Intro To Machine Learning

John Urbanic
Parallel Computing Scientist
Pittsburgh Supercomputing Center

Using MLlib

One of the reasons we use spark is for easy access to powerful data analysis tools. The MLlib library gives us a machine learning library that is easy to use and utilizes the scalability of the Spark system.

It has supported APIs for Python (with NumPy), R, Java and Scala.

We will use the Python version in a generic manner that looks very similar to any of the above implementations.

There are good example documents for the clustering routine we are using, as well as alternative clustering algorithms, here:

http://spark.apache.org/docs/latest/mllib-clustering.html

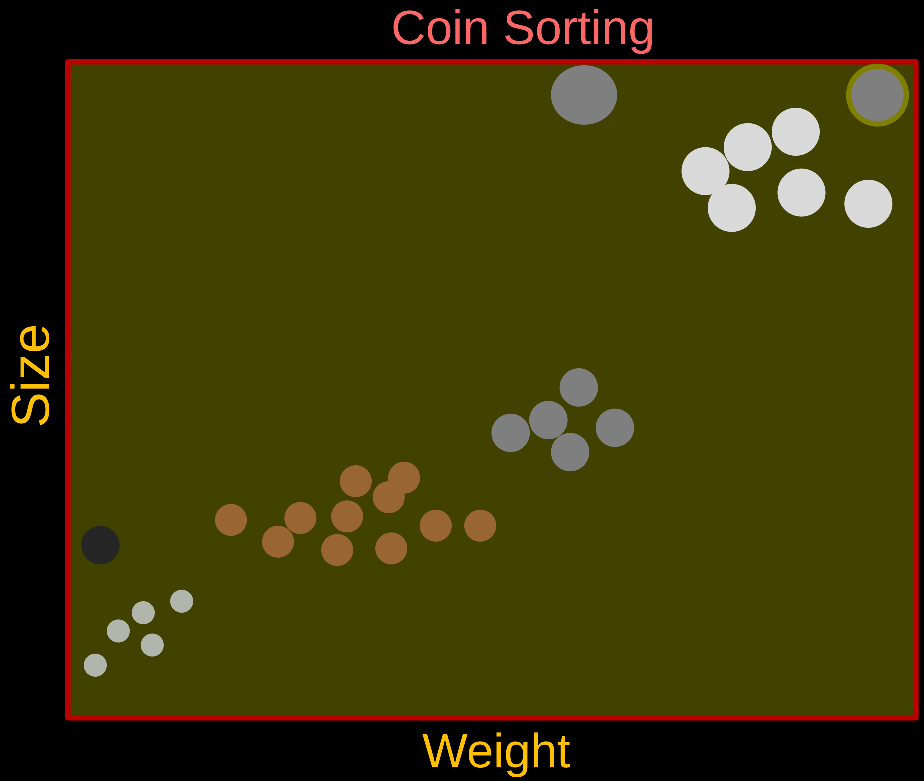
And an excellent API reference document here:

http://spark.apache.org/docs/latest/api/python/pyspark.mllib.html#pyspark.mllib.clustering.KMeans

I suggest you use these pages for all your Spark work.

Clustering

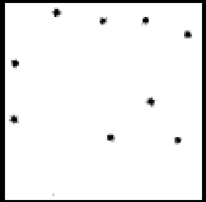
Clustering is a very common operation for finding grouping in data and has countless applications. This is a very simple example, but you will find yourself reaching for a clustering algorithm frequently in pursuing many diverse machine learning objectives, sometimes as one part of a pipeline.



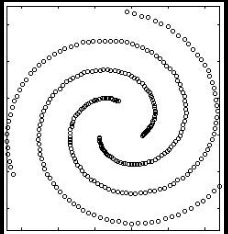
Clustering

As intuitive as clustering is, it presents challenges to implement in an efficient and robust manner.

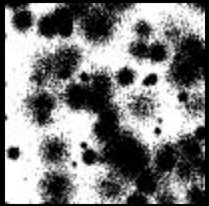
You might think this is trivial to implement in lower dimensional spaces.



But it can get tricky even there.



Sometimes you know how many clusters you have to start with. Often you don't.
How hard can it be to count clusters? How many are here?



