optimal parameter set. For instance, you might choose run number two based on the 0.0% error, low tree depth, and low number of training rounds. The classification results for run two will be found in predictions[2]. You can create a data frame containing the best results for further analysis.

```
df = DataFrame(predictions[2], :auto)
```

```
rename!(df, :x1=>"Predicted", :x2 => "Known", :x3 => "Prob_0", :x4 =>
"Prob_1")
```

3. Build the booster model

Now we will use the training data to create a XGBooster for fast classification of datasets. First, set the best model parameters using a dictionary and the information from the cross-validation training above.

```
my_model_params = Dict("objective"=>"multi:softprob",
"max_depth"=>5,"eta"=>0.2,"alpha"=>0.0, "gamma"=>0.0, "lambda"=>1.0,
"min_child_weight"=>0.0, “max_delta_step”=>0.0)
```

Now create the classifier using the dictionary and the optimized values from the training runs. The Dmatrix from the initial data set (dtrain) and optimized num_rounds are required. Set the number of classes with num_class. Set the evaluation metric(s) using an array.

```
bst = build_model(dtrain, 141; num_class=2, param=my_model_params, metrics=[“mlogloss"])
```

The build_model function automatically saves the booster to disk. This classifier model can be used perform classification of new mushroom data sets that contain the same variables.

4. Classifying new data

4.1 Load the binary XGBoost model for data classification.

```
mybstmodel = load_model(“bst.141.model”)
```

We will now predict the new dataset of ten mushrooms containing the same variables as training data. In this data set we know the the edibility of the ten mushrooms and have added the label as the second column of the infile. Load this small dataset called new_mushrooms.txt from the testdata directory.

```
dmatrix, features, ids = csv2dmat(“/path/to/testdata/new_mushrooms.txt”, weight=“none”, file_has_labels=true, file_has_ids=true);
```

4.2 Predict the edibility of each of the ten mushrooms using the predict function.

```
newpredictions, cm, err = prediction(mybstmodel, dpredict, num_obs=10, obj="multi:softprob", num_class=2, ids=ids);
```

The new predictions matrix variable contains our predictions. The data file had ids and labels and those variables are in the first two columns of the newpredictions matrix. Next is the predicted value. Note that 0 and 1 have been shifted to 1 and 2, that is, 0 is now 1 and 1 is now 2. The next column shows the difference between the best classification and the next best, times 100. Values near 100 indicate very high confidence in the prediction while values near 50 indicate little confidence in the prediction. Each of the following columns contain the classification probabilities. There is one column for each input class and the classes are in in numerical order. In our case, there are two classed (1 and 2).

Example output:

```
"M1"   2.0  2.0  100.0  5.14708e-6  0.999995
"M2"   1.0  1.0  100.0  0.999992    7.56894e-6
"M3"   2.0  2.0  100.0  5.14708e-6  0.999995
```

"M10" 1.0 2.0 100.0 7.47359e-6 0.999992

We see that the prediction for sample M10 does not match the known label despite very high confidence in the prediction. Perhaps this mushroom is very unusual. Alternatively, the data for this mushroom may be mislabeled. Never-the-less, this example serves to illustrate how an independent data set can be used to evaluate and validate the xgb classifier we build from a training data set.

When the prediction() function is run using labeled data, a confusion matrix (cm) is created. See https://en.wikipedia.org/wiki/Confusion_matrix for a detailed discussion of confusion matrices. The confusion matrix can be used to compare the actual labels to the predicted labels for all samples. The table below shows the confusion matrix for our run. For the 10 samples, all known edible mushrooms were predicted correctly. For the non-edible mushrooms four of five mushrooms were correctly predicted. The accuracy rate is 9/10 or 90%.

		Predicted	
		1	**2**
Actual	**1**	4	1
	2	0	5

After validating our model on one or more independent data sets containing known labels, we can now apply the new booster model to data sets containing only unknown samples. The process is the same as using input data containing labels except for setting the file_has_labels=false option when running csv2dmat.

