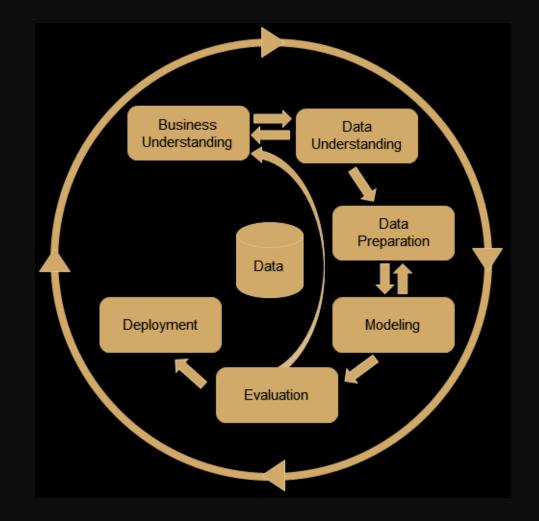
## mlpack: or, How I Learned To Stop Worrying and Love C++

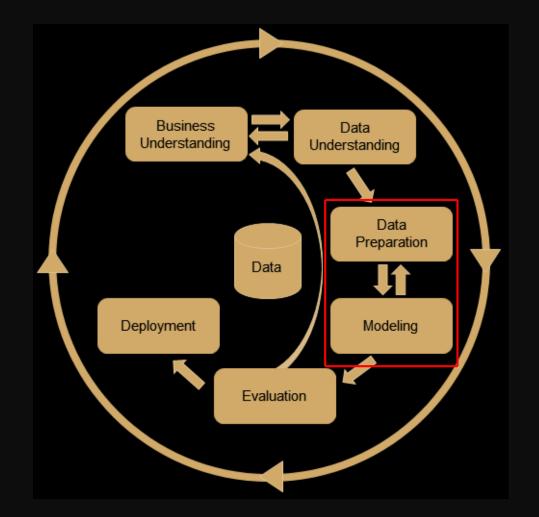
#### Ryan R. Curtin ryan.curtin@relational.ai May 30, 2019



#### Introduction: the data science cycle

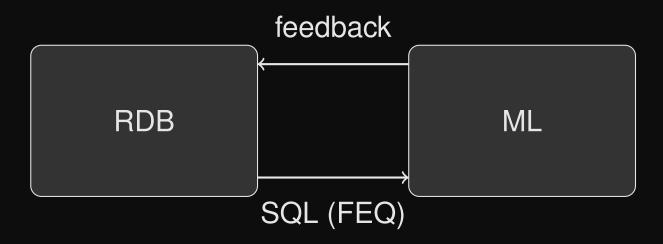


#### Introduction: the data science cycle



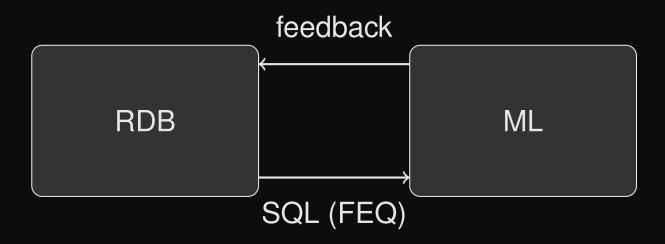
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**How long can this take?** Case study: at Symantec, to train neural networks to detect malicious domains, the FEQ took 8–16 hours and the ML training took 24 hours.

