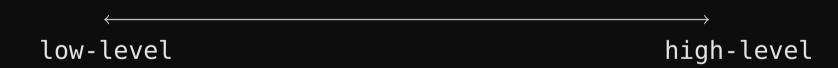
## mlpack: or, How I Learned To Stop Worrying and Love C++

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ODSC East 2019 #ODSC
May 2, 2019



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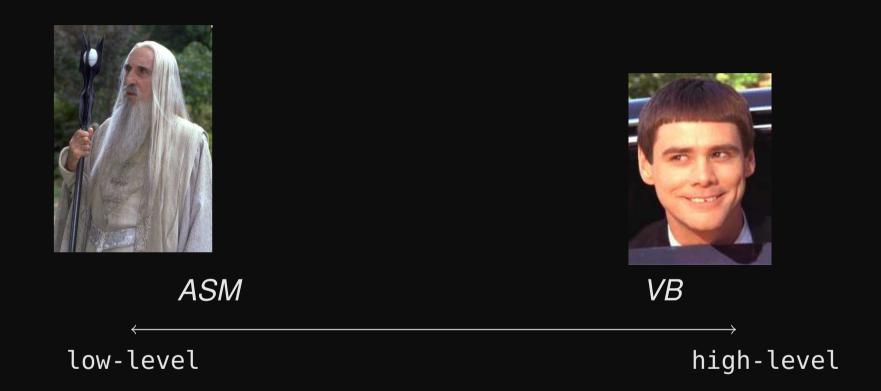


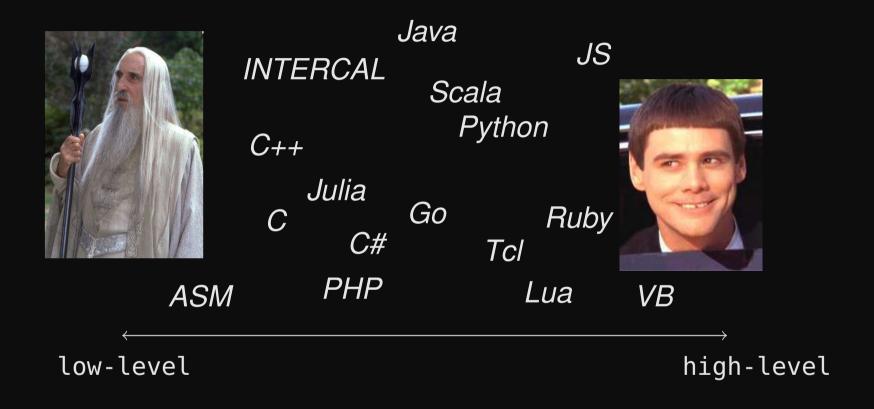
ASM

low-level

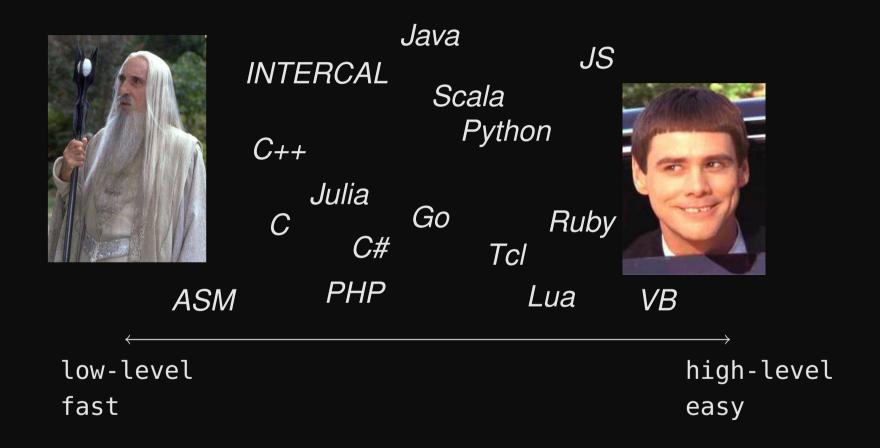
high-level



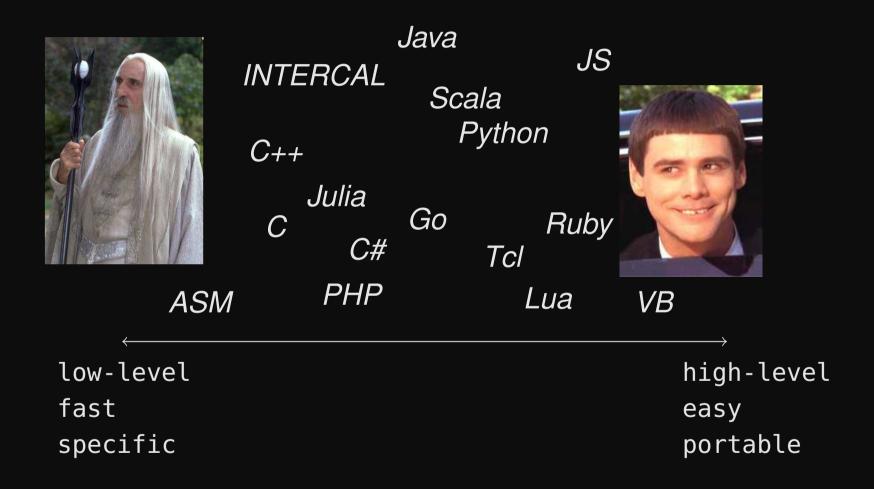




Note: this is not a scientific or particularly accurate representation.



