Designing and building the mlpack open-source machine learning library

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Abstract

mlpack is an open-source C++ machine learning library with an emphasis on speed and flexibility. Since its original inception in 2007, it has grown to be a large project implementing a wide variety of machine learning algorithms, from standard techniques such as decision trees and logistic regression to modern techniques such as deep neural networks as well as other recently-published cutting-edge techniques not found in any other library. mlpack is quite fast, with benchmarks showing mlpack outperforming other libraries' implementations of the same methods. mlpack has an active community, with contributors from around the world—including some from PUST. This short paper describes the goals and design of mlpack, discusses how the open-source community functions, and shows an example usage of mlpack for a simple data science problem.

1 Introduction

The broad field of machine learning has seen a huge surge in popularity in the past few decades, with compelling results for problems like image recognition [7], automatic medical diagnostics [14], recommender systems [4], and speech recognition [11]. Loosely speaking, any machine learning algorithm depends on data, and the quality of the algorithm's results can be increased by adding more data [12]. Since mass quantities of data are now so widely available, it is important to enable practitioners to run machine learning algorithms on large datasets. Thus, it is important to provide high-quality implementations of these algorithms.

This reality has motivated us to design, build, and maintain the open-source **mlpack** machine learning library, which focuses on providing high-quality implementations of both typical and cutting-edge machine learning algorithms to machine learning practitioners around the world. The library is free to use under the terms of the BSD open-source license, and accepts contributions from anyone.

mlpack development began in 2007 at the Georgia Institute of Technology, and the first stable release of the library was in 2011 [8]. Since then, the project has grown to have nearly 100 individual contributors from around the world, and at the time of this writing has been downloaded over 50,000 times and used in close to 100 academic papers. The growth and success of mlpack can be attributed in part to its open community and its participation in open-source initiatives such as Google Summer of Code (`https://summerofcode.withgoogle.com/`).

This short document aims to discuss the design and usage of mlpack, as well as how the open-source community functions. Section 2 discusses the design of mlpack, providing an overview of its functionality. Section 3 discusses the open-source community of mlpack and its participation in programs such as Google Summer of Code, and how someone new to the library might get involved and contribute. Then, Section 4 discusses the design and API considerations of mlpack. Section 5 shows a simple example of how mlpack can be used to solve a typical data science problem. Lastly, Section 6 briefly discusses the future planned functionality and directions of mlpack.

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2 Description of mlpack

The mlpack library aims to balance four major goals:

- implement **fast, scalable** machine learning algorithms;
- design an **intuitive, consistent, and simple** API for non-expert users;
- implement a **variety** of machine learning methods; and
- provide **cutting-edge** machine learning algorithms unavailable elsewhere.

In order to provide efficient implementations, mlpack is written in the C++ language, and uses C++ template metaprogramming to optimize mathematical expressions when the program is compiled. In addition, mlpack uses the fast Armadillo linear algebra library as its core [18].

Inside of mlpack, a breadth of machine learning algorithms are available. A basic list is given below; but note that the list is not exhaustive, and to find an up-to-date list one should consult the mlpack website.

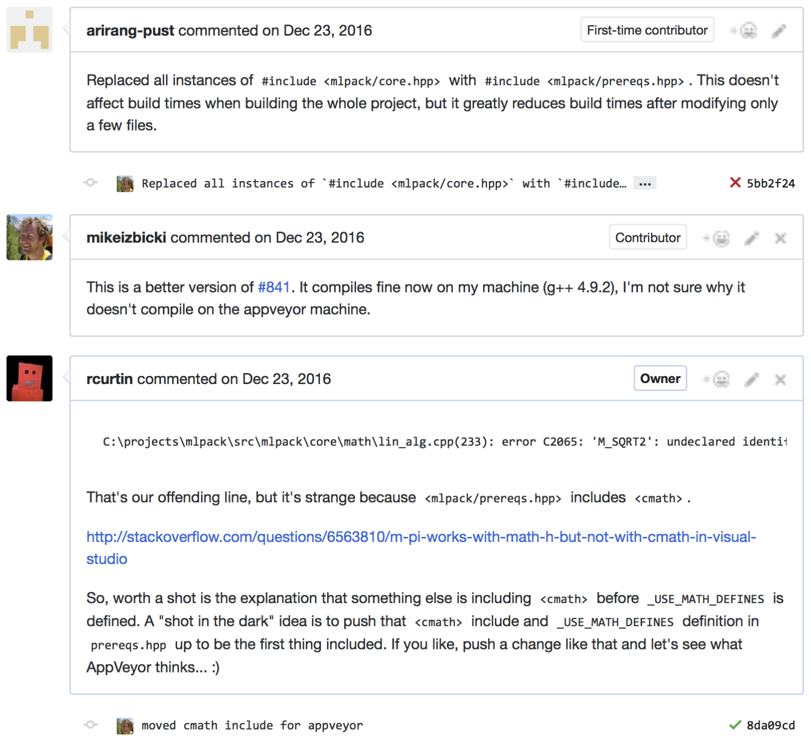
- **Classification**: logistic regression, softmax regression, deep neural networks, AdaBoost, perceptrons, Naive Bayes classifier, decision trees, decision stumps, Hoeffding trees
- **Regression**: linear regression, ridge regression, LARS, LASSO
- **Clustering**: k-means, DBSCAN, minimum spanning tree calculation
- **Data transformations**: PCA, kernel PCA, sparse coding, local coordinate coding, RADICAL, NMF
- **Distance-based tasks**: (approximate and exact) nearest neighbor search, furthest neighbor search, range search, max-kernel search, locality sensitive hashing
- **Optimization algorithms**: L-BFGS, SGD, gradient descent, simulated annealing, AdaGrad, ADAM, RMSprop, AdaDelta, augmented Lagrangian solver
- **Other**: collaborative filtering/recommender systems, data preprocessing tools, neighborhood components analysis, SVD matrix decompositions, density estimation trees