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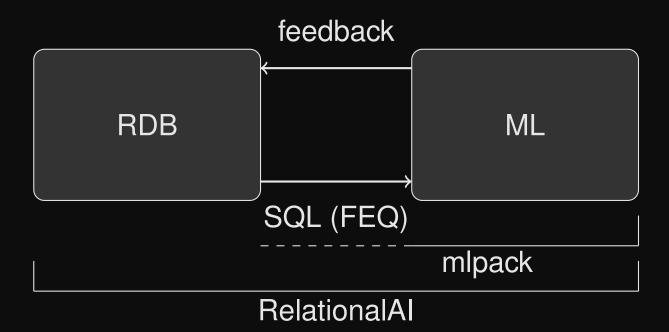
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neural ours and the

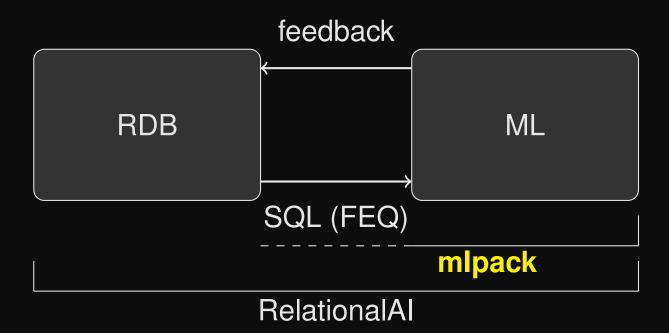
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We can do better: we can combine both of these operations and get massive speedups in some cases!

M.A. Khamis, H.Q. Ngo, A. Rudra. FAQ: Questions Asked Frequently. In *Proceedings of the 35th ACM SIGMOD-SIGACT-SIGAI Symposium on Principles of Database Systems*, pp. 13–28, 2016.

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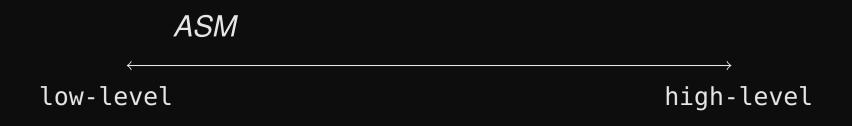
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low-level