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## **The Big Tradeoff**

speed vs. portability and readability

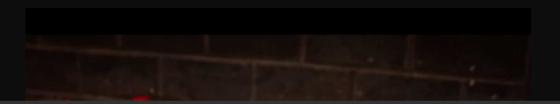
## **The Big Tradeoff**

speed vs. portability and readability



## **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?



## So, mlpack.



#### 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 (Julia, Go, Java?)
- 100+ developers from around the world
- frequent participation in the Google Summer of Code program

#### So, mlpack.

# mlpack

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http://www.mlpack.org/

https://github.com/mlpack/mlpack/

R.R. Curtin, M. Edel, M. Lozhnikov, Y. Mentekidis, S. Ghaisas, S. Zhang. "**mlpack 3**: a fast, flexible machine learning library", in *The Journal of Open Source Software*, vol. 3, issue 26, 2018.

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 Decision Stumps
Hidden Markov Models
Perceptrons Softmax Regression
Logistic Regression Decision Trees

Deep Learning
Random Forests Sparse SVM
Reinforcement Learning
Hoeffding Trees

## Regression

Collaborative Filtering
Deep Learning
Linear Regression
LARS HMM Regression

## Distance-Based Techniques

Kernel PCA
Rank-Approximate kNNNystroem Method
Range SearchEMSTSparse Coding
Locality-Sensitive Hashing
Locality-Sensitive Hashing
K-Nearest-Neighbor Search
Density Estimation Trees NCAk-Furthest-Neighbor Search
Max-Kernel Search Local Coordinate Coding
Approximate KFN

## Other Tools

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

## Clustering

K-means DBSCAN
Gaussian Mixture Models
Mean Shift

#### How do we get mlpack?

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```
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
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/doc/mlpack-3.1.0/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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```
# Train AdaBoost model.
$ mlpack_adaboost -t training_file.h5 -l training_labels.h5 \
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# Predict with AdaBoost model.
$ 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.

```
# 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
# 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
```



Can be dropped directly into a Python workflow.

>>> import numpy as np

```
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>>>
```

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>>> 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
```

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

```
>>> 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)
```

```
>>> 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)
[INFO ] Performing PCA on dataset...
```

```
>>> 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)
[INFO ] Performing PCA on dataset...
[INFO ] 99.9491% of variance retained (5 dimensions).
```

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



A simple example: collaborative filtering for item recommendations.

>>> import numpy as np

```
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>>>
```

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

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

```
>>> 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

```
With hegaetve macriax raccorazacton water accornating teast 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, guery=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 (CFType): Trained CF model to load.

```
(100000, 3)
>>> help(cf)
>>>
```

```
(100000, 3)
>>> help(cf)
>>> output = cf(training=x, algorithm='NMF', verbose=True)
```

```
(100000, 3)
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[INFO ] Performing CF matrix decomposition on dataset...
```

```
(100000, 3)
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[INFO ] Performing CF matrix decomposition on dataset...
[INFO ] No rank given for decomposition; using rank of 11 calculated by density-based heuristic.
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[INFO ] Iteration 1; residue 0.710812.
```

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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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>>> 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
```

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

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$ cat recs.csv
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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.

C++ is great!

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- Low-level memory management.

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- Little to no runtime overhead.