3 Community description

mlpack is an open-source project whose development is primarily conducted on Github (`https://github.com/mlpack/mlpack`) and on IRC (internet relay chat). Github is a centralized open-source development website that allows any user to contribute easily to some open-source software project. The website can be used to do many things—a user can ask for help using mlpack, report a bug inside of mlpack, submit new code, discuss ideas with mlpack maintainers, update or add documentation, or run automatic tests on mlpack code, among other things. Thanks to Github's standard interface and wide adoption inside the open-source community, this means that it is quite simple and straightforward for anyone interested in mlpack to perform any of these tasks.

When a user submits new code to mlpack for inclusion as a *pull request*, the code must be reviewed by mlpack maintainers to ensure that the code meets the mlpack standards. These standards include simple requirements like formatting, and more complex standards like the standardized APIs described in the following section. In addition, any new code must be submitted with tests, so that it can be known that the new code functions properly. Typically the review process will include several comments from maintainers that need to be addressed by the contributor(s). When agreement is reached between the maintainers and the contributors that the code is ready, then the code can be merged into the mlpack codebase. Since the mlpack project is careful to accept only high-quality code, this process can typically take several days to several weeks, depending on the complexity and quality of the original submission. An example of this process can be seen at `https://github.com/mlpack/mlpack/pull/842`. A screenshot of some of the discussion is pictured in Figure 1.

Because the Github pull request interface and process is standardized across all Github projects, it is straightforward for new contributors to get involved with mlpack and start getting their contributions merged into the code. Since the mlpack project moved to Github in the fall of 2014, the number of contributors to the project has grown more rapidly than before.


arirang-pust commented on Dec 23, 2016 First-time contributor

Replaced all instances of `#include <mlpack/core.hpp>` with `#include <mlpack/prereqs.hpp>`. This doesn't affect build times when building the whole project, but it greatly reduces build times after modifying only a few files.

```
Replaced all instances of `#include <mlpack/core.hpp>` with `#include… …    ✕ 5bb2f24
```

mikeizbicki commented on Dec 23, 2016 Contributor

This is a better version of #841. It compiles fine now on my machine (g++ 4.9.2), I'm not sure why it doesn't compile on the appveyor machine.

rcurtin commented on Dec 23, 2016 Owner

```
C:\projects\mlpack\src\mlpack\core\math\lin_alg.cpp(233): error C2065: 'M_SQRT2': undeclared identi
```

That's our offending line, but it's strange because `<mlpack/prereqs.hpp>` includes `<cmath>`.

http://stackoverflow.com/questions/6563810/m-pi-works-with-math-h-but-not-with-cmath-in-visual-studio

So, worth a shot is the explanation that something else is including `<cmath>` before `_USE_MATH_DEFINES` is defined. A "shot in the dark" idea is to push that `<cmath>` include and `_USE_MATH_DEFINES` definition in `prereqs.hpp` up to be the first thing included. If you like, push a change like that and let's see what AppVeyor thinks... :)

```
moved cmath include for appveyor    ✓ 8da09cd
```

Figure 1: Typical pull request discussion for an mlpack contribution.

Another factor contributing to the growth of the project is mlpack's participation in the Google Summer of Code program (`https://summerofcode.withgoogle.com`). The Google Summer of Code program is an open-source initiative led by Google, with the goal of getting more students to participate in the development of open-source software. In Summer of Code, the mlpack library selects a number of promising students for acceptance into the program. These students each prepare a proposal for a project that they will complete over the course of the summer, with a detailed description and timeline. Those students who are selected are paid a stipend and a t-shirt by Google to work full-time on their project over the summer, and usually at the end of the summer their work will be incorporated into the library. Communication during the summer is done usually via real-time IRC or on Github, and the use of real-time chat allows students and mentors to build relationships, which in turn strengthens the community.