high-level

 $\rightarrow$ 

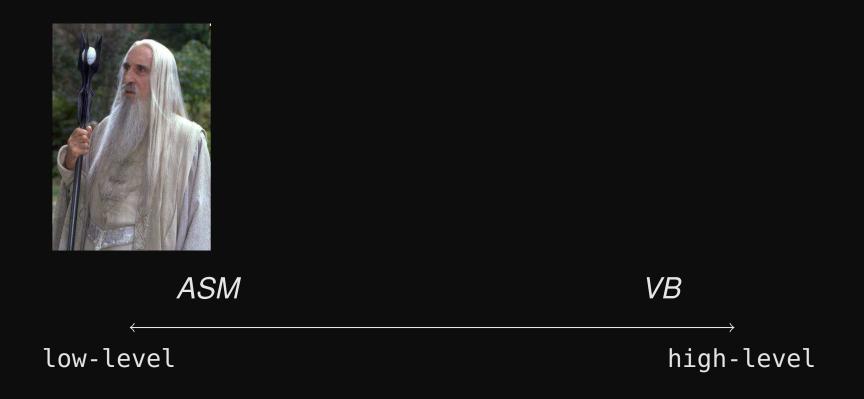


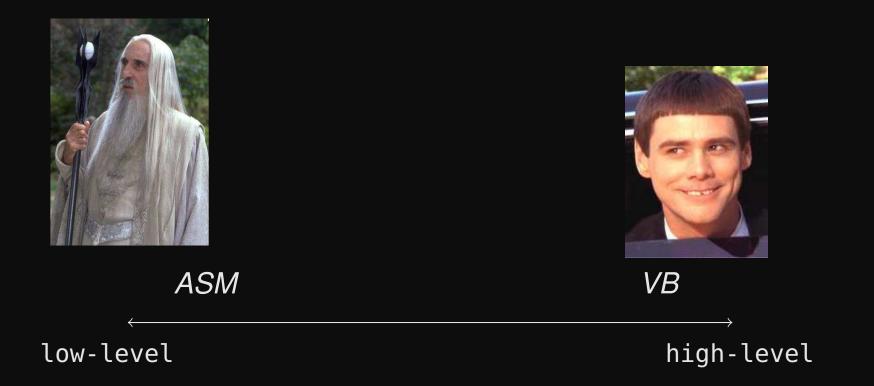


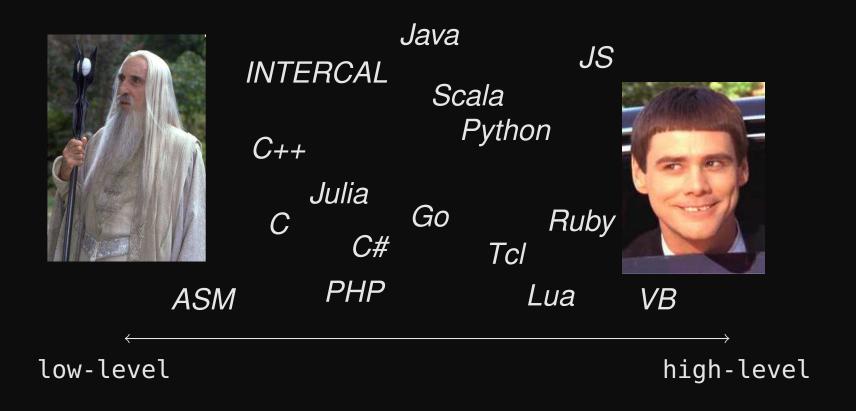
ASM

low-level

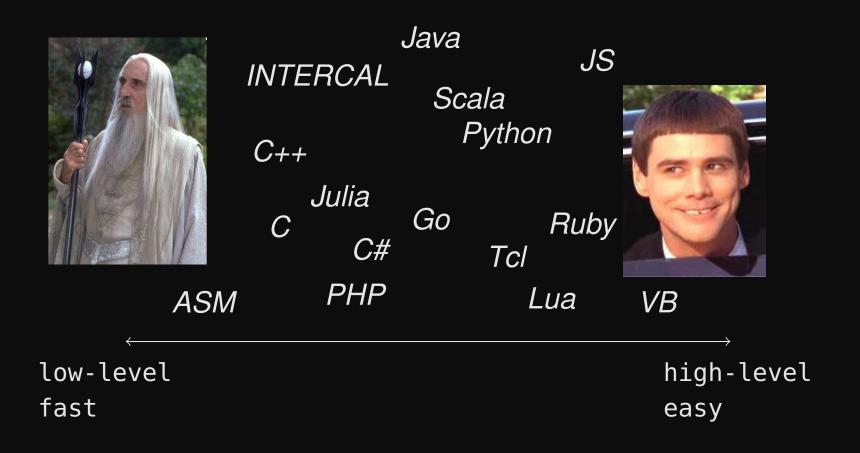
high-level



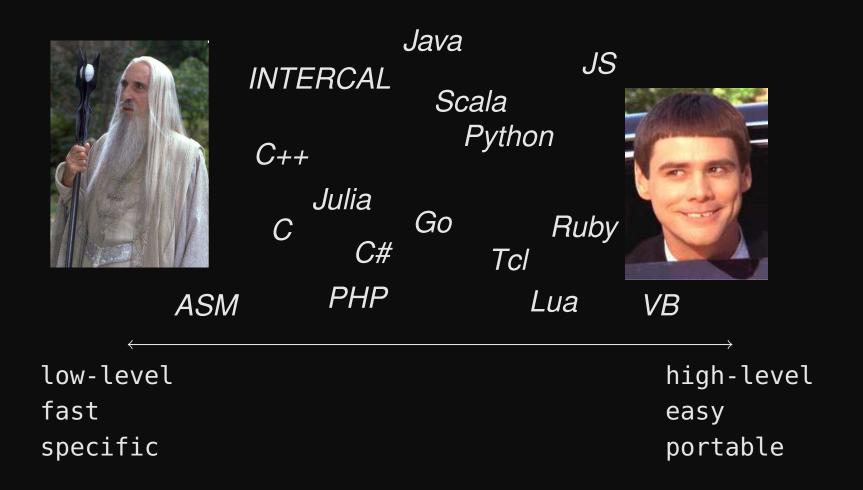




Note: this is not a scientific or particularly accurate representation.