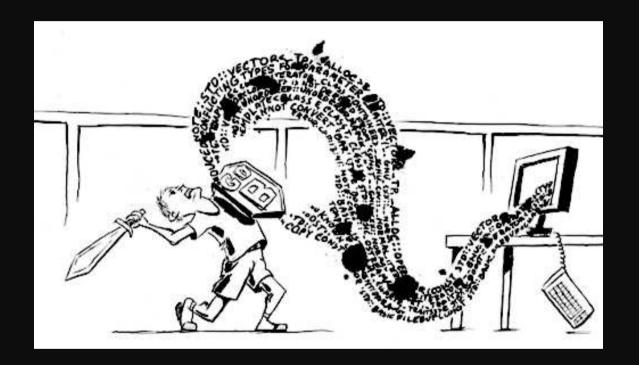
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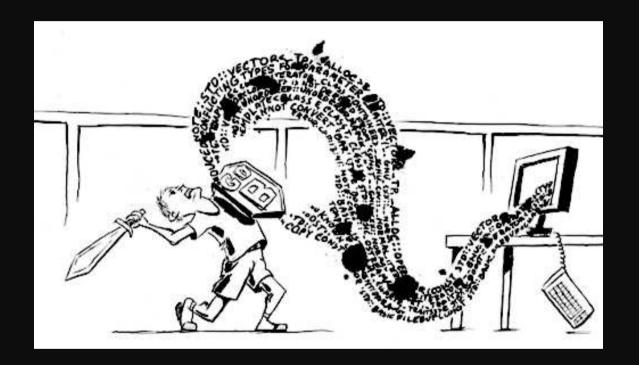
- Generic programming at compile time via templates.
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- Well-known!
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```
using namespace arma;
extern mat x, y;
mat z = (x + y) * chol(x) + 3 * chol(y.t());
```

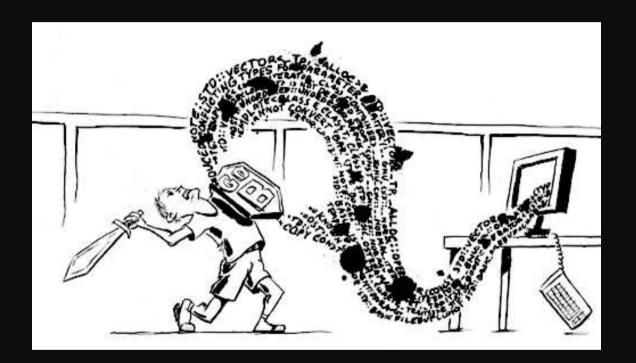
C++ is not great!



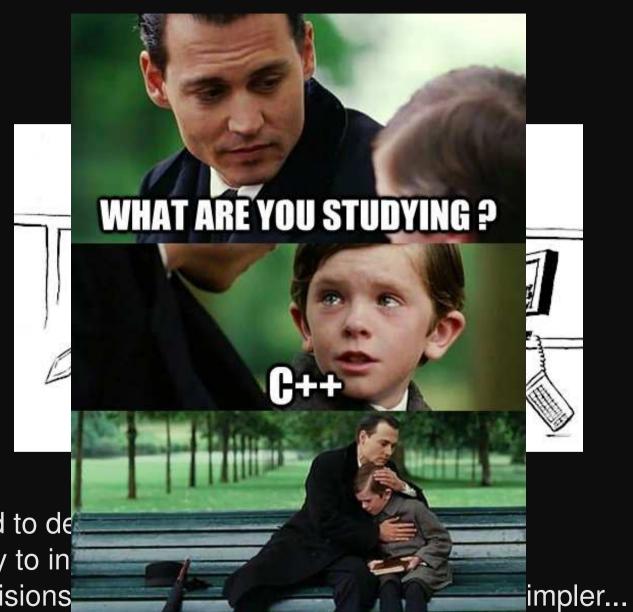
Templates can be hard to debug because of error messages.



- Templates can be hard to debug because of error messages.
- Memory bugs are easy to introduce.



- 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...



- Templates can be hard to de
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- The new language revisions

Why write an algorithm for one specific situation?

Why write an algorithm for one specific situation?

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

What if I don't want the Euclidean distance?

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!

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.

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);
```

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);
```

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.

Why write an algorithm for one specific situation?

# // Nearest neight NearestNeighborSe NearestNeighborSe NearestNeighborSe NearestNeighborSe NearestNeighborSe NearestNeighborSe NearestNeighborSe NearestNeighborSe

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Why write an algorithm for one specific situation?

// Nearest neight
NearestNeighborSe
NearestNeighborSe
NearestNeighborSe
NearestNeighborSe
NearestNeighborSe
NearestNeighborSe
NearestNeighborSe



What about virtual inheritance?

What about virtual inheritance?

What about virtual inheritance?

Using inheritance to call a function costs us instructions:

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

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);

// Call Evaluate()

call _ZN1B1aEd.isra.0.constprop.1
```

Using inheritance to call a function costs us instructions:

Up to 10%+ performance penalty in some situations!

What about math? (Armadillo)



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);
```



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.
```



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.
mat_add4_into(e, a, b, c, d, rows, cols);
```

Fastest! (one pass)



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.
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)</pre>
    for (int c = 0; c < cols; ++c)</pre>
      e[r][c] = a[r][c] + b[r][c] + c[r][c] + d[r][c];
```



What about math? (Armadillo)

In MATLAB:

$$e = a + b + c + d$$



What about math? (Armadillo)

In MATLAB:

$$e = a + b + c + d$$

Beautiful!



What about math? (Armadillo)



What about math? (Armadillo)





What about math? (Armadillo)

```
In C++ (with Armadillo):
```

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





```
What about math? (Armadillo)
In C++ (with Armadillo):
```

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

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);
```



```
What about math? (Armadillo)
In C++ (with Armadillo):
using namespace arma;
extern mat a, b, c, d;
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);
    mat + mat

ightarrow op<mat, mat, add>
```



```
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    mat + mat + mat
        \rightarrow op<mat, mat, add> + mat
```



```
What about math? (Armadillo)
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    mat + mat

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    mat + mat + mat
        \rightarrow op<op<mat, mat, add>, mat, add>
```



```
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    mat + mat + mat
        \rightarrow op<op<mat, mat, add>, mat, add>
    mat + mat + mat + mat
        \rightarrow op<mat, mat, add> + mat + mat
```



```
What about math? (Armadillo)
In C++ (with Armadillo):
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extern mat a, b, c, d;
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);
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    mat + mat + mat
        \rightarrow op<op<mat, mat, add>, mat, add>
    mat + mat + mat + mat
        \rightarrow op<op<mat, mat, add>, mat, add> + mat
```



```
What about math? (Armadillo)
In C++ (with Armadillo):
using namespace arma;
extern mat a, b, c, d;
mat e = a + b + c + d;
C++ allows us templated operator overloading:
template<typename T1, typename T2>
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    mat + mat + mat + mat

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```



```
What about math? (Armadillo)
In C++ (with Armadillo):
using namespace arma;
extern mat a, b, c, d;
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<mat, mat, add>, 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);
```



What about math? (Armadillo) In C++ (with Armadillo): using namespace arma; extern mat a, b, c, d; 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<mat, mat, add>, 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 is a fundamental machine learning problem:

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

Optimization is a fundamental machine learning problem:

```
\operatorname{argmin}_{x} f(x)
```

mlpack provides some nice facilities to do this, via the new ensmallen library: https://github.com/mlpack/ensmallen. 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);
```

Let's take linear regression as an example:

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

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- b: data responses
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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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We want to minimize f(x).

Let's take linear regression as an example:

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

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

And the gradient:

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

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.)