Examples of previous improvements include an automatic benchmarking system [10], a collaborative filtering framework [1], implementation of different tree types [17], addition of new deep learning techniques [3], and others. Since 2013, mlpack has mentored 24 students from around the world.

4 Design of mlpack

An important consideration of any library is the interface it implements (the API). If the interface is confusing, then it will be difficult for end users to solve their problems. Therefore, in the design of mlpack we have endeavored to make each piece of the library match a consistent and intuitive interface. This is similar to the efforts of the Python open-source machine learning library `scikit-learn` [6].

The top-level interface to mlpack is its machine learning algorithms, listed earlier in Section 2. Each of these classes of algorithms is typically used to solve a different task. To take an example, for a classification algorithm, given a data point, we wish to select a distinct class that the data point belongs to. An example in the field of malware detection would be to classify a file (which is a data point) as `malicious` or `benign`.

Inside of mlpack, each class of algorithm must implement an identical API. This allows easy combination and substitution of mlpack algorithms: a common requirement in data science tasks is to try multiple different algorithms to solve a single problem. If each of these algorithms implements the same API, then the developer can simply switch the type of algorithm used without needing to adapt their support code.

All classification algorithms inside of mlpack, such as the Naive Bayes classifier or the decision tree, must implement the same interface for two methods: `Train()` and `Classify()`. The `Train()` function takes training data and labels and trains the classifier on the data. The `Classify()` function then can use this trained model to predict classes for the given test points. For instance, the code below could be used to train an mlpack classifier on the matrix `dataset` with labels `labels`, and then predict the class of the test point `(1.3, 2.4, 1.0)`.

```
// Here we will use the DecisionTree class, but we could easily use another
// mlpack classifier.
typedef DecisionTree<> ClassifierType;

// Train the model.
ClassifierType classifier;
classifier.Train(dataset, labels);

// Now predict on the test point.
arma::vec point("1.3, 2.4, 1.0");
const size_t predictedClass = classifier.Classify(point);

std::cout << "Predicted class is " << predictedClass << "." << std::endl;
```

In addition to this top-level interface, lower-level interfaces inside mlpack are also required to implement identical APIs for easy composability. Examples of this include the `TreeType` API, which provides a generic interface for space partitioning trees such as the *kd*-tree [9], the `OptimizerType` API, which provides a simple interface for numerical optimization tasks, and the `KernelType` API, which provides a simple interface for machine learning kernel functions [13].

The description of the mlpack API given here is certainly not comprehensive; we would refer readers to the documentation found at `http://www.mlpack.org/docs.html` for more information.

Another important component of mlpack design is flexibility. To this end, we use a C++ programming paradigm known as *policy-based design* [2]. In short, this means that the behavior of mlpack algorithms is easily controllable by the user, simply by specifying template parameters. For example, the `DualTreeBoruvka` class, which is used to calculate minimum spanning trees [16], accepts a template parameter `MetricType`. Thus, if the user wants to find a minimum spanning tree in a metric space that mlpack does not have support for, they merely need to implement a distance metric class, and then they can use the type `DualTreeBoruvka<MyCustomMetric>` to calculate the minimum spanning tree in the custom metric space. Additionally, because templates are being used, there is no additional overhead, as there would be when providing this type of support through inheritance or in other languages such as Python or C.

5 Example data science application

This section details the usage of mlpack for a simple data science task. In this example, we would like to predict the primary type of tree in a forest based only on cartographic variables such as elevation, slope, azimuth, soil type, and others. The dataset we use for this task is known as the `covertype` dataset [5], and is available on the UCI machine learning dataset repository [15]. The version of mlpack used in this example is mlpack 2.2.3, released on May 24, 2017.

In this example, we will show how we can use mlpack's decision tree to build a classifier for this task, and we will obtain the accuracy of the classifier on a held-out test dataset.

First, we would like to load the dataset and labels. Suppose these are in the files `covertype.csv` and `covertype.labels.csv`, respectively. We will load the dataset into an Armadillo matrix called `dataset`, and we will load the labels into an unsigned Armadillo matrix called `labels`. This can be done with mlpack's `Load()` function, in the code shown below.

```
Load("covertype.csv", dataset);
Load("covertype.labels.csv", labels);
```

Next we need to split the dataset into a training set (only used for the training process) and a test set (which is what we will use to obtain the accuracy of the classifier). We can do this using the `Split()` function, setting aside 20% of the data for the test set:

```
// Split dataset/labels into trainingData/trainingLabels and
// testData/testLabels.  The 'labels' object needs to be cast into an
// arma::Row<size_t> object.
Split(dataset, arma::Row<size_t>(labels.row(0)), trainingData,
    testData, trainingLabels, testLabels, 0.2);
```

