

mlpack: or, How I Learned To Stop Worrying and Love C++

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May 3, 2018



Introduction

Why are we here?

Introduction

Why are we here?

speed

Introduction

Why are we here?

speed | programming languages

Introduction

Why are we here?

speed | programming languages | machine learning

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C++

Introduction

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C++ | mlpack

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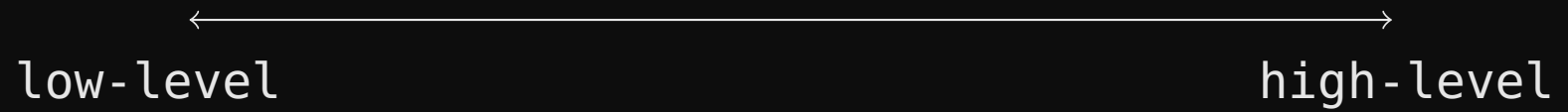
C++ | mlpack | fast



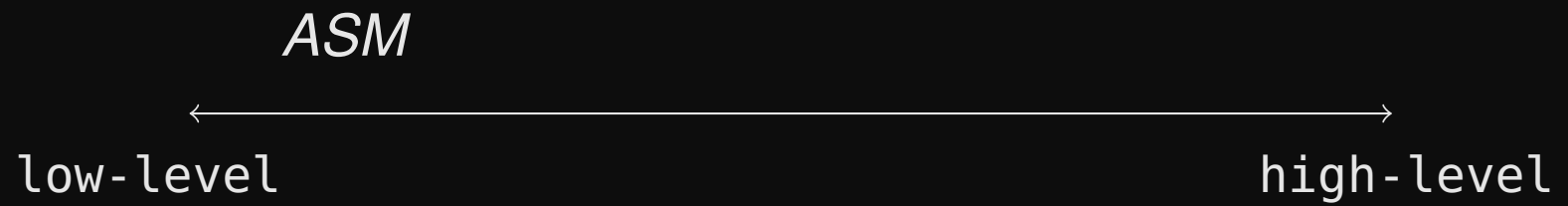
Graph #1



Graph #1



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Graph #1



ASM

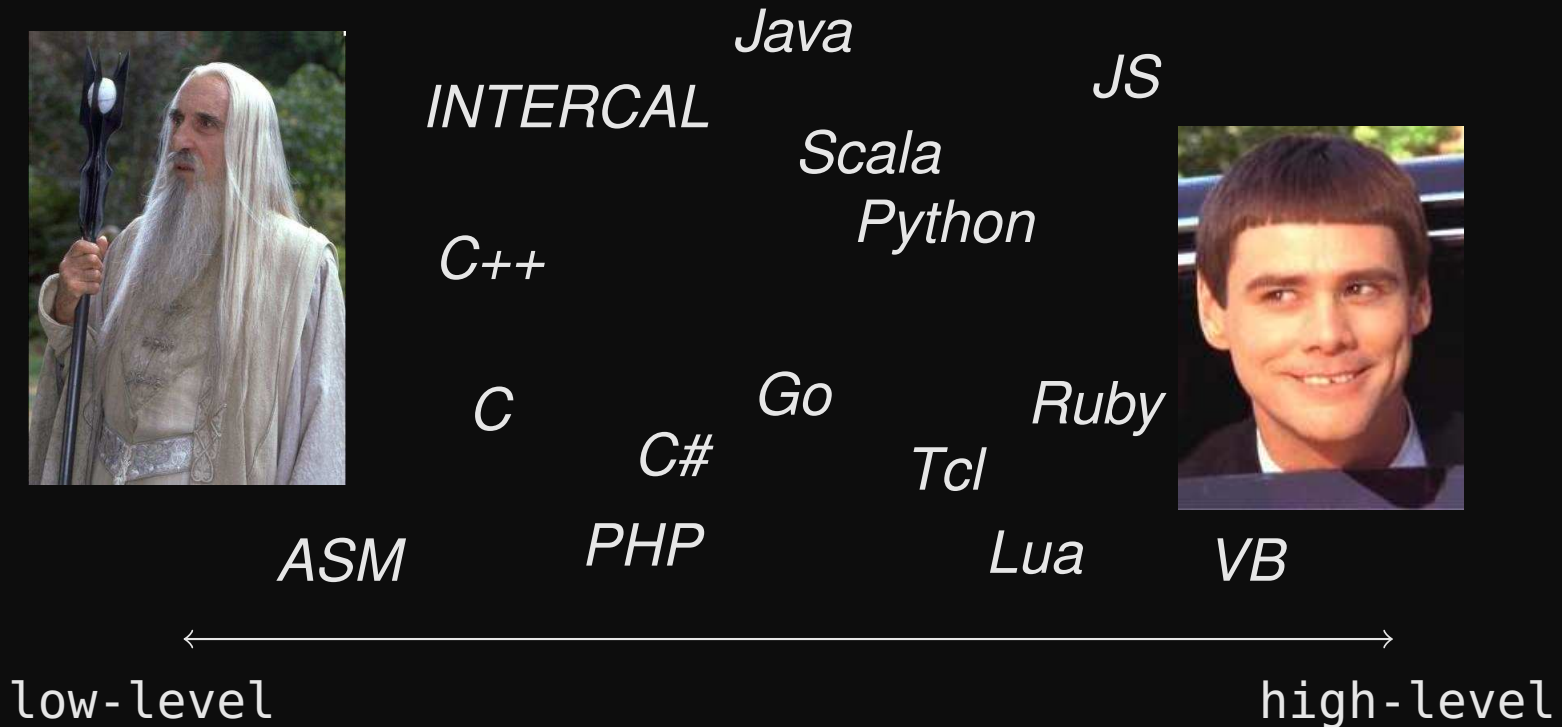
VB

low-level

high-level

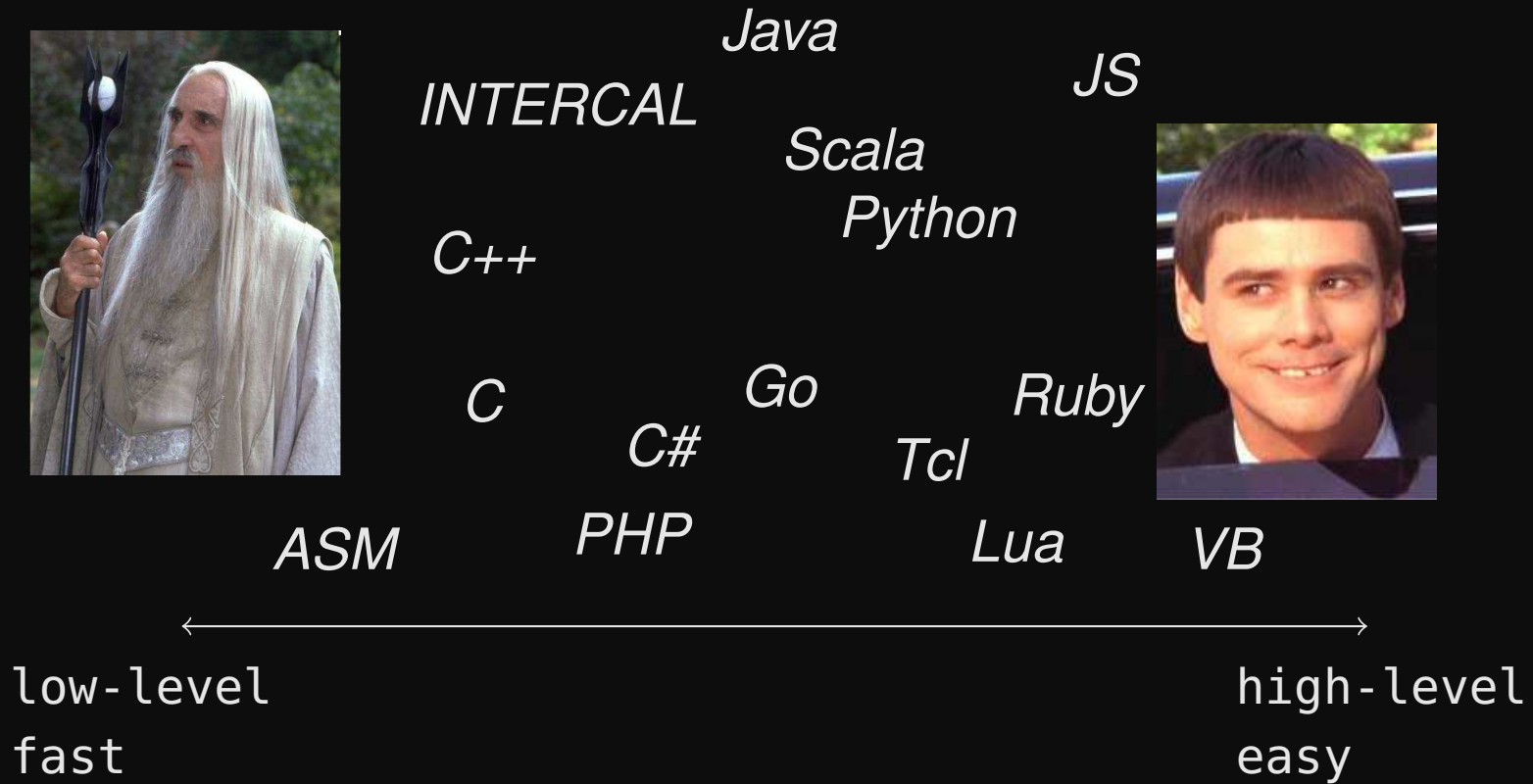


Graph #1



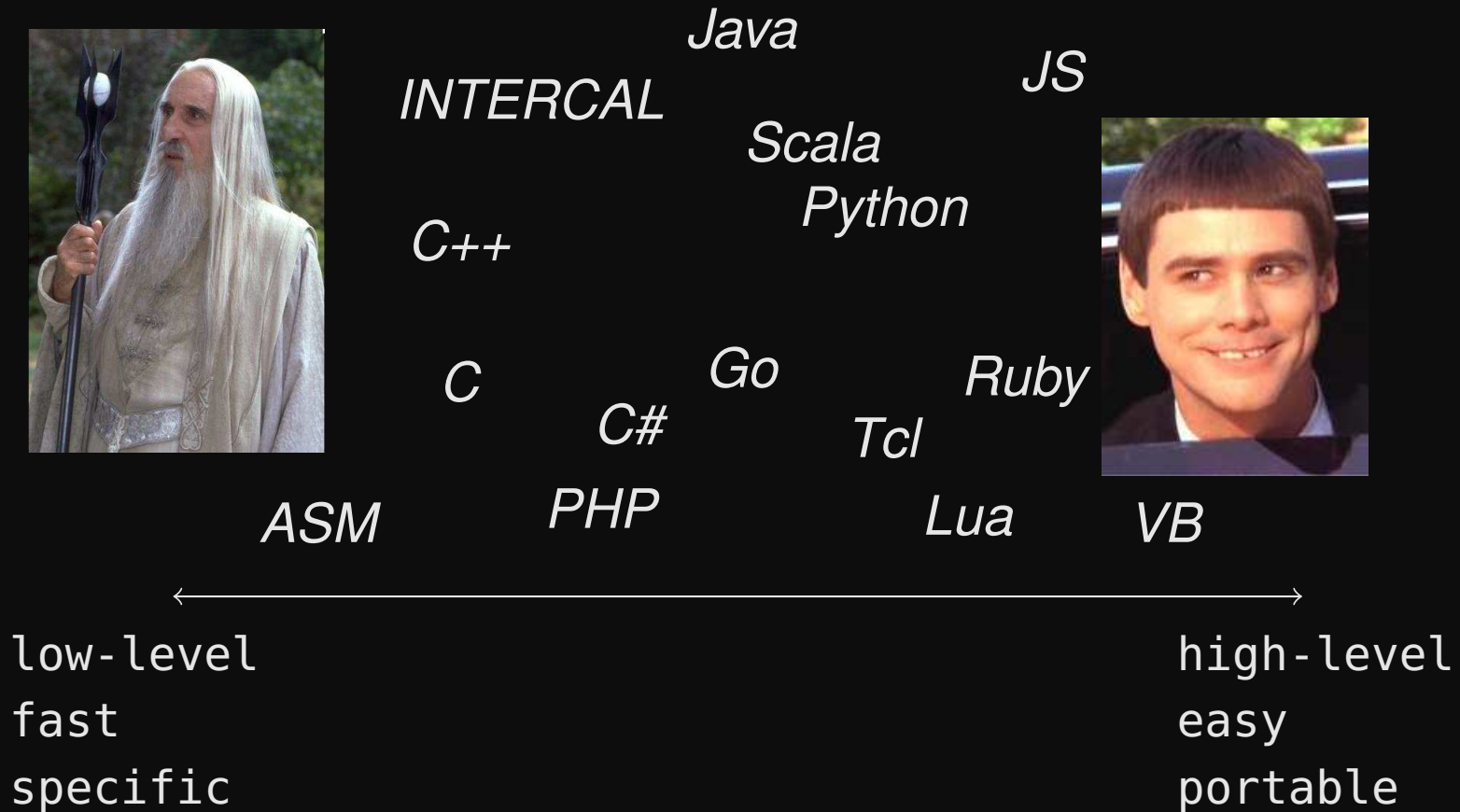
Note: this is not a scientific or particularly accurate representation.

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The Big Tradeoff

speed vs. portability and readability

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The Big Tradeoff

speed vs. portability and readability



If we're careful, we can get speed, portability, *and* readability by using C++.



So, mlpack.

What is it?

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What is it?

- a fast general-purpose C++ machine learning library
- contains flexible implementations of common and cutting-edge machine learning algorithms
- for fast or big runs on single workstations
- bindings are available for R, Python, and the command line, and are coming for other languages

- 100+ developers from around the world
- frequent participation in the Google Summer of Code program

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<http://www.mlpack.org/>

<https://github.com/mlpack/mlpack/>

R.R. Curtin, J.R. Cline, N.P. Slagle, W.B. March, P. Ram, N.A. Mehta, A.G. Gray, “**mlpack**: a scalable C++ machine learning library”, in *The Journal of Machine Learning Research*, vol. 14, p. 801–805, 2013.

What does mlpack implement?

mlpack implements a lot of standard machine learning techniques and also new, cutting-edge techniques.