```
class LinearRegressionFunction
{
```

```
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) { }
```

```
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) { }

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

```
class LinearRegressionFunction
 private:
        arma::mat& data; // Store a reference to the data.
  const arma::rowvec& responses;
                                       f(x) = (Ax - b)^T (Ax - b).
  LinearRegressionFunc<sup>-</sup>
                                                                                      data(data),
      responses(responses) { }
  double Evaluate(const arma::mat& x)
    return (data * x - responses).t() * (data * x - responses);
```

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       arma::mat& data; // Store a reference to the data.
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  LinearRegressionFunction(const arma::mat& data, const arma::rowvec& responses) : data(data),
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    return (data * x - responses).t() * (data * x - responses);
  void Gradient(const arma::mat& x, arma::mat& gradient)
    gradient = data.t() * (data * x - responses);
```

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

```
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.
```

```
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.

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

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SA s; // Simulated Annealing.
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```

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

# A wide range of optimizers for different problem types

ensmallen 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, Padam, Nadam, WNGrad, AMSGrad
- Genetic variants: Conventional Neuro-evolution (CNE), Covariance Matrix Adaptation Evolution Strategy (CMA-ES)
- Other: Conditional Gradient Descent, Frank-Wolfe algorithm, Simulated Annealing, SPSA

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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, SPSA

And it is also easy to implement new optimizers. https://ensmallen.org/

# **Deep Neural Networks with mlpack**

With ensmallen, we can do deep learning.

### **Deep Neural Networks with mlpack**

With ensmallen, we can 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, 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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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);
```

Did C++ get us what we wanted?

```
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	fail	36.730s

```
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.

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
```

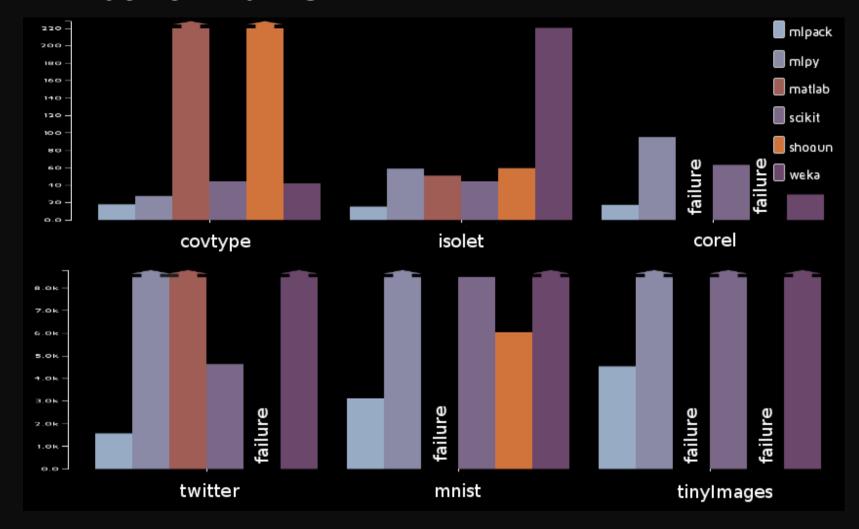
n	arma	numpy	octave	R	Julia
1000	0.042s	0.051s	0.033s	0.056s	0.037s
3000	0.642s	0.812s	0.796s	0.846s	0.844s
10000	16.320s	26.815s	26.478s	26.957s	26.576s
30000	329.87s	708.16s	706.10s	707.12s	704.032s