There are many additional features in the XGBtk package. The confusion matrix can be evaluated using the cm_stats() function. For highly asymmetric data, the softprobs_bayes_correction() function may be useful. The importance, frequency, and coverage of the top features can be visualized using the plot_feature_info() function. Although XGBtk is focused on multi-class prediction and analysis, additional functionality for other types of classification is planned for future versions of the toolkit. Explore and have fun.

Package functions

Package functions are listed in alphabetical order. Each function is specified as function(). Each function's return values are also specified. For instance, a function called analyze_data() that processes some data set called my_big data and returns two result objects will be shown as

```
result1, results2 = analyze_data(my_big_data)
```

Each function may have keyword arguments that guide the function's operations. Every keyword has a default setting shown in brackets. Importantly, all inputs into a function must conform to the proper type. The types are indicated in the description of the command and are shown in the example command as input_object::Type. For instance, if a input is shown as num_class::Int, the input to num_class must be an integer like 3, not a floating point number like 3.0. An array input must be specified in the form ["a", "b", "c"] not "a, b, c", etc. Thus, to use the build_model command and all keywords, you would enter:

```
bst = build_model(dtrain, num_rounds=150, num_class=5,
metrics=["mlogloss"], seed=42, param=myparamdictionary)
```

In the example above, the metrics array is specified directly as an array in the command, but the param dictionary is pre-made and passed as a variable whose type is Dict. If in doubt of the type of some variable called x, please check its type using typeof(x). Although knowing and specifying types may seem tedious, it improve the speed of execution and can help to prevent inadvertent errors in analysis workflows.

---

build_model

```
bst = build_model(dtrain::DMatrix, num_rounds::Int, num_class::Int,
metrics::Array, seed::Int, param::Dict)
```

The build_model function builds and saves a booster model to disk.

Keyword options:

num_class	Number of classes	[2]
metrics	Evaluation metrics	[mlogloss]
seed	Random seed values	[0]
param	Dictionary of all model parameters	[]

A parameters dictionary must include all the optimized parameters you want in your model. An example of the param dictionary might look like:

```
myparams = Dict("objective"=>"multi:softprob",  “max_depth"=>16,
“eta"=>0.15, "alpha"=>0.2, "gamma"=>0.0, "lambda"=>1.0,
"min_child_weight"=>1.0, "max_delta_step"=>0.0)
```

The general form for a final model-building command would look like:

```
bst = build_model(dtrain, num_rounds=108, num_class=5, param=myparams,
seed=4917, metrics=["mlogloss", "auc"])
```

---

cm_stats

```
stats_table = cm_stats(cm::Matrix; percent::Bool)
```

Get the typical statistics from a confusion matrix. If the matrix is larger than 2x2, analyze each variable class separately against all others.

Keyword options:

```
percent    Output numerical data as percentages  [false]
```

---

csv2dmat

```
dmatrix, features = csv2dmat(filename::String; weight::String,
file_has_labels::Bool, file_has_ids::Bool, data_only::Bool)
```

The csv2dmat() function converts your comma-separated data table to a sparse Dmatrix for input into XGBoost. This is the starting point for all analyses.

Keyword options:

```
weight                "none"|"equal"|"weightfile.csv"  [none]
data_only              false|true                       [false]
file_has_ids           true|false                       [true]
File_has_labels        true|false                       [true]
```

Discussion: Most real world data is collected in tables with observations in rows and variables in columns. Typically, these tables can be easily formatted as simple csv files. The input for csv2dmat is a table of numerical observations with with sample ids and the truth labels in columns one and two. All additional columns contain variables. Sample ids, if provided, must be in the first column only.

The truth labels may start with zero or one, but they must be sequential integer values, as in 0, 1, …, N, or 1, 2, …, N.

Each column in the csv file must have a heading. The column headings for the data variables are converted into a list of features for further use. The data values are converted into a sparse DMatrix using SpareArrays.