Classification

Naive Bayes Classifier ID3
Hidden Markov Models
Perceptrons Decision Stumps
Logistic Regression Softmax Regression
Deep Learning Q Learning
Random Forests Sparse SVM
Reinforcement Learning AdaBoost.MH
Hoeffding Trees

Regression

Collaborative Filtering
Deep Learning
Linear Regression
LARS HMM Regression

Distance-Based Techniques

Kernel PCA
Rank-Approximate kNN Nystroem Method
Range Search EMST Sparse Coding
Locality-Sensitive Hashing PCA
k-Nearest-Neighbor Search
Density Estimation Trees NCA k-Furthest-Neighbor Search
Max-Kernel Search Local Coordinate Coding
Approximate KFN Sparse Autoencoder

Other Tools

Randomized SVD
Matrix Completion Hyper-Parameter Tuner
Preprocessing Utilities
Non-Negative Matrix Factorization QUIC-SVD
Regularized SVD
Optimization Toolkit
Collaborative Filtering
Incremental SVD

Clustering

k-means DBSCAN
Gaussian Mixture Models
Mean Shift

How do we get mlpack?

Linux (Debian/Ubuntu): `$ sudo apt-get install libmlpack-dev`
Linux (Red Hat/Fedora): `$ sudo dnf install mlpack-devel`
OS X (Homebrew): `$ brew tap brewsci/science &&`
`brew install mlpack`
Windows (nuget): `> nuget add mlpack-windows`

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Or install from source:

```
$ git clone https://github.com/mlpack/mlpack
$ mkdir mlpack/build && cd mlpack/build
$ cmake ../
$ make -j8 # Probably good to use many cores.
$ sudo make install
```

<https://www.mlpack.org/docs/mlpack-3.0.0/doxygen/build.html>
<https://keon.io/mlpack/mlpack-on-windows/>

Installing from Python

Use pip:

```
$ pip install mlpack3
```

Or use conda:

```
$ conda install -c mlpack mlpack
```

Command-line programs

You don't need to be a C++ expert.

```
# Train AdaBoost model.
```

```
$ mlpack_adaboost -t training_file.h5 -l training_labels.h5 \  
> -M trained_model.bin
```

```
# Predict with AdaBoost model.
```

```
$ mlpack_adaboost -m trained_model.bin -T test_set.csv \  
> -o test_set_predictions.csv
```

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$ mlpack_adaboost -m trained_model.bin -T test_set.csv \  
> -o test_set_predictions.csv
```

```
# Find the 5 nearest neighbors of the data in dataset.txt, storing the  
# indices of the neighbors in 'neighbors.csv'.
```

```
$ mlpack_knn -r dataset.txt -k 5 -n neighbors.csv
```

Command-line programs

You don't need to be a C++ expert.

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# Train AdaBoost model.
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$ mlpack_adaboost -t training_file.h5 -l training_labels.h5 \  
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```

```
# Find the 5 nearest neighbors of the data in dataset.txt, storing the  
# indices of the neighbors in 'neighbors.csv'.
```

```
$ mlpack_knn -r dataset.txt -k 5 -n neighbors.csv
```

```
# Impute missing values ("NULL") in the input dataset to the  
# mean in that dimension.
```

```
$ mlpack_preprocess_imputer -i dataset.h5 -s mean -o imputed.h5
```

Python bindings

Can be dropped directly into a Python workflow.

```
>>>
```

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```
>>> import numpy as np
>>> from mlpack import pca
>>> x = np.genfromtxt('my_data.csv', delimiter=',')
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```
>>> import numpy as np
>>> from mlpack import pca
>>> x = np.genfromtxt('my_data.csv', delimiter=',')
>>> x.shape
```

Python bindings

Can be dropped directly into a Python workflow.

```
>>> import numpy as np
>>> from mlpack import pca
>>> x = np.genfromtxt('my_data.csv', delimiter=',')
>>> x.shape
(2048, 10)
>>>
```

Python bindings

Can be dropped directly into a Python workflow.

```
>>> import numpy as np
>>> from mlpack import pca
>>> x = np.genfromtxt('my_data.csv', delimiter=',')
>>> x.shape
(2048, 10)
>>> result = pca(input=x, new_dimensionality=5, verbose=True)
```


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>>> import numpy as np
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>>> x = np.genfromtxt('my_data.csv', delimiter=',')
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>>> result = pca(input=x, new_dimensionality=5, verbose=True)
[INFO ] Performing PCA on dataset...
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>>> x = np.genfromtxt('my_data.csv', delimiter=',')
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(2048, 10)
>>> result = pca(input=x, new_dimensionality=5, verbose=True)
[INFO ] Performing PCA on dataset...
[INFO ] 99.9491% of variance retained (5 dimensions).
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>>> result = pca(input=x, new_dimensionality=5, verbose=True)
[INFO ] Performing PCA on dataset...
[INFO ] 99.9491% of variance retained (5 dimensions).
>>> result['output'].shape
```

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Can be dropped directly into a Python workflow.

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>>> import numpy as np
>>> from mlpack import pca
>>> x = np.genfromtxt('my_data.csv', delimiter=',')
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(2048, 10)
>>> result = pca(input=x, new_dimensionality=5, verbose=True)
[INFO ] Performing PCA on dataset...
[INFO ] 99.9491% of variance retained (5 dimensions).
>>> result['output'].shape
(2048, 5)
>>>
```

Python bindings

A simple example: collaborative filtering for item recommendations.

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Python bindings

A simple example: collaborative filtering for item recommendations.

```
>>> import numpy as np
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```
>>> from mlpack import cf
```

```
>>> x = np.genfromtxt('GroupLens100k.csv', delimiter=',')
```

Python bindings

A simple example: collaborative filtering for item recommendations.

```
>>> import numpy as np
>>> from mlpack import cf
>>> x = np.genfromtxt('GroupLens100k.csv', delimiter=',')
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```
>>> import numpy as np
>>> from mlpack import cf
>>> x = np.genfromtxt('GroupLens100k.csv', delimiter=',')
>>> x.shape
```

Python bindings

A simple example: collaborative filtering for item recommendations.

```
>>> import numpy as np
>>> from mlpack import cf
>>> x = np.genfromtxt('GroupLens100k.csv', delimiter=',')
>>> x.shape
(100000, 3)
>>>
```

Python bindings

A simple example: collaborative filtering for item recommendations.

```
>>> import numpy as np
>>> from mlpack import cf
>>> x = np.genfromtxt('GroupLens100k.csv', delimiter=',')
>>> x.shape
(100000, 3)
>>> help(cf)
```

Help on built-in function cf in module mlpack.cf:

cf(...)

Collaborative Filtering

This program performs collaborative filtering (CF) on the given dataset. Given a list of user, item and preferences (the 'training' parameter), the program will perform a matrix decomposition and then can perform a series of actions related to collaborative filtering. Alternately, the program can load an existing saved CF model with the 'input_model' parameter and then use that model to provide recommendations or predict values.

The input matrix should be a 3-dimensional matrix of ratings, where the first dimension is the user, the second dimension is the item, and the third dimension is that user's rating of that item. Both the users and items should be numeric indices, not names. The indices are assumed to start from 0.

A set of query users for which recommendations can be generated may be specified with the 'query' parameter; alternately, recommendations may be generated for every user in the dataset by specifying the 'all_user_recommendations' parameter. In addition, the number of recommendations per user to generate can be specified with the 'recommendations' parameter, and the number of similar users (the size of the neighborhood) to be considered when generating recommendations can be specified with the 'neighborhood' parameter.

For performing the matrix decomposition, the following optimization algorithms can be specified via the 'algorithm' parameter:

'RegSVD' -- Regularized SVD using a SGD optimizer

NMF Non-negative matrix factorization with alternating least squares
update rules
'BatchSVD' -- SVD batch learning
'SVDIncompleteIncremental' -- SVD incomplete incremental learning
'SVDCompleteIncremental' -- SVD complete incremental learning
A trained model may be saved to with the 'output_model' output parameter.