Armadillo can automatically select the correct ordering for multiplication.

```
Task 4: z=a'(\mathrm{diag}(b)^{-1})c. extern int n; vec a(n, fill::randu); vec b(n, fill::randu); vec c(n, fill::randu); double z=\mathrm{as\_scalar}(\mathrm{a.t}()*\mathrm{inv}(\mathrm{diagmat}(\mathrm{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	fail	0.002s	fail	fail
1M	0.009s	fail	0.024s	fail	fail
10M	0.088s	fail	0.205s	fail	fail
100M	0.793s	fail	1.972s	fail	fail
1B	8.054s	fail	19.520s	fail	fail

# **kNN** benchmarks

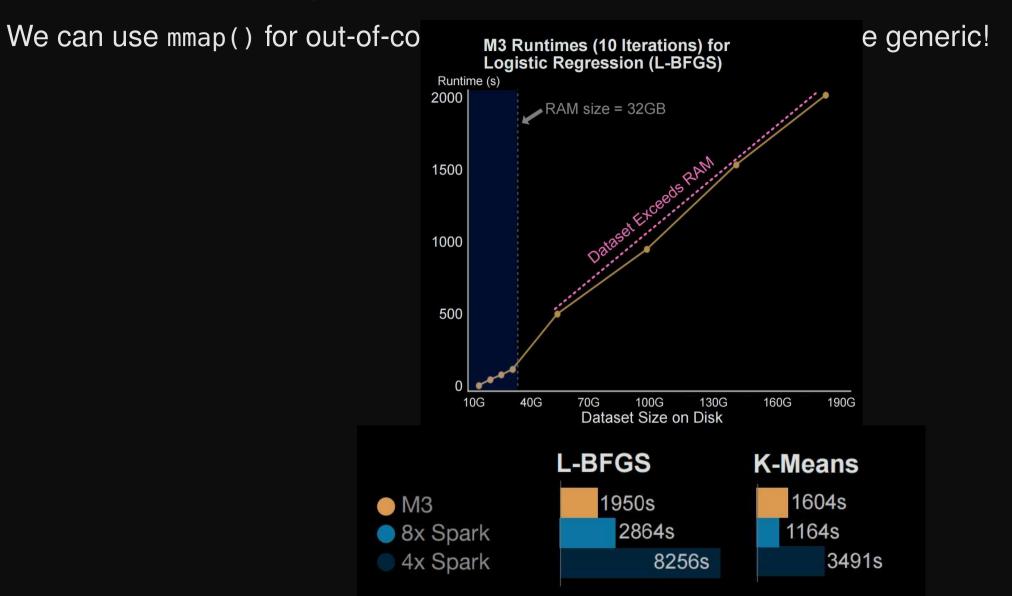


dataset	d	N	mlpack	mlpy	matlab	scikit	shogun	Weka
isolet	617	8k	15.65s	59.09s	50.88s	44.59s	59.56s	220.38s
corel	32	68k	17.70s	95.26s	fail	63.32s	fail	29.38s
covertype	54	581k	18.04s	27.68s	>9000s	44.55s	>9000s	42.34s
twitter	78	583k	1573.92s	>9000s	>9000s	4637.81s	fail	>9000s
mnist	784	70k	3129.46s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



D. Fang, P. Chau. M3: scaling up machine learning via memory mapping, SIGMOD/PODS 2016.

#### ensmallen benchmarks

Runtimes for the linear regression function on various dataset sizes, with n indicating the number of samples, and d indicating the dimensionality of each sample. All Julia runs do not count compilation time.

algorithm	d: 100, n: 1k	d: 100, n: 10k	d: 100, n: 100k	d: 1k, n: 100k
ensmallen-2	0.002s	0.016s	0.182s	2.522s
Optim.jl	0.006s	0.030s	0.337s	4.271s
scipy	0.003s	0.017s	0.202s	2.729s
bfgsmin	0.071s	0.859s	23.220s	2859.81s
ForwardDiff.jl	0.497s	1.159s	4.996s	603.106s
autograd	0.007s	0.026s	0.210s	2.673s

S. Bhardwaj, R.R. Curtin, M. Edel, Y. Mentekidis, C. Sanderson, "ensmallen: a flexible C++ library for efficient function optimization", *Systems for ML Workshop at NeurIPS 2018*, 2018.

#### ensmallen benchmarks

Runtimes for the linear regression function on various dataset sizes, with n indicating the number of samples, and d indicating the dimensionality of each sample. All Julia runs do not count compilation time.

algorithm	d: 100, n: 1k	d: 100, n: 10k	d: 100, n: 100k	d: 1k, n: 100k
ensmallen-1	0.001s	0.009s	0.154s	2.215s
ensmallen-2	0.002s	0.016s	0.182s	2.522s
Optim.jl	0.006s	0.030s	0.337s	4.271s
scipy	0.003s	0.017s	0.202s	2.729s
bfgsmin	0.071s	0.859s	23.220s	2859.81s
ForwardDiff.jl	0.497s	1.159s	4.996s	603.106s
autograd	0.007s	0.026s	0.210s	2.673s

S. Bhardwaj, R.R. Curtin, M. Edel, Y. Mentekidis, C. Sanderson, "ensmallen: a flexible C++ library for efficient function optimization", *Systems for ML Workshop at NeurIPS 2018*, 2018.

## Application: low-latency webserver comment filtering

Let's talk about how we can use mlpack in a deployment environment. Here's our (hypothetical) situation:

- We run a news website for some locality or region.
- We get lots of comment spam.
- Our boss has told us we better fix the comment spam issue or else!

# **Current spam-filtering workflow**

1. User submits comment.