Example input files:

```
LABEL,FEATURE1,FEATURE2
1,0,1
3,1,1
2,0,0

IID,LABEL,FEATURE1,FEATURE2
IID3,1,0,1
SAM7,3,1,1
UNQ9,2,0,0
```

Truth data can be weighted for training. The default is no weight, (ie. weight="none"). Specifying weights="equal" will down-weight each category according to its frequency in the data set. Custom weights can be applied to each label by specifying line-by-line, in a separate text file, the relative weight for each label.

Example weight file for three labels:

```
1,0.10
2,0.40
3,0.50
```

If the input file is a simple numerical matrix without ids or labels, use the data_only=true keyword argument. This type of input matrix cannot contain ids, labels, or headers, and weighting is not allowed. However, this option is very fast and useful for prediction of large datasets of unknowns once a validated model is build.

---

load_model

```
bst = load_model(filename::String)
```

The load_model function loads a saved booster model into the REPL environment for use. The booster model is a binary file created by the build_model() function.

plot_feature_info

```
info, gainplot, freqplot, covplot = plot_feature_info(bst::Booster,
features::Array; n::Int, newnames::Dict)

Keyword options:

n          Number of features to include [1-30]       [10]
newnames   Dictionary to replace long feature name    []
```

Discussion: A function to plot the gain, frequency, and coverage for the most informative features (traits) in a XGbooster model. The features input array is generated by the csv2dmat function or can be read from a disk file using readdlm("filename.txt"). The outputs are plot objects which can be viewed using the display function, for example, display(gainplot).

prediction

```
predictions, cm, miss = prediction(bst::Booster, data::Dmatrix,
obj::String, num_class::Int, num_obs::Int, ntree_limit::Int,
ids::Array)

The prediction() functions predicts a labeled or an unlabeled data set
using a previously made booster model. The input data and booster
model must contain the same features. If the input is labeled, the
function creates a confusion matrix to evaluate the accuracy of the
predictions.


Keyword options:
obj              Objective of the model     [binary:logistic]
num_class        Number of classes in model [2]
num_obs          Total number of samples    [0]
ntree_limit      Max number of trees (DART) [0]
ids              An array of ids, in order  []

Discussion:

The prediction wrapper simplifies predicting and analyzing data sets.
You may want to see how your booster model works on a replication data
set where the labels (truth) are known. First, enter your data as a
labeled DMatrix (see csv2dmat). Specify the objective (obj), number of
classes (num_class), the number of samples (num_obs), and the optional
tree limit (ntree_limit). Inputting the samples ids in an array is
optional but can be very helpful for downstream analyses.
```

Example:

```
predictions, cm, err = prediction(bst, dtrain; obj="multi:softprob",
num_class=5, num_obs=3000, ids=idlist);
```

The results are returned as a matrix in the predictions variable. When known labels are provided in the DMatrix input, a confusion matrix is also produced, and the err variable gives the overall error rate by comparison to the known labels.

Often, you will want to predict only unknowns. First, create the DMatrix. This matrix can contain ids or can be a data-only matrix (see csv2dmat). Load your booster (bst) model with load_model(), and then predict the labels for the unknown data based on the model. For example:

```
predout = prediction(bst, dmat; obj="multi:softprob", num_class=5,
num_obs=14765, ids=ids);
```

Note that the obj must match the objective in the booster model that you loaded. If you built the model with multi:softprob you must use multi:softprob in the prediction. You will need to provide the num_class and total number of observations (lines of data). Ids corresponding to each line in the input data in order may also be passed in as an array.

---

runCVtrain

```
pred, cvdat, cvheader, trainerr, bestcvround = runCVtrain(dtrain,
many_options …)
```

The runCVtrain function is used to find the best parameters for a data set to then build a classifier model. This function runs cross-validation training to optimize parameters. Extensive output data can be plotted to visualize the parameter space. Inputs and their types are shown below.