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### The Big Tradeoff

#### speed vs. portability and readability

# The Big Tradeoff

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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?

# 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 (Go, Julia, etc.)
- 140+ developers from around the world
- regular participation in the Google Summer of Code program

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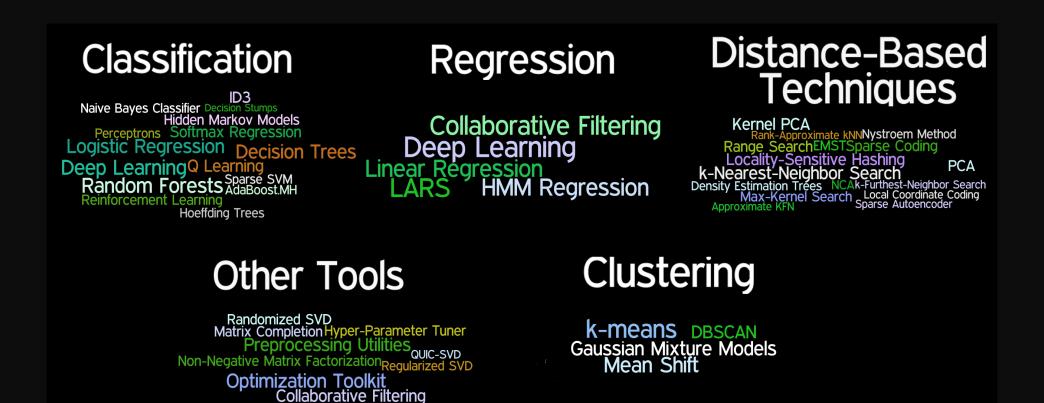
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http://www.mlpack.org/
https://github.com/mlpack/mlpack/

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.



### How do we get mlpack?

Linux (Debian/Ubuntu): Linux (Red Hat/Fedora): OS X (Homebrew):

Windows (nuget):

Or install from source:

```
Linux (Debian/Ubuntu): $ sudo apt-get install libmlpack-dev
```

- Linux (Red Hat/Fedora): \$ sudo dnf install mlpack-devel
  - \$ brew tap brewsci/science &&
     brew install mlpack
    - > nuget add mlpack-windows

```
$ 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
```

# **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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# 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

Can be dropped directly into a Python workflow.

>>>

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- >>> x = np.genfromtxt('my\_data.csv', delimiter=',')

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- >>> x.shape

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

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>>> from mlpack import cf
>>>