We will start with 5000 2D points. We want to figure out how many clusters there are, and their centers. Let's fire up pyspark and get to it…

Finding Clusters

```
      ____              __
     / __/__  ___ _____/ /__
    _\ \/ _ \/ _ `/ __/  '_/
   /__ / .__/\_,_/_/ /_/\_\   version 1.6.0
      /_/

Using Python version 2.7.5 (default, Nov 20 2015 02:00:19)
SparkContext available as sc, HiveContext available as sqlContext.
>>>
>>> rdd1 = sc.textFil
>>>
>>> rdd2 = rdd1.map(l
>>> rdd3 = rdd2.map(l
>>>
```

to RDD

rm to words and integers

```
br06% interact
...
r288%
r288% module load spark
r288% pyspark
```

Finding Our Way

```
>>> rdd1 = sc.textFile("5000_points.txt")
>>> rdd1.count()
5000
>>> rdd1.take(4)
[u'    664159    550946', u'    665845    557965', u'    597173    575538', u'    618600    551446']
>>> rdd2 = rdd1.map(lambda x:x.split())
>>> rdd2.take(4)
[[u'664159', u'550946'], [u'665845', u'557965'], [u'597173', u'575538'], [u'618600', u'551446']]
>>> rdd3 = rdd2.map(lambda x: [int(x[0]),int(x[1])])
>>> rdd3.take(4)
[[664159, 550946], [665845, 557965], [597173, 575538], [618600, 551446]]
>>>
```

Finding Clusters

```
      ____              __
     / __/__  ___ _____/ /__
    _\ \/ _ \/ _ `/ __/  '_/
   /__ / .__/\_,_/_/ /_/\_\   version 1.6.0
      /_/

Using Python version 2.7.5 (default, Nov 20 2015 02:00:19)
SparkContext available as sc, HiveContext available as sqlContext.
>>>
>>> rdd1 = sc.textFile("5000_points.txt")
>>>
>>> rdd2 = rdd1.map(lambda x:x.split())
>>> rdd3 = rdd2.map(lambda x: [int(x[0]),int(x[1])])
>>>
>>>
>>> from pyspark.mllib.clustering import KMeans
```

Read into RDD

Transform

Import Kmeans

class pyspark.mllib.clustering.**KMeans**

New in version 0.9.0.

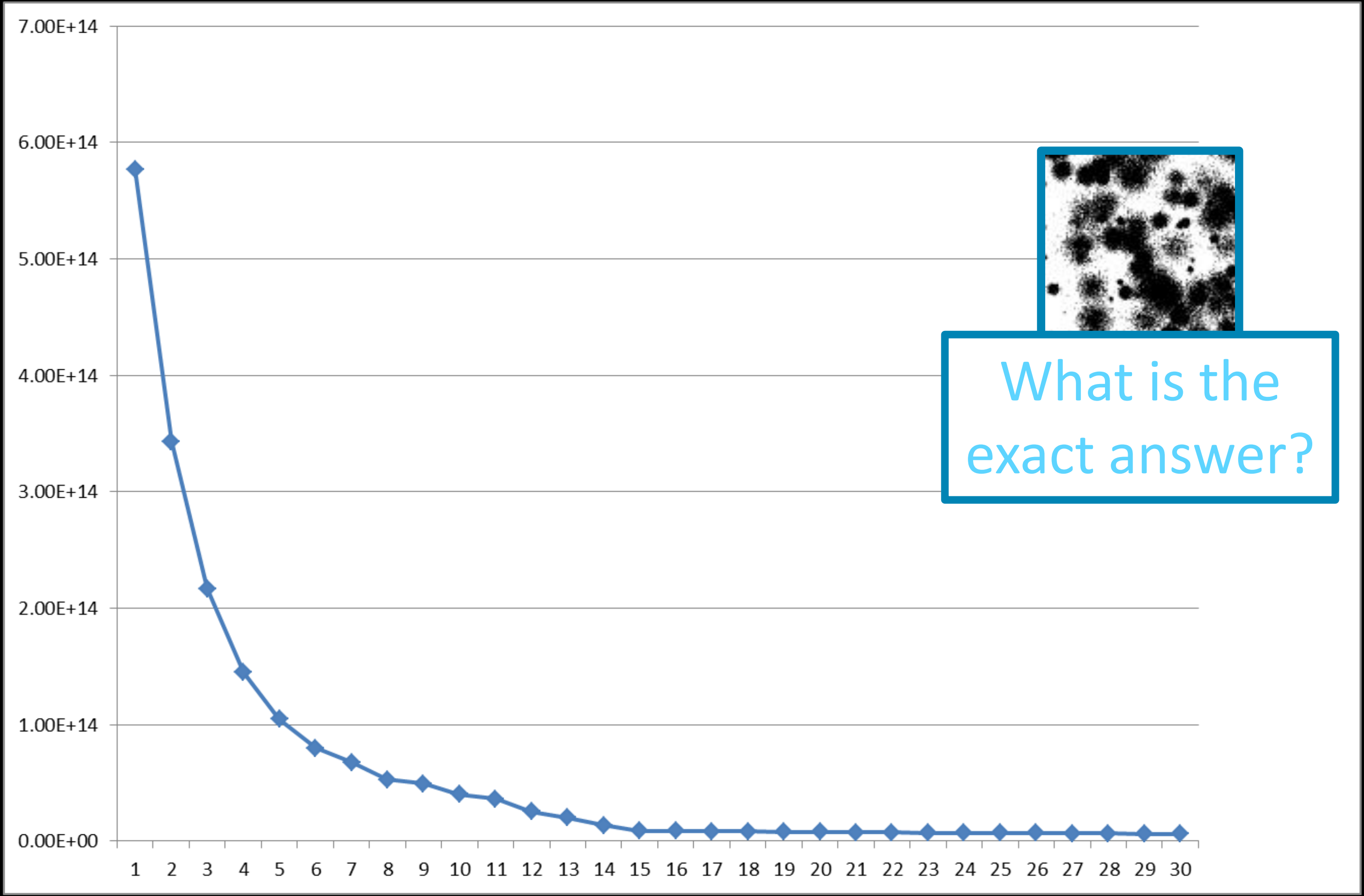
classmethod **train**(*rdd, k, maxIterations=100, runs=1, initializationMode='k-means||', seed=None, initializationSteps=5, epsilon=0.0001, initialModel=None*) ¶