To train a CF model on a dataset 'training_set' using NMF for decomposition and saving the trained model to 'model', one could call:

```
>>> cf(training=training_set, algorithm='NMF')  
>>> model = output['output_model']
```

Then, to use this model to generate recommendations for the list of users in the query set 'users', storing 5 recommendations in 'recommendations', one could call

```
>>> cf(input_model=model, query=users, recommendations=5)  
>>> recommendations = output['output']
```

Input parameters:

- algorithm (string): Algorithm used for matrix factorization. Default value 'NMF'.
- all_user_recommendations (bool): Generate recommendations for all users.
- copy_all_inputs (bool): If specified, all input parameters will be deep copied before the method is run. This is useful for debugging problems where the input parameters are being modified by the algorithm, but can slow down the code.
- input_model (CFTType): Trained CF model to load.

```
>>> help(ct)
```

```
>>>
```

```
>>> help(cf)
```

```
>>> output = cf(training=x, algorithm='NMF', verbose=True)
```

```
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```
[INFO ] Performing CF matrix decomposition on dataset...
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```
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```
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```

```
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```
[INFO ] No rank given for decomposition; using rank of 11  
calculated by density-based heuristic.
```

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>>> help(cf)
>>> output = cf(training=x, algorithm='NMF', verbose=True)
[INFO ] Performing CF matrix decomposition on dataset...
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>>> help(cf)
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[INFO ] Performing CF matrix decomposition on dataset...
[INFO ] No rank given for decomposition; using rank of 11
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[INFO ] Initialized W and H.
[INFO ] Iteration 1; residue 0.710812.
```

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>>> help(cf)
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[INFO ] Performing CF matrix decomposition on dataset...
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[INFO ] Iteration 1; residue 0.710812.
[INFO ] Iteration 2; residue 0.0627744.
```



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...
[INFO ] Iteration 26; residue 5.93531e-06.
```

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[INFO ] AMF converged to residue of 5.93531e-06 in 26
iterations.
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>>> model = output['output_model']
```

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>>> model = output['output_model']
>>> result = cf(input_model=model, query=[[1]],
               recommendations=3, verbose=True)
```



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>>> model = output['output_model']
>>> result = cf(input_model=model, query=[[1]],
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[INFO ] Generating recommendations for 1 user.
[INFO ] 41 node combinations were scored.
[INFO ] 40 base cases were calculated.
```

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[INFO ] Generating recommendations for 1 user.
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[INFO ] 40 base cases were calculated.
>>> print(result['output'])
[[123 8 136]]
```

From the command line

Actually, we could have done the exact same thing from the command line:

```
$ mlpack_cf -t GroupLens100k.csv -M model.bin -a NMF
```

From the command line

Actually, we could have done the exact same thing from the command line:

```
$ mlpack_cf -t GroupLens100k.csv -M model.bin -a NMF  
$ mlpack_cf -m model.bin -q query.csv -c 3 -o recs.csv
```

From the command line

Actually, we could have done the exact same thing from the command line:

```
$ mlpack_cf -t GroupLens100k.csv -M model.bin -a NMF
$ mlpack_cf -m model.bin -q query.csv -c 3 -o recs.csv
$ cat recs.csv
```

From the command line

Actually, we could have done the exact same thing from the command line:

```
$ mlpack_cf -t GroupLens100k.csv -M model.bin -a NMF
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$ cat recs.csv
123, 8, 136
```

Basically all mlpack algorithm bindings to the command-line, Python, or other languages operate like this.

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- Generic programming *at compile time* via templates.

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- Little to no runtime overhead.

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- Generic programming *at compile time* via templates.
- Low-level memory management.
- Little to no runtime overhead.
- Well-known!

Pros of C++

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Pros of C++

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- Well-known!
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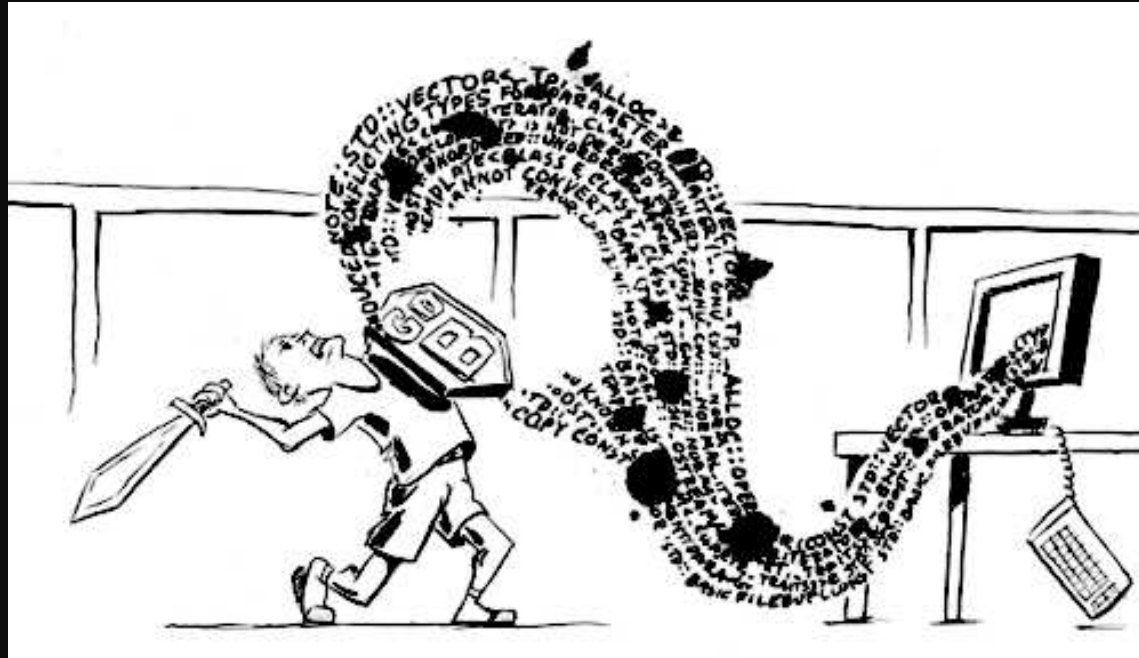
```
using namespace arma;  
extern mat x, y;  
mat z = (x + y) * chol(x) + 3 * chol(y.t());
```


Cons of C++

C++ is not great!

Cons of C++

C++ is not great!



- Templates can be hard to debug because of error messages.
- Memory bugs are easy to introduce.
- The new language revisions are not making the language any simpler...

Cons of C++

C++ is not great!



- Templates can
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essages.

uage any

Genericity

Why write an algorithm for one specific situation?

Genericity

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```
NearestNeighborSearch n(dataset);  
n.Search(query_set, 3, neighbors, distances);
```

What if I don't want the Euclidean distance?

Genericity

Why write an algorithm for one specific situation?

```
// The numeric parameter is the value of p for the p-norm to  
// use. 1 = Manhattan distance, 2 = Euclidean distance, etc.  
NearestNeighborSearch n(dataset, 1);  
n.Search(query_set, 3, neighbors, distances);
```

Ok, this is a little better!

Genericity

Why write an algorithm for one specific situation?

```
// ManhattanDistance is a class with a method Evaluate().  
NearestNeighborSearch<ManhattanDistance> n(dataset);  
n.Search(query_set, 3, neighbors, distances);
```

This is much better! The user can specify whatever distance metric they want, including one they write themselves.

Genericity

Why write an algorithm for one specific situation?