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```
>>> from mlpack import cf
>>> 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

```
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 (CFType): Trained CF model to load.

## **Documentation**

### The documentation is also readily available online. https://www.mlpack.org/docs.html



linear\_regression()

clustering:

- dbscan()
- gmm\_train()
- gmm\_generate() gmm\_probability()
- kmeans() mean\_shift()

#### geometry:

- approx\_kfn()
- emst() fastmks()
- Ish()
- knn()
- kfn()
- krann()

preprocessing:

- preprocess\_split()
- preprocess\_binarize()
- preprocess\_describe()

misc. / other:

An implementation of the Naive Bayes Classifier, used for classification. Given labeled data, an NBC model can be trained and saved, or, a pre-trained model can be used for classification.

#### Input options #

name	type	description	default	
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. Only exists in Python binding.	False	
incremental_variance	bool	The variance of each class will be calculated incrementally.	False	
input_model	NBCModelType	Input Naive Bayes model.	None	
labels	int vector	A file containing labels for the training set.	np.empty([0], dtype=np.uint64)	
test	matrix	A matrix containing the test set.	np.empty([0, 0])	
training	matrix	A matrix containing the training set.	np.empty([0, 0])	

## **Documentation**

### The documentation is also readily available online. https://www.mlpack.org/docs.html

#### mlpack\_nbc #

#### **Parametric Naive Bayes Classifier**

\$ mlpack\_nbc [--incremental\_variance] [--input\_model\_file <string>]
 [--labels\_file <string>] [--test\_file <string>] [--training\_file
 <string>] [--output\_file <string>] [--output\_model\_file <string>]
 [--output\_probs\_file <string>] [--predictions\_file <string>]
 [--probabilities\_file <string>]

An implementation of the Naive Bayes Classifier, used for classification. Given labeled data, an NBC model can be trained and saved, or, a pre-trained model can be used for classification. Detailed documentation.

#### Input options &

name	type	description	default
help (-h)	flag	Default help info. Only exists in CLI binding.	
incremental_variance (-I)	flag	The variance of each class will be calculated incrementally.	
info	string	Print help on a specific option. Only exists in CLI binding.	
input_model_file (-m)	NBCModel file	Input Naive Bayes model.	
labels_file (-l)	1-d index matrix file	A file containing labels for the training set.	
test_file (-T)	2-d matrix file	A matrix containing the test set.	
training_file (-t)	2-d matrix file	A matrix containing the training set.	
verbose (-v)	flag	Display informational messages and the full list of parameters and timers at the end of execution.	
version (-V)	flag	Display the version of mlpack. Only exists in CLI binding.	

#### mlpack\_softmax\_regression

mlpack\_nbc
 mlpack\_perceptron

mlpack-3.1.1

cli

overview
 quickstart
 tutorials

data formats

classification:

mlpack\_adaboost

mlpack\_decision\_stumpmlpack\_decision\_tree

mlpack\_random\_forest

mlpack\_hoeffding\_tree
 mlpack\_logistic\_regression

#### regression:

mlpack\_lars
 mlpack\_linear\_regression

#### clustering:

- mlpack\_dbscan
- mlpack\_gmm\_train
- mlpack\_gmm\_generate
- mlpack\_gmm\_probability
  mlpack\_kmeans
- mlpack\_mean\_shift

#### geometry:

- mlpack\_approx\_kfn