Train a k-means clustering model.

Parameters:

- **rdd** – Training points as an *RDD* of *Vector* or convertible sequence types.
- **k** – Number of clusters to create.
- **maxIterations** – Maximum number of iterations allowed. (default: 100)
- **runs** – This param has no effect since Spark 2.0.0.
- **initializationMode** – The initialization algorithm. This can be either "random" or "k-means||". (default: "k-means||")
- **seed** – Random seed value for cluster initialization. Set as None to generate seed based on system time. (default: None)
- **initializationSteps** – Number of steps for the k-means|| initialization mode. This is an advanced setting – the default of 5 is almost always enough. (default: 5)
- **epsilon** – Distance threshold within which a center will be considered to have converged. If all centers move less than this Euclidean distance, iterations are stopped. (default: 1e-4)
- **initialModel** – Initial cluster centers can be provided as a KMeansModel object rather than using the random or k-means|| initialization model. (default: None)

Finding Clusters



Finding Clusters

```
      ____              __
     / __/__  ___ _____/ /__
    _\ \/ _ \/ _ `/ __/  '_/
   /__ / .__/\_,_/_/ /_/\_\   version 1.6.0
      /_/

Using Python version 2.7.5 (default, Nov 20 2015 02:00:19)
SparkContext available as sc, HiveContext available as sqlContext.
>>>
>>> rdd1 = sc.textFile("5000_points.txt")
>>>
>>> rdd2 = rdd1.map(lambda x:x.split())
>>> rdd3 = rdd2.map(lambda x: [int(x[0]),int(x[1])])
>>>
>>> from pyspark.mllib.clustering import KMeans
>>>
>>> for clusters in range(1,30):
...     model = KMeans.train(rdd3, clusters)
...     print (clusters, model.computeCost(rdd3))
...
```

Let's see results for 1-30 cluster tries

```
1 5.76807041184e+14
2 3.43183673951e+14
3 2.23097486536e+14
4 1.64792608443e+14
5 1.19410028576e+14
6 7.97690150116e+13
7 7.16451594344e+13
8 4.81469246295e+13
9 4.23762700793e+13
10 3.65230706654e+13
11 3.16991867996e+13
12 2.94369408304e+13
13 2.04031903147e+13
14 1.37018893034e+13
15 8.91761561687e+12
16 1.31833652006e+13
17 1.39010717893e+13
18 8.22806178508e+12
19 8.22513516563e+12
20 7.79359299283e+12
21 7.79615059172e+12
22 7.70001662709e+12
23 7.24231610447e+12
24 7.21990743993e+12
25 7.09395133944e+12
26 6.92577789424e+12
27 6.53939015776e+12
28 6.57782690833e+12
29 6.37192522244e+12
```