```
// This will _definitely_ get me best paper at ICML! I can
// feel it!
class MyStupidDistance
{
    static double Evaluate(const arma::vec& a,
                          const arma::vec& b)
    {
        return 15.0 * std::abs(a[0] - b[0]);
    }
};

// Now we can use it!
NearestNeighborSearch<MyStupidDistance> n(dataset);
n.Search(query_set, 3, neighbors, distances);
```

Genericity

Why write an algorithm for one specific situation?

```
// We can also use sparse matrices instead!  
NearestNeighborSearch<MyStupidDistance, arma::sp_mat>  
    n(sparse_dataset);  
n.Search(sparse_query_set, 3, neighbors, distances);
```

Genericity

Why write an algorithm for one specific situation?

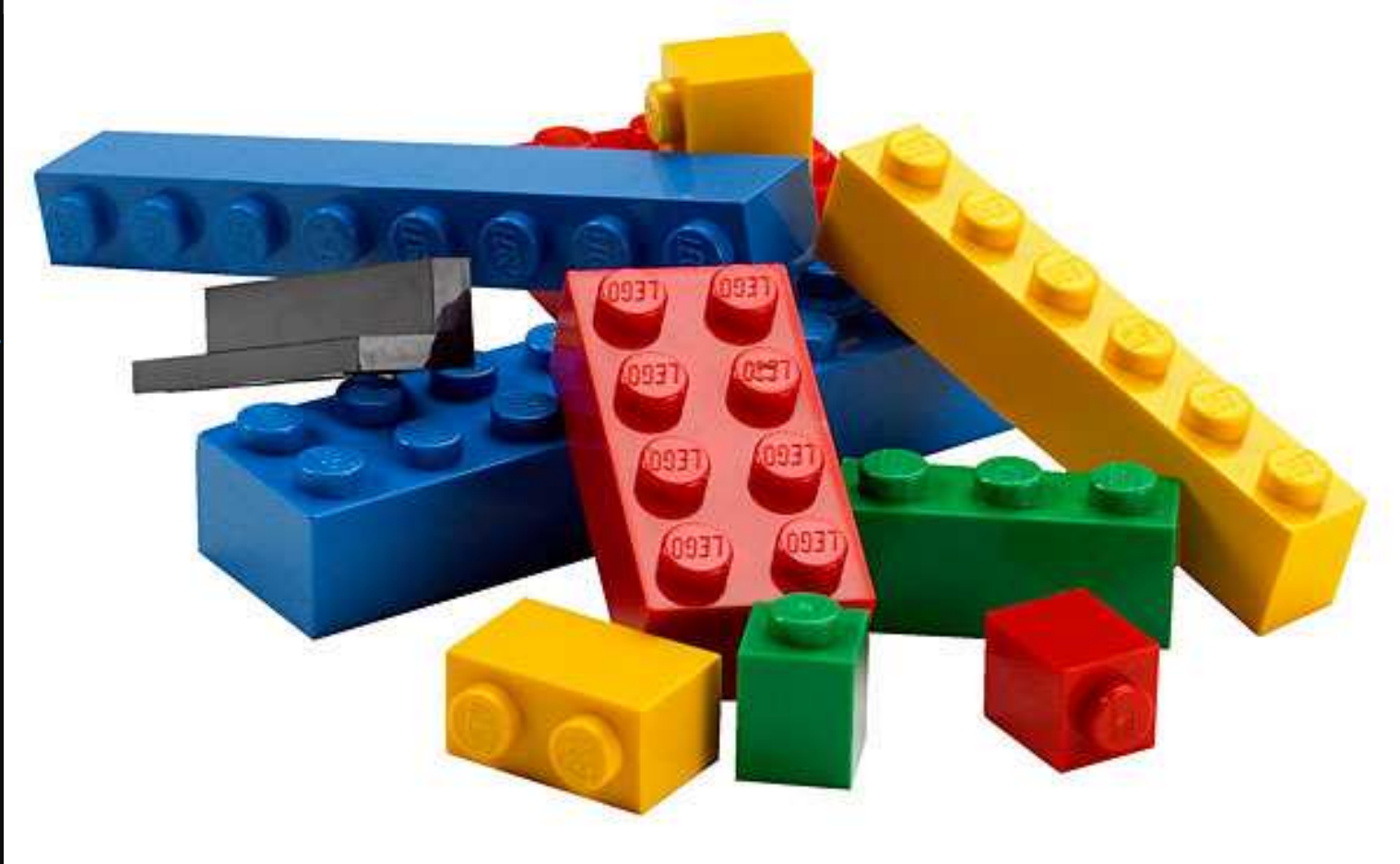
```
// Nearest neighbor search with arbitrary types of trees!  
NearestNeighborSearch<EuclideanDistance, arma::mat, KDTree> kn;  
NearestNeighborSearch<EuclideanDistance, arma::sp_mat, CoverTree> cn;  
NearestNeighborSearch<ManhattanDistance, arma::mat, Octree> on;  
NearestNeighborSearch<ChebyshevDistance, arma::sp_mat, RPlusTree> rn;  
NearestNeighborSearch<MahalanobisDistance, arma::mat, RPTree> rpn;  
NearestNeighborSearch<EuclideanDistance, arma::mat, XTree> xn;
```

R.R. Curtin, "Improving dual-tree algorithms". *PhD thesis, Georgia Institute of Technology, Atlanta, GA, 8/2015.*

Genericity

Why write an algorithm for one specific situation?

```
// Near  
Nearest  
Nearest  
Nearest  
Nearest  
Nearest  
Nearest
```



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Genericity

Why wr

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Nearest



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Why templates?

What about virtual inheritance?

Why templates?

What about virtual inheritance?

```
class MyStupidDistance : public Distance
{
    virtual double Evaluate(const arma::vec& a,
                           const arma::vec& b)
    {
        return 15.0 * std::abs(a[0] - b[0]);
    }
};
```

```
NearestNeighborSearch n(dataset, new MyStupidDistance());
n.Search(3, neighbors, distances);
```


Why templates?

What about virtual inheritance?

```
class MyStupidDistance : public Distance
{
    virtual double Evaluate(const arma::vec& a,
                           const arma::vec& b)
    {
        return 15.0 * std::abs(a[0] - b[0]);
    }
};
```

```
NearestNeighborSearch n(dataset, new MyStupidDistance());
n.Search(3, neighbors, distances);
```

vtable lookup penalty!

Why templates?

Using inheritance to call a function costs us instructions:

```
Distance* d =  
    new MyStupidDistance();  
d->Evaluate(a, b);
```

```
MyStupidDistance::Evaluate(a, b);
```

Why templates?

Using inheritance to call a function costs us instructions:

```
Distance* d =  
    new MyStupidDistance();  
d->Evaluate(a, b);
```

```
; push stack pointer  
movq %rsp, %rdi  
; get location of function  
movq $_ZTV1A+16, (%rsp)  
; call Evaluate()  
call _ZN1A1aEd
```

```
MyStupidDistance::Evaluate(a, b);
```

```
; just call Evaluate()  
call _ZN1B1aEd.isra.0.constprop.1
```

Why templates?

Using inheritance to call a function costs us instructions:

```
Distance* d =  
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; push stack pointer  
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; get location of function  
movq  $_ZTV1A+16, (%rsp)  
; call Evaluate()  
call  _ZN1A1aEd
```