Now, we can use the training data and labels to train a decision tree classifier.

```
// Optionally, the constructor can be used to set specific algorithm
// parameters.  We will leave them as the defaults here.  7 is the
// number of classes in the dataset.
DecisionTree<> treeClassifier;
treeClassifier.Train(trainingData, trainingLabels, 7);
```

The training may take some time. Following training, we want to obtain predictions for the test set. We will store the predictions of the decision tree in the variable `predictions`.

```
// Predict the classes of the points in testData and store them in the output
// predictions vector.
arma::Row<size_t> predictions;
treeClassifier.Classify(testData, predictions);
```

Lastly, we would like to calculate the accuracy of each classifier. We can do this by using an Armadillo expression that will sum the number of identical elements in the test labels and the prediction vectors.

```
// Calculate the number of points that the classifier got right.
const size_t correct = arma::accu(predictions == testLabels);

// Now print the accuracy.
const double accuracy = double(correct) / double(testLabels.n_elem);
std::cout << "Decision tree classifier accuracy on test set: "
    << (accuracy * 100.0) << "." << std::endl;
```

Using this code, we can compile the program[1], and when we run it we receive the following output:

```
Decision tree classifier accuracy on test set: 71.0022.
```

So we can see that the decision tree classifier can obtain reasonable accuracy on our data. If we were to tune the parameters of the classifier, we could likely achieve better accuracy. Also, if we desired more predictions for new test points, as in a production machine learning application, we could easily use the `Classify()` method. This simple example, of course, does not discuss all the intricacies of good data science work, but instead presents how mlpack could be used in a simple data science context. Adapting the example to a real-life application would be more complex but straightforward.

6 Conclusion and Future Goals

We have introduced the open-source mlpack C++ machine learning library and discussed its general design philosophy, as well as its open-source development process. However, mlpack is under active development continually, so the library is far from complete or static. New versions are released typically every few months with enhanced functionality, bugfixes, and efficiency improvements. The next major release, mlpack 3.0.0, is currently planned for late in 2017 with the following major functionality improvements and changes:

- Bindings to Python and other languages
- Addition of random forests

[1]Full sources and compilation instructions given in the appendix.

- Addition of deep neural network toolkit
- Addition of several optimizers and changes to optimizer API
- Cross-validation and hyper-parameter tuning framework

This list, of course, is non-comprehensive; for a more clear list of goals, the mlpack website (`http://www.mlpack.org/`) and the Github website (`https://github.com/mlpack/mlpack`) have more details both about the future goals of the project and the current status of the project.

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A Data science example code

The full code for the example in Section 5 is given below.

```
/**
 * Build a decision tree classifier on the covertype dataset, then print the
 * accuracy of the classifier on the held-out testing data.
 */
#include <mlpack/core.hpp>
#include <mlpack/core/data/split_data.hpp>
#include <mlpack/core/data/load_impl.hpp>
#include <mlpack/methods/decision_tree/decision_tree.hpp>

using namespace mlpack;
using namespace mlpack::data;
using namespace mlpack::tree;

int main()
{
  // Load the dataset.
  arma::mat dataset;
  arma::Mat<size_t> labels;

  Load("covertype.csv", dataset);
  Load("covertype.labels.csv", labels);

  // Split into training and test dataset.
  arma::mat trainingData, testData;
  arma::Row<size_t> trainingLabels, testLabels;

  // Split dataset/labels into trainingData/trainingLabels and
  // testData/testLabels.
  Split(dataset, arma::Row<size_t>(labels.row(0)), trainingData, testData,
      trainingLabels, testLabels, 0.2);

  // Optionally, the constructor can be used to set specific algorithm
  // parameters.  We will leave them as the defaults here.  7 is the
  // number of classes in the dataset.
  DecisionTree<> treeClassifier;
  treeClassifier.Train(trainingData, trainingLabels, 7);

  // Predict the classes of the points in testData and store them in the output
  // predictions vector.
  arma::Row<size_t> predictions;
  treeClassifier.Classify(testData, predictions);

  // Calculate the number of points that the classifier got right.
  const size_t correct = arma::accu(predictions == testLabels);

  // Now print the accuracy.
  const double accuracy = double(correct) / double(testLabels.n_elem);
  std::cout << "Decision tree classifier accuracy on test set: "
      << (accuracy * 100.0) << "." << std::endl;
}
```

Assuming that mlpack is installed on the system, then this code (`code.cpp`) can be compiled with `g++` or another compiler:

```
$ g++ -o code code.cpp -std=c++11 -lmlpack -larmadillo
```

Typically, installing mlpack is easy, especially if a Linux distribution such as Ubuntu, Debian, or Fedora is being used. Installing mlpack on an Ubuntu system can be done with the following command:

```
$ sudo apt-get install libmlpack-dev
```