Right Answer?

```
>>> for trials in range(10):
...     print
...     for clusters in range(12,18):
...         model = KMeans.train(rdd3,clusters)
...         print (clusters, model.computeCost(rdd3))
```

```
12 2.45472346524e+13
13 2.00175423869e+13
14 1.90313863726e+13
15 1.52746006962e+13
16 8.67526114029e+12
17 8.49571894386e+12

12 2.62619056924e+13
13 2.90031673822e+13
14 1.52308079405e+13
15 8.91765957989e+12
16 8.70736515113e+12
17 8.49616440477e+12

12 2.5524719797e+13
13 2.14332949698e+13
14 2.11070395905e+13
15 1.47792736325e+13
16 1.85736955725e+13
17 8.42795740134e+12

12 2.31466242693e+13
13 2.10129797745e+13
14 1.45400177021e+13
15 1.52115329071e+13
16 1.41347332901e+13
17 1.31314086577e+13

12 2.47927778784e+13
13 2.43404436887e+13
14 2.1522702068e+13
15 8.91765000665e+12
16 1.4580927737e+13
17 8.57823507015e+12
```

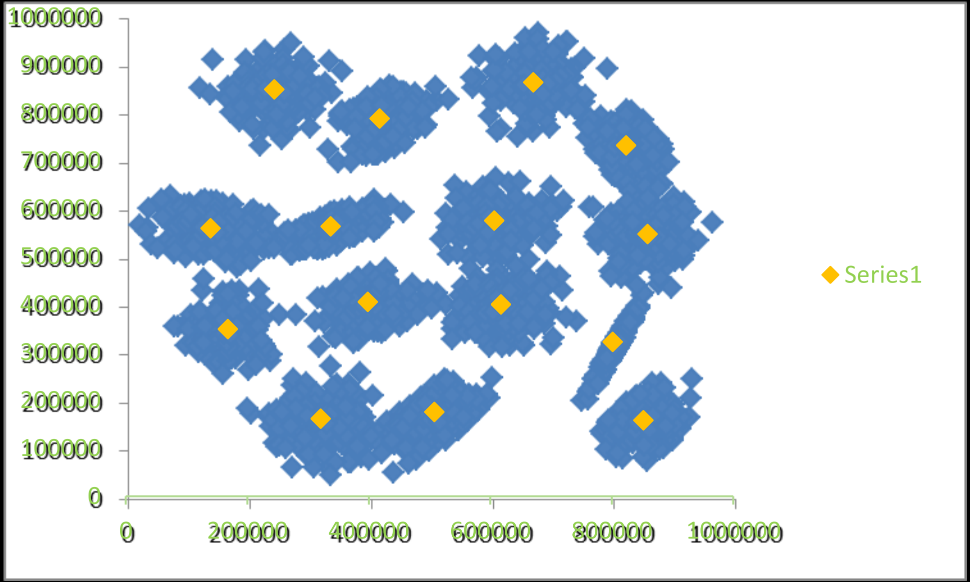
```
12 2.31466520037e+13
13 1.91856542103e+13
14 1.4933202312e+13
15 1.3506302755e+13
16 8.7757678836e+12
17 1.60075548613e+13

12 2.5187054064e+13
13 1.83498739266e+13
14 1.96076943156e+13
15 1.41725666214e+13
16 1.41986217172e+13
17 8.46755159547e+12

12 2.38234539188e+13
13 1.85101922046e+13
14 1.91732620477e+13
15 8.91769396968e+12
16 8.64876051004e+12
17 8.54677681587e+12

12 2.5187054064e+13
13 2.04031903147e+13
14 1.95213876047e+13
15 1.93000628589e+13
16 2.07670831868e+13
17 8.47797102908e+12

12 2.39830397362e+13
13 2.00248378195e+13
14 1.34867337672e+13
15 2.09299321238e+13
16 1.32266735736e+13
17 8.50857884943e+12
```

Find the Centers

```
>>> for trials in range(10):                          #Try ten times to find best result
...     for clusters in range(12, 16):                #Only look in interesting range
...         model = KMeans.train(rdd3, clusters)
...         cost = model.computeCost(rdd3)
...         centers = model.clusterCenters            #Let's grab cluster centers
...         if cost<1e+13:                            #If result is good, print it out
...            print (clusters, cost)
...            for coords in centers:
...              print (int(coords[0]), int(coords[1]))
...            break
...
```