- mlpack\_emst
  mlpack\_fastmks
- mlpack\_lsh
- mlpack\_knn
- mlpack\_kfn
- mlpack\_range\_search
- mlpack\_krann
- preprocessing:
- mlpack\_preprocess\_split
- mlpack\_preprocess\_binarize
- mlpack\_preprocess\_describe
   mlpack\_preprocess\_imputer
- mpack\_preproceso\_mpater

# Under the hood



C++ is great!

• Generic programming *at compile time* via templates.

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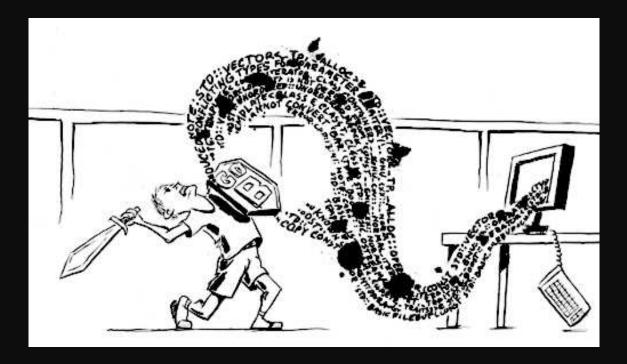
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- The Armadillo library gives us good linear algebra primitives.

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

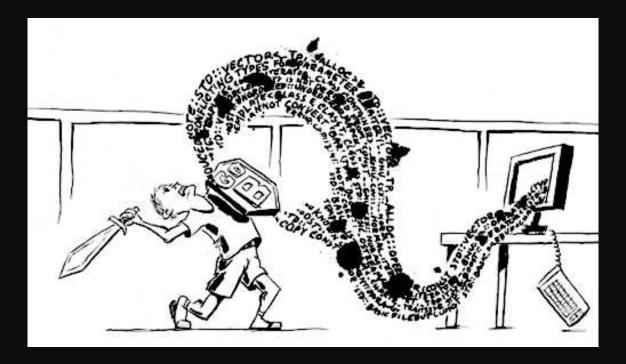
C++ is not great!

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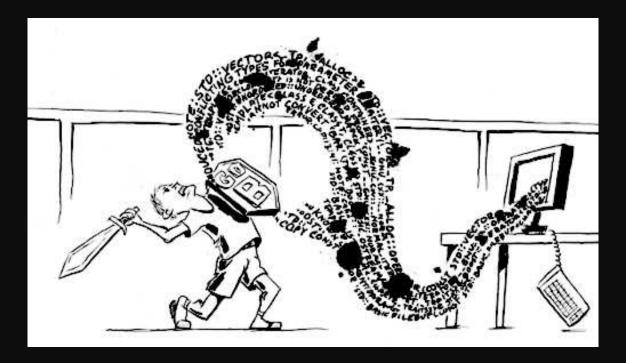
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#### C++ is not great!



- 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...

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?

#### // Now we can use it!

NearestNeighborSearch<MyStupidDistance> n(dataset); n.Search(query\_set, 3, neighbors, distances);

Why write an algorithm for one specific situation?

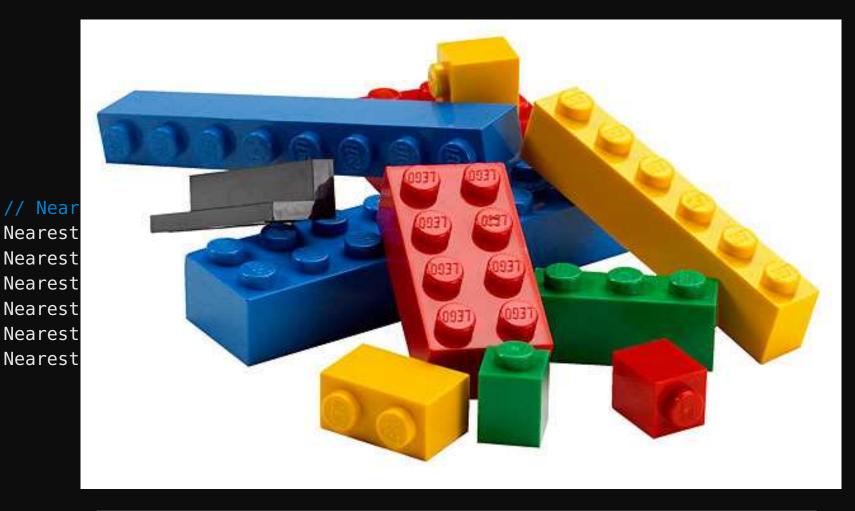
// We can also use sparse matrices instead!
NearestNeighborSearch<MyStupidDistance, arma::sp\_mat>
 n(sparse\_dataset);
n.Search(sparse\_query\_set, 3, neighbors, distances);

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.

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What about virtual inheritance?

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

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vtable lookup penalty!

Using inheritance to call a function costs us instructions:

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

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<pre>; push stack pointer movq %rsp, %rdi ; get location of function movq \$_ZTV1A+16, (%rsp) ; call Evaluate() call _ZN1A1aEd</pre>	; just call Evaluate()! call _ZN1B1aEd.isra.0.constprop.1

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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:

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mat\_add4\_into(e, a, b, c, d, rows, cols);

Fastest! (one pass)



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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;

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



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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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 $\rightarrow$  op<op<mat, mat, add>, mat, add>



What about math? (Armadillo)

In C++ (with Armadillo):

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

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

C++ allows us templated operator overloading:

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

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

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



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



## Take-home

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

With ensmallen, we can do deep learning.

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```
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);
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#### // Predict on test points.