```
MyStupidDistance::Evaluate(a, b);
```

```
; just call Evaluate()!  
call  _ZN1B1aEd.isra.0.constprop.1
```

Up to 10%+ performance penalty in some situations!

Compile-time expressions

What about math? (Armadillo)



Compile-time expressions

What about math? (Armadillo)

In C:

```
extern double** a, b, c, d, e;  
extern int rows, cols;  
  
// We want to do  $e = a + b + c + d$ .  
mat_copy(e, a, rows, cols);  
mat_add(e, b, rows, cols);  
mat_add(e, c, rows, cols);  
mat_add(e, d, rows, cols);
```



Compile-time expressions

What about math? (Armadillo)

In C with a custom function:

```
extern double** a, b, c, d, e;  
extern int rows, cols;
```

```
// We want to do e = a + b + c + d.
```



Compile-time expressions

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In C with a custom function:

```
extern double** a, b, c, d, e;  
extern int rows, cols;
```

```
// We want to do  $e = a + b + c + d$ .  
mat_add4_into(e, a, b, c, d, rows, cols);
```

Fastest! (one pass)



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```
extern double** a, b, c, d, e;  
extern int rows, cols;
```

```
// We want to do e = a + b + c + d.  
mat_add4_into(e, a, b, c, d, rows, cols);
```

Fastest! (one pass)

```
void mat_add4_into(double** e, double** a, double** b,  
                  double** c, double** d, int rows, int cols)  
{  
    for (int r = 0; r < rows; ++r)  
        for (int c = 0; c < cols; ++c)  
            e[r][c] = a[r][c] + b[r][c] + c[r][c] + d[r][c];  
}
```



Compile-time expressions

What about math? (Armadillo)

In MATLAB:

```
e = a + b + c + d
```



Compile-time expressions

What about math? (Armadillo)

In MATLAB:

```
e = a + b + c + d
```

Beautiful!



Compile-time expressions

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Compile-time expressions

What about math? (Armadillo)

In C++ (with Armadillo):

```
using namespace arma;  
extern mat a, b, c, d;
```

```
mat e = a + b + c + d;
```

No temporaries, only one pass! Just as fast as the fastest C implementation.



Compile-time expressions

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```
using namespace arma;  
extern mat a, b, c, d;
```

```
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C++ allows us templated operator overloading:

```
template<typename T1, typename T2>  
const op<T1, T2, add> operator+(const T1& x, const T2& y);
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- `mat + mat`
→ `op<mat, mat, add>`



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Compile-time expressions



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mat e = a + b + c + d;
```

C++ allows us templated operator overloading:

```
template<typename T1, typename T2>  
const op<T1, T2, add> operator+(const T1& x, const T2& y);
```

The expression yields type `op<op<op<mat, mat, add>, mat, add>, mat, add>`.

```
// This can accept an op<...> type.  
template<typename T1, typename T2>  
mat::operator=(const op<T1, T2, add>& op);
```

Compile-time expressions



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mat e = a + b + c + d;
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The expression yields type `op<op<op<mat, mat, add>, mat, add>, mat, add>`.

```
// This can accept an op<...> type.  
template<typename T1, typename T2>  
mat::operator=(const op<T1, T2, add>& op);
```

The assignment operator "unwraps" the operation and generates optimal code.

Take-home

- Templates give us generic code.
- Templates allow us to generate fast code.

Optimization in C++ with mlpack

Optimization is a fundamental machine learning problem:

$$\operatorname{argmin}_x f(x)$$

Optimization in C++ with mlpack

Optimization is a fundamental machine learning problem:

$$\operatorname{argmin}_x f(x)$$

mlpack provides some nice facilities to do this. In order to optimize a differentiable function we just need a class with two methods:

```
// Return the value of f(x).  
double Evaluate(const arma::mat& x);  
  
// Compute the gradient of f(x) with respect to x.  
void Gradient(const arma::mat& x, arma::mat& gradient);
```

Optimization in C++ with mpack

Let's take linear regression as an example:

- A : data matrix
- b : data responses
- x : parameters for linear regression

Optimization in C++ with mlpack

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$$f(x) = (Ax - b)^T (Ax - b).$$

And the gradient:

$$\nabla f(x) = A^T (Ax - b).$$

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And the gradient:

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We want to minimize $f(x)$.

(The point of the demo here is to show how easy it is to implement, not to detail the intricacies of linear regression, so don't worry about the math much.)

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Remember, we just need two functions inside of a class.

```
class LinearRegressionFunction  
{
```

Optimization in C++ with mlpack

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```
class LinearRegressionFunction
{
private:
    const arma::mat& data; // Store a reference to the data.
    const arma::rowvec& responses;

public:
    LinearRegressionFunction(const arma::mat& data, const arma::rowvec&
        responses) : data(data), responses(responses) { }
```


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    double Evaluate(const arma::mat& x)
    {
```

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```
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{
private:
    const arma::mat& data; // Store a reference to the data.
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```

```
public:
```

```
LinearRegressionFunction(const arma::mat& data, const arma::rowvec& responses) : data(data), responses(responses) {}

    double Evaluate(const arma::mat& x) const {
        return responses * (x - data) * (x - data).t();
    }
};
```

```
double Evaluate(const arma::mat& x)
{
```

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public:
    LinearRegressionFunction(const arma::mat& data, const arma::rowvec& responses) : data(data), responses(responses) {}

    double Evaluate(const arma::mat& x)
    {
        return (data * x - responses).t() * (data * x - responses);
    }
};
```

$$f(x) = (Ax - b)^T (Ax - b).$$

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    double Evaluate(const arma::mat& x)
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    void Gradient(const arma::mat& x, arma::mat& gradient)
    {
```

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$$\nabla f(x) = A^T (Ax - b).$$


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        responses) : data(data), responses(responses) { }

    double Evaluate(const arma::mat& x)
    {
        return (data * x - responses).t() * (data * x - responses);
    }

    void Gradient(const arma::mat& x, arma::mat& gradient)
    {
        gradient = data.t() * (data * x - responses);
    }
};
```

Optimization in C++ with mlpack

Now we can take our `LinearRegressionFunction` and optimize it!

Optimization in C++ with mlpack

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```
using namespace mlpack::optimization;

// Create the function.
LinearRegressionFunction lrf(data, responses);

arma::mat x;
L_BFGS l; // Construct optimizer with default parameters.
l.Optimize(lrf, x); // Find the minimum of lrf and store the parameters in x.
```

Optimization in C++ with mlpack

Now we can take our `LinearRegressionFunction` and optimize it!

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LinearRegressionFunction lrf(data, responses);

arma::mat x;
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l.Optimize(lrf, x); // Find the minimum of lrf and store the parameters in x.

GradientDescent g;
g.Optimize(lrf, x);
```

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SA s; // Simulated Annealing.
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```

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s.Optimize(lrf, x);

IQN i;
i.Optimize(lrf, x);
```

A wide range of optimizers for different problem types

mlpack has a huge collection of optimizers.

- **Quasi-Newton variants:** Limited-memory BFGS (L-BFGS), incremental Quasi-Newton method (IQN), Augmented Lagrangian Method
- **SGD variants:** Stochastic Gradient Descent (SGD), Stochastic Coordinate Descent (SCD), Parallel Stochastic Gradient Descent (Hogwild!), Stochastic Gradient Descent with Restarts (SGDR), SMORMS3, AdaGrad, AdaDelta, RMSProp, Adam, AdaMax
- **Genetic variants:** Conventional Neuro-evolution (CNE), Covariance Matrix Adaptation Evolution Strategy (CMA-ES)
- **Other:** Conditional Gradient Descent, Frank-Wolfe algorithm, Simulated Annealing

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- **Genetic variants:** Conventional Neuro-evolution (CNE), Covariance Matrix Adaptation Evolution Strategy (CMA-ES)
- **Other:** Conditional Gradient Descent, Frank-Wolfe algorithm, Simulated Annealing

And it is also easy to implement new optimizers.