Options:

num_rounds	number of training rounds (Int)	[100]
nfold	cross-validation value (Int)	[5]
seed	set a seed (Int)	[0]
randseed	force random seed (Bool)	false
subsample	subsample this fraction (Int)	[1]
reps	reps, reruns to estimate error (Int)	[1]
num_class	set the number of label classes (Int)	[2]
metrics	logloss/mlogloss (Array {String})	["mlogloss"]

param	A dictionary of initial parameters (Dict)	[Dict()]
verbosity	verbosity for debugging (Int)	[1]
nthreads	treads to use, 0=all available (Int)	[1]
early_stop	number of non-improving metrics (Int)	[40]
print_every_n	output screen info every n lines (Int)	[1]

Grid options:

These options are iterators with the input format: (start, increment, stop). Use a range to iterate over any combination of these parameters. The increment value must be greater than zero, but if start and stop are the same value no iteration will occur and that parameter is constant for the run. Each range below shows a "range" that runs only the standard default value for that parameter.

max_depth	tree depth range	(6,1,6)
eta	learning rate range	(0.3,0.1,0.3)
alpha	L1 regularization on leaf weights	(0.0,0.1,0.0)
gamma	Regularization of model complexity	(0.0,0.1,0.0)
lambda	L2 regularization on leaf weights	(1.0,0.1,1.0)
max_delta_step	Constrain tree splitting	(0,1,0)
min_child_weight	Min sum of weights to partition	(0,1,0)

Discussion:

This function runs a grid search over several parameters to identify the best combination of parameters as judged by the logloss or mlogloss metric and the cross-validation (CV) error rate. Important: try several simple runs to get into a parameter space that will yield a productive search. Setting all the parameters iterators over a larger range will result in high run times that may be intractable.

A simple example:

Start by initializing the dictionary of parameters, then try a run changing the maximum tree depth. Be sure to include the objective.

```
param = Dict("objective"=>"multi:softprob", "max_depth"=>6,
"eta"=>0.3, "alpha"=>0.0, "gamma"=>0.0, "lambda"=>1.0,
"max_delta_step"=>0, "min_child_weight"=>0)

pred, cvdat, cvheader, trainerr, bestcvround = runCVtrain(dtrain;
num_rounds=100, nfold=5, seed=0, num_class=5, metrics=["mlogloss"],
param=params, max_depth=(5,1,7) )
```

Three runs are performed at tree depths of 5, 6, and 7. Each run has 100 rounds. After the three runs, one run will have the minimum cv-test-mlogloss and one will have a minimum test classification error rate. These two best runs are shown in the summary. Ideally, they will

be the same run. This is result is uncommon, but it represents a very good parameter space. That is, a test minimum mlogloss with the lowest classification error rate. Perform some additional runs to find the lowest value of max_depth where there is little change in mlogloss and classification error.

Now, try varying the learning rate (eta) over a small range that surrounds your optimized value for the max_depth. Generally, start eta below the default (0.3) to keep learning slow and prevent possible over-fitting.

```
pred, cvdat, cvheader, trainerr, bestcvround = runCVtrain(dtrain;
num_rounds=100, nfold=5, seed=0, num_class=5, metrics=["mlogloss"],
param=params, max_depth=(5,1,7), eta=(0.1, 0.1, 0.3))
```

The run above performs three runs for eta (0.1, 0.2, 0.3) each for three max_depth values (5, 6, 7) for a total of nine runs. Again, look at the summary for the overall results. To find out which of the nine runs produced the lowest classification error, type argmin(trainerr) to get the index for the run.

Let say that index value was 5, indicating the fifth run (max_depth=6, eta=0.2). We can now get additional information about that run from the other return values as follows.

bestcvround[5] - shows the run parameters, mlogloss values, and classification error.

cvdat[5] - shows the testing and training values for all metrics

pred[5] - shows the predicted labels, the known labels and the probabilities of each observation and label class for that run.