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- 4. Extract more features from the request for spam filtering.

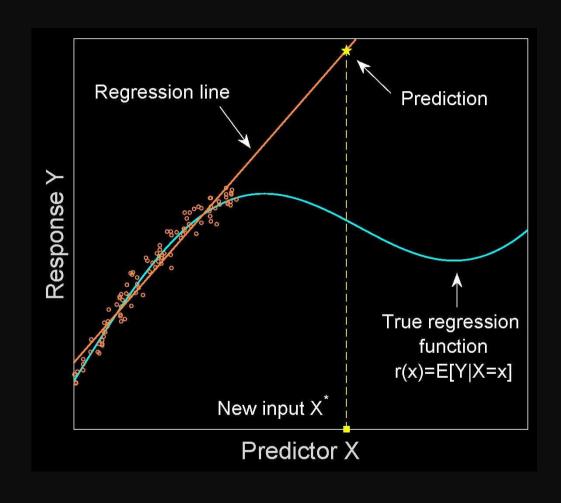
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- 5. Pass extracted features into a fast logistic regression classifier.

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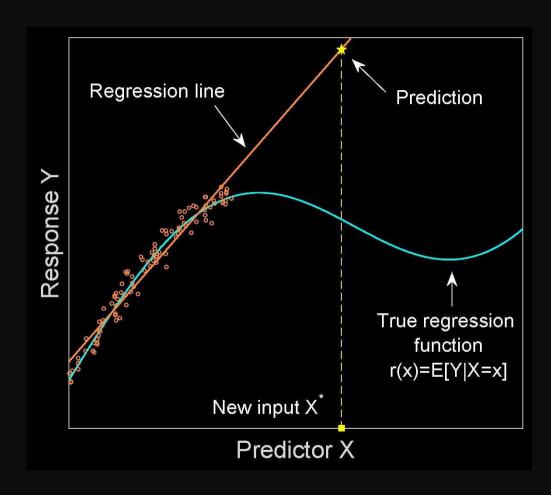
# Why KDE?

Model extrapolation is a problem.



# Why KDE?

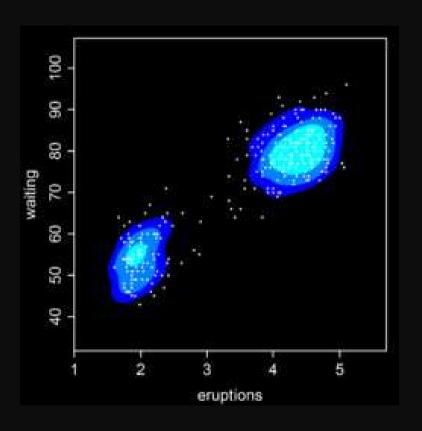
**Model extrapolation** is a problem.



We don't want the model to make predictions for comments coming from locations it wasn't trained on. We don't have much idea what the model would do in that case!

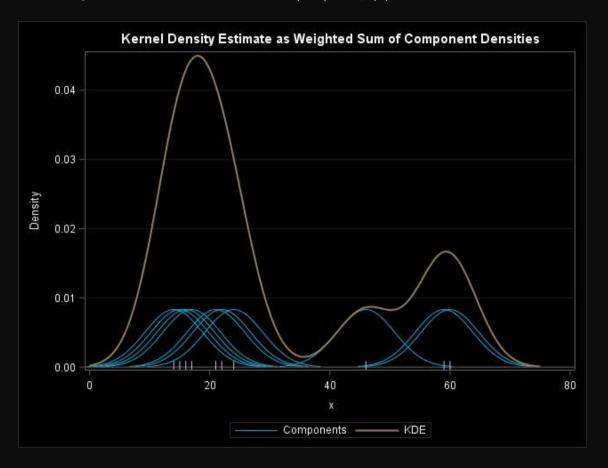
#### What is KDE?

**Kernel density estimation** gives us an estimate of the probability density function at a given location based on the training data.



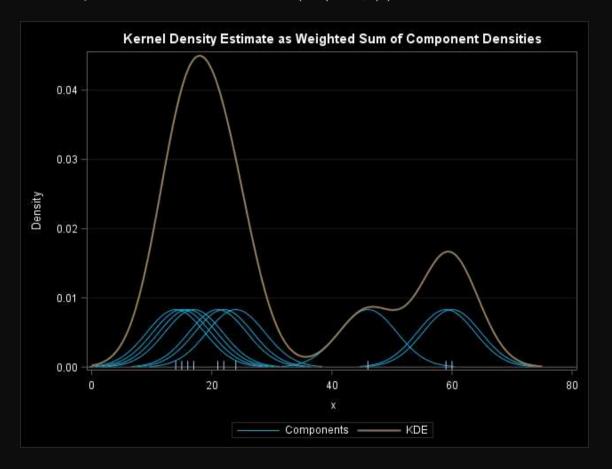
#### What is KDE?

To compute a prediction we compute and sum K(d(x,y)) for some distance  $d(\cdot,\cdot)$  and kernel  $K(\cdot)$ .



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To compute a prediction we compute and sum K(d(x,y)) for some distance  $d(\cdot,\cdot)$  and kernel  $K(\cdot)$ .



mlpack's KDE<> uses dual-tree and single-tree algorithms to provide fast approximate density estimates!

A.G. Gray, A.W. Moore. "Nonparametric density estimation: toward computational tractability." In *Proceedings of the 2003 SIAM International Conference on Data Mining (SIAM Data Mining 2003)*, p. 203–211, 2003.

## Why logistic regression?

We choose logistic regression here because it's *fast* and we are interested in low-latency. To get a prediction, it is just a quick vector-vector dot product, and it won't slow down our pipeline much.

$$y = e^{-(x^T \beta + c)}$$

Hang on: we'll talk about making it more complex later.

## Why logistic regression?

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$$y = e^{-(x^T \beta + c)}$$

Hang on: we'll talk about making it more complex later.

We can use mlpack's LogisticRegression<> for this.

#### Feature engineering

As input to our logistic regression model, we'll use brutally simple slide-optimized features:

- Number of comments from this IP
- Percentage of spam comments from this IP
- Number of comments from this region
- Percentage of spam comments from this region
- Unigram character counts (number of a's, b's, etc.)

#### **Feature engineering**

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- Number of comments from this IP
- Percentage of spam comments from this IP
- Number of comments from this region
- Percentage of spam comments from this region
- Unigram character counts (number of a's, b's, etc.)

In a real situation you'd pick more/different features...

#### "Before" code

We have some auxiliary functions available to us:

```
// Get the string part of a comment.
std::string getCommentString(const Http::Request& reg);
// Post a comment and return the user to the page.
void postComment(const Http::Request& reg, Http::ResponseWriter& response);
// Make the user fill out a captcha and post comment if successful.
void captcha(const Http::Reguest& reg, Http::ResponseWriter& response);
// Return radian long/lat coordinates from an IP.
std::pair<double, double> geolocate(const Http::Request& reg);
// Log information about a request.
void logRequest(const Http::Request& reg);
// Log query functionality.
size_t getNumCommentsFromIP(const Http::Request& reg);
size_t getNumCommentsFromRegion(const Http::Reguest& reg);
double getSpamPercentageFromIP(const Http::Reguest& reg);
double getSpamPercentageFromRegion(const Http::Reguest& reg);
size_t getNumComments();
Http::Request& getComment(const size_t id);
// Get whether or not a comment was spam.
bool wasSpam(const Http::Request& reg);
```

### "Before" comment handler

Written in Pistache. http://pistache.io/

```
struct CommentHandler : public Http::Handler {
  void onRequest(const Http::Request& req, Http::ResponseWriter response) {
    // TODO: GDPR (wait until we get sued)
    logRequest(req);

  // Just post the comment! Don't check for spam, it might reduce our
    // engagement numbers!
    postComment(req, response);
  }
};
```

### **Training the KDE model**

We need a KDE model ready for use. But the KDE model should work with a distance over the surface of the Earth...

### Training the KDE model

Before we run our server, let's train our KDE model.

```
// Build the training dataset. mlpack/Armadillo is column major!
arma::mat dataset(2, getNumComments());
for (size_t currentCol = 0, i = 0; i < dataset.n_cols; ++i) {</pre>
 if (!wasSpam(getComment(i))) {
    std::pair<double, double> latLong = geolocate(getComment(i));
    dataset(0, currentCol) = latLong.first;
    dataset(1, currentCol) = latLong.second;
    ++currentCol;
dataset.shed_cols(currentCol, dataset.n_cols - 1); // Remove any extra columns.
// Train the model.
KDE<GaussianKernel, GreatCircleDistance> kde(0.05 /* relative error tolerance */,
                                             0.0, /* absolute error tolerance */,
                                             GaussianKernel(BANDWIDTH));
kde.Train(dataset);
// Save the model.
data::Save("kde_model.bin", "model", kde);
```

## Training the logistic regression model: feature extraction

Let's write a utility function to turn a Http::Request into an arma::vec.

```
// Process a point in the dataset.
arma::vec extractFeatures(const Http::Request& req) {
  arma::vec result(30, arma::fill::zeros);
  result(0) = (double) getNumCommentsFromIP(reg);
  result(1) = getSpamPercentageFromIP(reg);
  result(2) = (double) getNumCommentsFromRegion(reg);
  result(3) = getSpamPercentageFromRegion(reg);
  std::string comment = getCommentString(reg);
  for (size_t j = 0; j < comment.size(); ++j)</pre>
    if (std::tolower(comment[j]) >= 'a' && std::tolower(comment[j]) <= 'z')</pre>
      result(4 + size_t(std::tolower(comment[j]) - 'a'))++;
  return result;
```

Training the logistic regression model is simple: create the dataset, then train.

```
// Build the logistic regression training dataset. One observation per comment.
arma::mat dataset(30, getNumComments());
arma::Row<size_t> labels(getNumComments()); // 0: clean; 1: spam
for (size_t i = 0; i < dataset.n_cols; ++i)
{
    dataset.col(i) = extractFeatures(getComment(i));
    labels(i) = (size_t) wasSpam(getComment(i));
}
LogisticRegression<> lr(dataset, labels, 0.1 /* lambda (penalty) */);
data::Save("lr_model.bin", "model", lr);
```

Training the logistic regression model is simple: create the dataset, then train.

```
// Build the logistic regression training dataset. One observation per comment.
arma::mat dataset(2, getNumComments());
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But... how do we know we chose the best lambda so we didn't overfit? We can use the hyperparameter tuner.

We can also select the best lambda using the hyperparameter tuner.

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// Build the logistic regression training dataset. One observation per comment.
arma::mat dataset(2, getNumComments());
arma::Row<size_t> labels(getNumComments()); // 0: clean; 1: spam
for (size_t i = 0; i < dataset.n_cols; ++i)
{
    dataset.col(i) = extractFeatures(getComment(i));
    labels(i) = (size_t) wasSpam(getComment(i));
}

// Create the hyperparameter tuner; it will use 20% of the data as the validation set.
HyperParameterTuner<LogisticRegression, F1<Binary>, SimpleCV> hpt(0.2, dataset, labels);
```

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arma::mat dataset(2, getNumComments());
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for (size_t i = 0; i < dataset.n_cols; ++i)</pre>
  dataset.col(i) = extractFeatures(getComment(i));
  labels(i) = (size_t) wasSpam(getComment(i));
// Create the hyperparameter tuner; it will use 20% of the data as the validation set.
HyperParameterTuner<LogisticRegression, F1<Binary>, SimpleCV> hpt(0.2, dataset, labels);
// Use grid search on a set of lambdas.
arma::vec lambdas { 0.0, 0.01, 0.05, 0.1, 0.5, 1.0, 5.0, 10.0 };
double bestLambda;
std::tie(bestLambda) = hpt.Optimize(lambdas);
```

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arma::vec lambdas { 0.0, 0.01, 0.05, 0.1, 0.5, 1.0, 5.0, 10.0 };
double bestLambda;
std::tie(bestLambda) = hpt.Optimize(lambdas);
// Finally train the model with the best lambda.
LogisticRegression<> lr(dataset, labels, bestLambda);
data::Save("lr_model.bin", "model", lr);
```

The hyperparameter tuner supports continuous optimization! So we can use gradient descent too.