Deep Neural Networks with mpack

With the optimization infrastructure, we can also do deep learning.

Deep Neural Networks with mlpack

With the optimization infrastructure, we can also do deep learning.

```
using namespace mlpack::ann;
extern arma::mat data, responses, testData;

// Create a 3-layer sigmoid neural network with 10 outputs.
FFN<NegativeLogLikelihood<>, RandomInitialization> model;
model.Add<Linear<>>(data.n_rows, 100);
model.Add<SigmoidLayer<>>();
model.Add<Linear<>>(100, 100);
model.Add<SigmoidLayer<>>();
model.Add<Linear<>>(100, 10);
model.Add<LogSoftMax<>>();
```


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model.Add<Linear<>>(100, 100);
model.Add<SigmoidLayer<>>();
model.Add<Linear<>>(100, 10);
model.Add<LogSoftMax<>>();

// Train the model.
SGD<> optimizer(0.001 /* step size */, 1024 /* batch size */,
               100000 /* max iterations */);
model.Train(data, responses, optimizer);
```

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FFN<NegativeLogLikelihood<>, RandomInitialization> model;
model.Add<Linear<>>(data.n_rows, 100);
model.Add<SigmoidLayer<>>();
model.Add<Linear<>>(100, 100);
model.Add<SigmoidLayer<>>();
model.Add<Linear<>>(100, 10);
model.Add<LogSoftMax<>>();

// Train the model.
SGD<> optimizer(0.001 /* step size */, 1024 /* batch size */,
               100000 /* max iterations */);
model.Train(data, responses, optimizer);

// Predict on test points.
arma::mat predictions;
model.Predict(testData, predictions);
```

Benchmarks

Did C++ get us what we wanted?

Benchmarks

Task 1: $z = 2(x' + y) + 2(x + y')$.

```
extern int n;  
mat x(n, n, fill::randu);  
mat y(n, n, fill::randu);  
mat z = 2 * (x.t() + y) + 2 * (x + y.t()); // only time this line
```

n	arma	numpy	octave	R	Julia
1000	0.029s	0.040s	0.036s	0.052s	0.027s
3000	0.047s	0.432s	0.376s	0.344s	0.041s
10000	0.968s	5.948s	3.989s	4.952s	3.683s
30000	19.167s	62.748s	41.356s	<i>fail</i>	36.730s

Benchmarks

Task 2: $z = (x + 10 * I)^\dagger - y$.

```
extern int n;  
mat x(n, n, fill::randu);  
mat y(n, n, fill::randu);  
mat z = pinv(x + 10 * eye(n, n)) - y; // only time this line
```

n	arma	numpy	octave	R	Julia
300	0.081s	0.080s	0.324s	0.096s	0.098s
1000	1.321s	1.354s	26.156s	1.444s	1.236s
3000	28.817s	28.955s	648.64s	29.732s	29.069s
10000	777.55s	785.58s	17661.9s	787.201s	778.472s

The computation is dominated by the calculation of the pseudoinverse.

Benchmarks

Task 3: $z = abcd$ for decreasing-size matrices.

```
extern int n;  
mat a(n, 0.8 * n, fill::randu);  
mat b(0.8 * n, 0.6 * n, fill::randu);  
mat c(0.6 * n, 0.4 * n, fill::randu);  
mat d(0.4 * n, 0.2 * n, fill::randu);  
mat z = a * b * c * d; // only time this line
```

n	arma	numpy	octave	R	Julia
1000	0.042s	0.051s	0.033s	0.056s	0.037s
3000	0.642s	0.812s	0.796s	0.846s	0.844s
10000	16.320s	26.815s	26.478s	26.957s	26.576s
30000	329.87s	708.16s	706.10s	707.12s	704.032s

Armadillo can automatically select the correct ordering for multiplication.

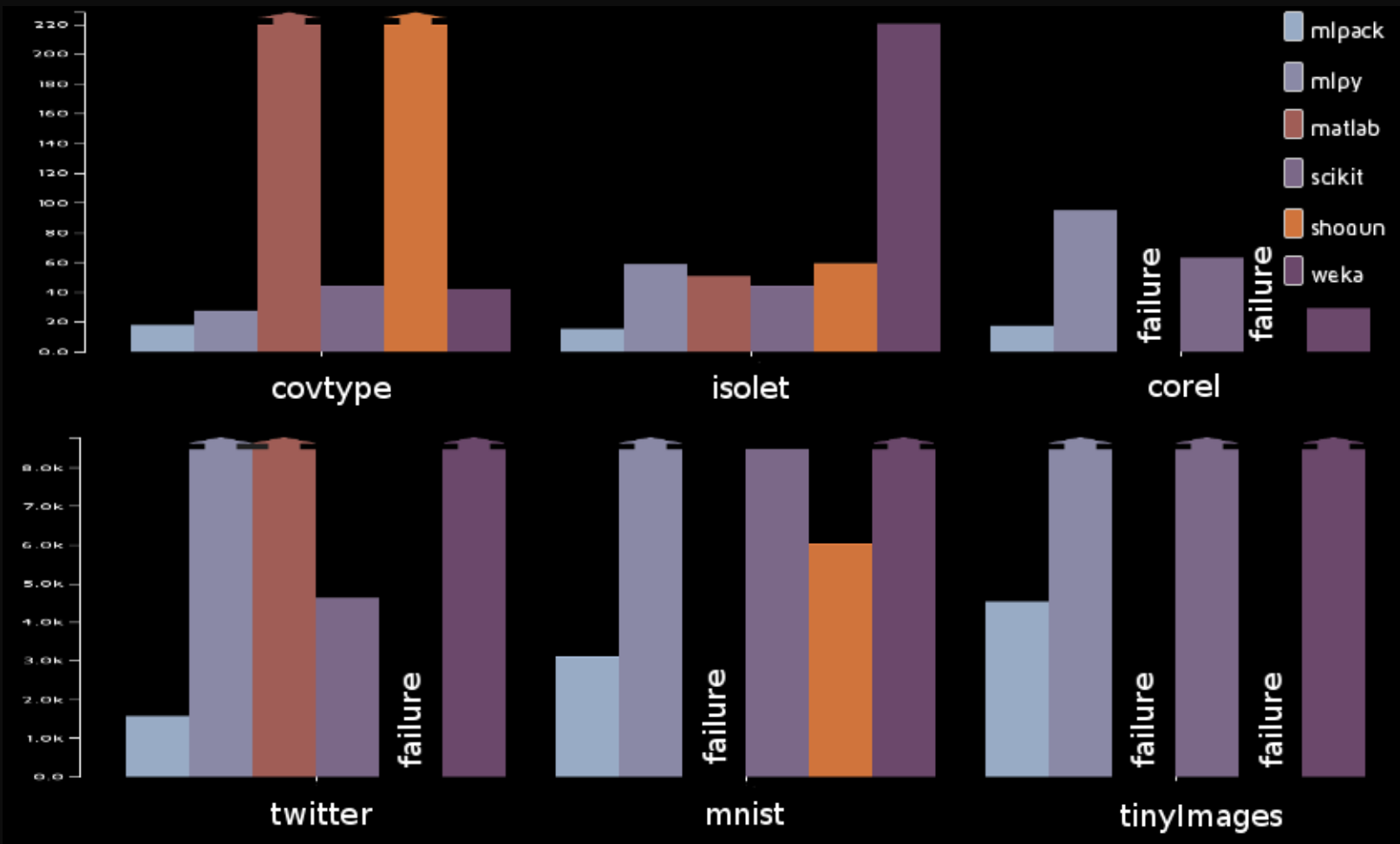
Benchmarks

Task 4: $z = a'(\text{diag}(b)^{-1})c$.

```
extern int n;  
vec a(n, fill::randu);  
vec b(n, fill::randu);  
vec c(n, fill::randu);  
double z = as_scalar(a.t() * inv(diagmat(b)) * c); // only time this line
```