Continue to optimize the various run parameters to find the best overall parameter space. With a little work, you can get the approximate range for several parameters which can then be iterated to find the best error rate at the minimum mlogloss. Because XGBoost is multi-threaded, multi-core server runs are fast, and it is practical to complete several hundred to a few thousand runs in a day, depending on exact parameters. Use nthreads to utilize more cores/threads. If you have sole access to a server, set ntreads to 0 to utilize all cores.

Once you have an approximate parameter space to explore, execute a more granular grid search. Such a search might look something like:

```
pred, cvdat, cvheader, trainerr, bestcvround = runCVtrain(dtrain,
num_rounds=500, nfold=5, randseed=true, num_class=5,
metrics=["mlogloss","auc"], param=param, reps=1, subsample=0.5,
```

max_depth=(4, 1, 10), eta=(0.10, 0.02, 0.2), alpha=(0.0, 0.2, 1.0), gamma=(0, 1, 3), print_every_n=10);

By default, an early stop is performed when the evaluation metric (mlogloss) fails to improve after multiple iterations. Therefore, setting num_rounds to a high number will not, generally, slow down the grid search. Setting the early_stop option to a high value (e.g. 10000) will prevent early_stopping.

After a "big" run surrounding the best approximate parameters, plot the evaluation metrics for all runs over combinations of 2 or 3 parameters to evaluate the shape of the parameter space. For instance, plot max_depth vs. eta vs. mlogloss in a 3d plot. This type of plot can give you some confidence that a true best parameter space, not just a local minimum, has been reached.

Hints:

1) Think about the parameters that you are testing:

a) learning rate: scales the new feature weights after each step to slow the learning. Lower is more conservative. Range [0 – 1]

b) alpha: Regularization (L1) on leaf weights. Higher is more conservative. Range [0 – inf]

c) lambda: Regularization (L2) on leaf weights. Higher is more conservative. Range [0 – inf]

d) max_delta_step: max step size for a leaf node. Max leaf values ≤ learning rate times max_delta_step. Higher is more conservative. [0 – inf], typically 0–10

e) max_depth: the maximum depth of the tree. Shallow trees are more conservative, run faster, and use less memory than deep trees. Be cautious about using trees with depths > 20. Range [0 – inf]

f) min_child_weight: minimum sum of hessians to keep a child node. Higher is more conservative. [0 – inf]

g) gamma: (min_split_loss) the minimum loss reduction needed to partition a leaf node and higher values are more conservative. Range [0 – inf]

2) Make sure you are running enough rounds that cv-test-mlogloss hits a minimum and is flat or starts to increase. The a default of 100 is

often too low, but there is usually no need to perform excessive rounds.

3) The evaluation metrics will bounce around, so expect a small range for mlogloss and for classification error at any given set of parameters. Don't fixate on small differences, especially early in the optimization process; it wastes time. Setting a seed will allow you reproduce a given run.

4) Using only the minimum classification error as an evaluation metric can lead to over-fitting. The ideal parameter set is the one with the lowest classification error at a mlogloss value that is very near the minimum of the test mlogloss curve. You should also subsample the data to reduce overfitting.

See also: [https://www.kaggle.com/prashant111/a-guide-on-xgboost-hyperparameters-tuning]

---

softprobs_bayes_correction

```
bc = softprobs_bayes_correction(predictions::Matrix)
```

Apply a naive Bayesian correction to the multi:softprob prediction probabilities. Re-predict the original predicted labels. The input is a table in matrix form with the following columns: [truelabels, predicted_labels, mxn_prob_matrix]. The input matrix is numerical and is not labeled. The output is a matrix containing the following columns: [truelabels, predicted_labels, bayes_predicted_labels, bayes_corrected_mxn_prob_matrix].

Bibliography

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2. The Distributed (Deep) Machine Learning Community 2022 [https://github.com/orgs/dmlc].
3. The Julia Community. XGBoost.jl. 2022 [https://github.com/dmlc/XGBoost.jl].