```
arma::mat predictions;
model.Predict(testData, predictions);
```

Did C++ get us what we wanted?

```
Task 1: \overline{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 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

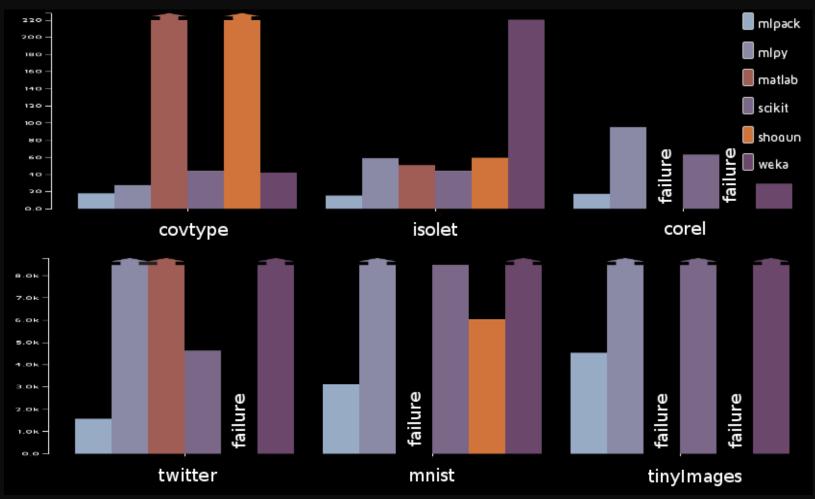
Armadillo can automatically select the correct ordering for multiplication.

```
Task 4: z = a'(\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	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



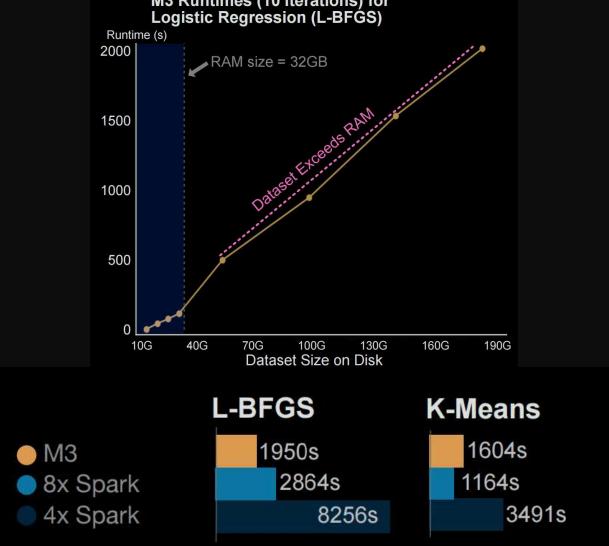
dataset	d	N	mlpack	mlpy	matlab	scikit	shogun	Weka
isolet	617	8k	15.65s	59.09s	50.88s	44.59s	59.56s	220.38s
corel	32	68k	17.70s	95.26s	fail	63.32s	fail	29.38s
covertype	54	581k	18.04s	27.68s	>9000s	44.55s	>9000s	42.34s
twitter	78	583k	1573.92s	>9000s	>9000s	4637.81s	fail	>9000s
mnist	784	70k	3129.46s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

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We can use mmap() for out-of-core learning since our algorithms are generic! M3 Runtimes (10 Iterations) for



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

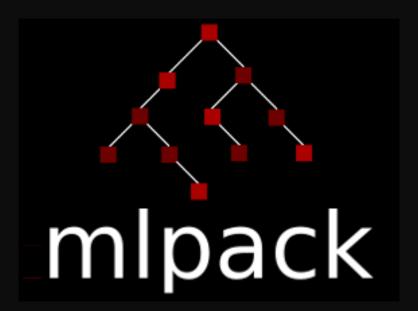
# What didn't I talk about in depth?

- optimization toolkit (ensmallen)
- 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 3.1.1 was just 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 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?**



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