n	arma	numpy	octave	R	Julia
1k	8e-6s	0.100s	2e-4s	0.014s	0.057s
10k	8e-5s	49.399s	4e-4s	0.208s	18.189s
100k	8e-4s	<i>fail</i>	0.002s	<i>fail</i>	<i>fail</i>
1M	0.009s	<i>fail</i>	0.024s	<i>fail</i>	<i>fail</i>
10M	0.088s	<i>fail</i>	0.205s	<i>fail</i>	<i>fail</i>
100M	0.793s	<i>fail</i>	1.972s	<i>fail</i>	<i>fail</i>
1B	8.054s	<i>fail</i>	19.520s	<i>fail</i>	<i>fail</i>

kNN benchmarks



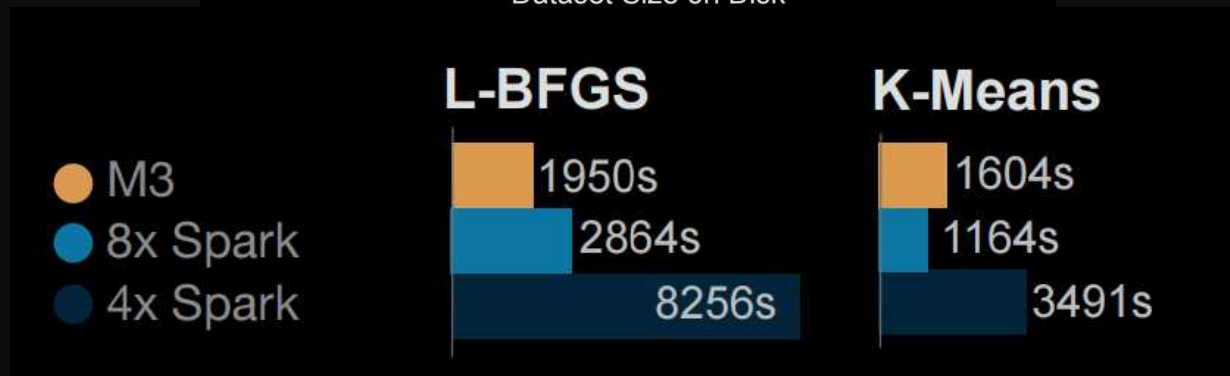
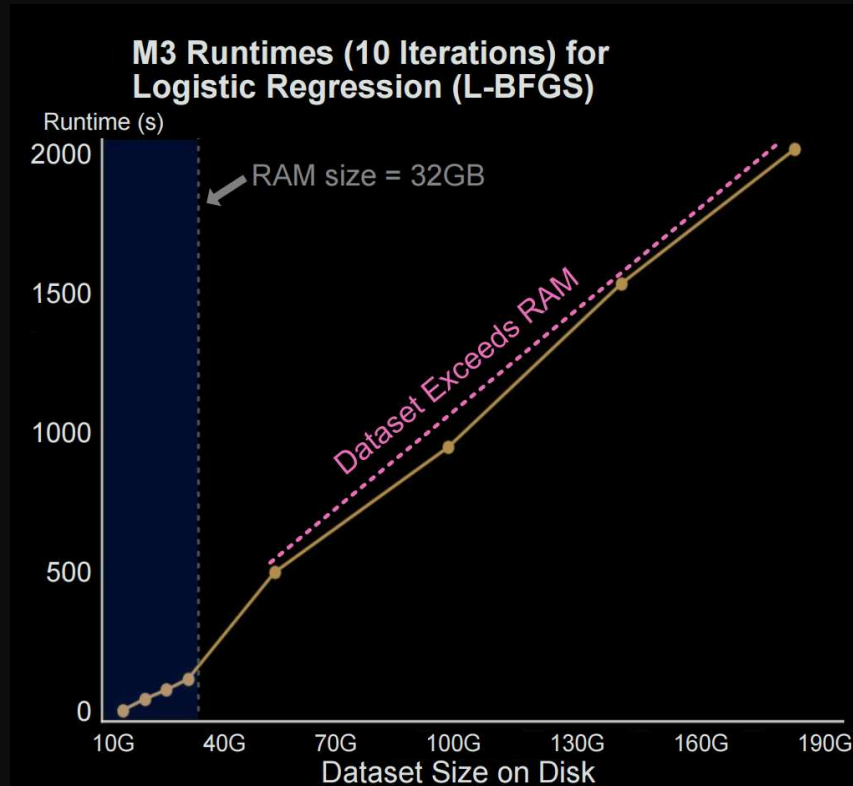
dataset	d	N	mlpack	mlpy	matlab	scikit	shogun	Weka
isolet	617	8k	15.65s	59.09s	50.88s	44.59s	59.56s	220.38s
corel	32	68k	17.70s	95.26s	fail	63.32s	fail	29.38s
covertyp	54	581k	18.04s	27.68s	>9000s	44.55s	>9000s	42.34s
twitter	78	583k	1573.92s	>9000s	>9000s	4637.81s	fail	>9000s
mnist	784	70k	3129.46s	>9000s	fail	8494.24s	6040.16s	>9000s
tinyImages	384	100k	4535.38s	9000s	fail	>9000s	fail	>9000s

vs. Spark

We can use `mmap()` for out-of-core learning since our algorithms are generic!

vs. Spark

We can use `mmap()` for out-of-core learning since our algorithms are generic!



What didn't I talk about in depth?

- hyper-parameter tuner
- tree infrastructure for problems like nearest neighbor search
- reinforcement learning code
- matrix decomposition infrastructure
- benchmarking system
- automatic binding generator
- preprocessing utilities
- ...and surely more I am not thinking of...

What's coming?

mlpack 3 is released and ready for production use!

<http://mlpack.org/blog/mlpack-3-released.html>



<http://www.mlpack.org/>
<https://github.com/mlpack/mlpack/>

Further out

Armadillo-like library for GPU matrix operations: **Bandicoot**



<http://coot.sourceforge.io/>

Two separate use case options:

- Bandicoot can be used as a drop-in accelerator to Armadillo, offloading intensive computations to the GPU when possible.
- Bandicoot can be used as its own library for GPU matrix programming.

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Armadillo-like library for GPU matrix operations: **Bandicoot**



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- Bandicoot can be used as its own library for GPU matrix programming.

```
using namespace coot;  
mat x(n, n, fill::randu); // matrix allocated on GPU  
mat y(n, n, fill::randu);  
mat z = x * y; // computation done on GPU
```

Questions and comments?



<http://www.mlpack.org/>
<https://github.com/mlpack/mlpack/>