```
// Build the logistic regression training dataset. One observation per comment.
arma::mat dataset(2, getNumComments());
arma::Row<size_t> labels(getNumComments()); // 0: clean; 1: spam
for (size_t i = 0; i < dataset.n_cols; ++i)</pre>
  dataset.col(i) = extractFeatures(getComment(i));
  labels(i) = (size_t) wasSpam(getComment(i));
// Create the hyperparameter tuner; it will use 20% of the data as the validation set.
HyperParameterTuner<LogisticRegression, F1<Binary>, SimpleCV, GradientDescent> hpt(0.2, dataset, labels);
hpt.StepSize() = 0.01; // More parameters to tune... :)
hpt.Tolerance() = 1e-5; // Tolerance before terminating search.
// Use gradient descent to find lambda.
double bestLambda;
std::tie(bestLambda) = hpt.Optimize(0.01);
// Finally train the model with the best lambda.
LogisticRegression<> lr(dataset, labels, bestLambda);
data::Save("lr_model.bin", "model", lr);
```

```
struct CommentHandler : public Http::Handler {
  void onRequest(const Http::Request& req, Http::ResponseWriter response) {
    // TODO: GDPR (wait until we get sued)
    logRequest(req);

  // Just post the comment! Don't check for spam, it might reduce our
    // engagement numbers!
    postComment(req, response);
  }
};
```

```
struct CommentHandler : public Http::Handler {
 CommentHandler() {
    data::Load("kde_model.bin", "model", kde);
    data::Load("lr_model.bin", "model", lr);
  void onRequest(const Http::Request& req, Http::ResponseWriter response) {
   // TODO: GDPR (wait until we get sued)
    logRequest(req);
    // Just post the comment! Don't check for spam, it might reduce our
    // engagement numbers!
    postComment(req, response);
 KDE<GaussianKernel, GreatCircleDistance> kde;
 LogisticRegression<> lr;
};
```

```
struct CommentHandler : public Http::Handler {
 CommentHandler() {
    data::Load("kde_model.bin", "model", kde);
    data::Load("lr_model.bin", "model", lr);
  void onRequest(const Http::Request& req, Http::ResponseWriter response) {
    // TODO: GDPR (wait until we get sued)
    logRequest(req);
    std::pair<double, double> latLong = geolocate(reg);
    arma::vec result, point { latLong.first, latLong.second };
    kde.Evaluate(point, result);
    if (result[0] < THRESHOLD) {</pre>
      captcha(req, response);
      return;
    // TODO: more machine learning...
    postComment(req, response);
  KDE<GaussianKernel, GreatCircleDistance> kde;
 LogisticRegression<> lr;
};
```

```
struct CommentHandler : public Http::Handler {
  CommentHandler() {
    data::Load("kde_model.bin", "model", kde);
    data::Load("lr_model.bin", "model", lr);
  void onReguest(const Http::Reguest& reg, Http::ResponseWriter response) {
    // TODO: GDPR (wait until we get sued)
    logRequest(req);
    std::pair<double, double> latLong = geolocate(reg);
    arma::vec result, point { latLong.first, latLong.second };
    kde.Evaluate(point, result);
    if (result[0] < THRESHOLD) {</pre>
      captcha(reg, response);
      return;
    // We did not filter, so use the logistic regression model.
    point = extractFeatures(req);
    size_t predClass = lr.Predict(point); // Could use custom threshold.
    (predClass == 1) ? captcha(reg, response) : postComment(reg, responses);
  KDE<GaussianKernel, GreatCircleDistance> kde;
  LogisticRegression<> lr;
};
```

### We saved our job



#### What did mlpack get us?

- Fast distance implementation via template type GreatCircleDistance
- Flexibility via templates to implement GreatCircleDistance
- Fast KDE via dual-tree and single-tree algorithms
- Hyperparameter tuner for easy optimization of LogisticRegression<> model.
- Easy integration with performance-optimized C++ code.

### We saved our job



How do we keep our job in the future?

- Add a character-RNN after LogisticRegression<> to filter more points
- Hyperparameter tuning, different/custom kernels for KDE
- Better embeddings or features for the comment text, additional features
- ...

We should be employable for at least the next ten years!

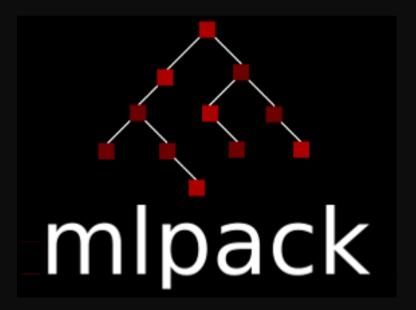
# What didn't I talk about in depth?

- hyper-parameter tuner (there's a lot more to it!)
- 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 3.1.0 was just released and is 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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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.

```
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?**