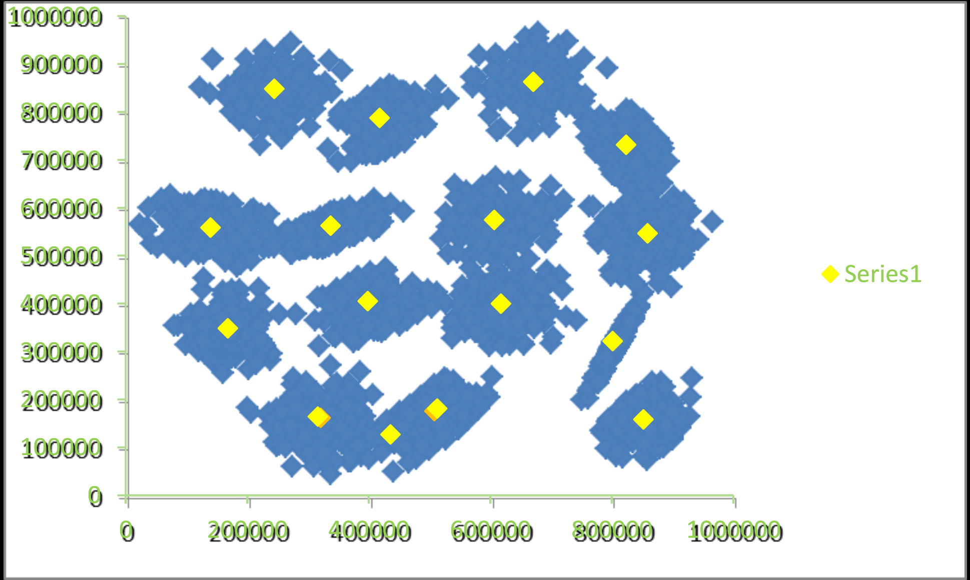
```
15 8.91761561687e+12
852058 157685
606574 574455
320602 161521
139395 558143
858947 546259
337264 562123
244654 847642
398870 404924
670929 862765
823421 731145
507818 175610
801616 321123
617926 399415
417799 787001
167856 347812
15 8.91765957989e+12
670929 862765
139395 558143
244654 847642
852058 157685
617601 399504
801616 321123
507818 175610
337264 562123
858947 546259
823421 731145
606574 574455
167856 347812
398555 404855
417799 787001
320602 161521
```

Fit?



1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
0
200000
400000
600000
800000
1000000
Series1

16 Clusters



1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
0
200000
400000
600000
800000
1000000
Series1

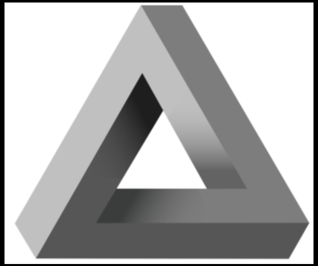
Dimensionality Reduction

We are going to find a recurring theme throughout machine learning:

- Our data naturally resides in higher dimensions
- Reducing the dimensionality makes the problem more tractable
- And simultaneously provides us with insight

This last two bullets highlight the principle that "learning" is often finding an effective compressed representation.

As we return to this theme, we will highlight these slides with our Dimensionality Reduction badge so that you can follow this thread and appreciate how fundamental it is.



Why all these dimensions?

The problems we are going to address, as well as the ones you are likely to encounter, are naturally highly dimensional. If you are new to this concept, lets look at an intuitive example to make it less abstract.

Category	Purchase Total ($)
Children's Clothing	$800
Pet Supplies	$0
Cameras (Dash, Security, Baby)	$450
Containers (Storage)	$350
Romance Book	$0
Remodeling Books	$80
Sporting Goods	$25
Children's Toys	$378
Power Tools	$0
Computers	$0
Garden	$0
Children's Books	$180

< 2900 Categories >

This is a 2900 dimensional vector.

Why all these dimensions?

If we apply our newfound clustering expertise, we might find we have 80 clusters (with an acceptable error).

People spending on “child’s toys “ and “children’s clothing” might cluster with “child’s books” and, less obvious, "cameras (Dashcams, baby monitors and security cams)", because they buy new cars and are safety conscious. We might label this cluster "Young Parents". We also might not feel obligated to label the clusters at all. We can now represent any customer by their distance from these 80 clusters.

80 dimensional vector.

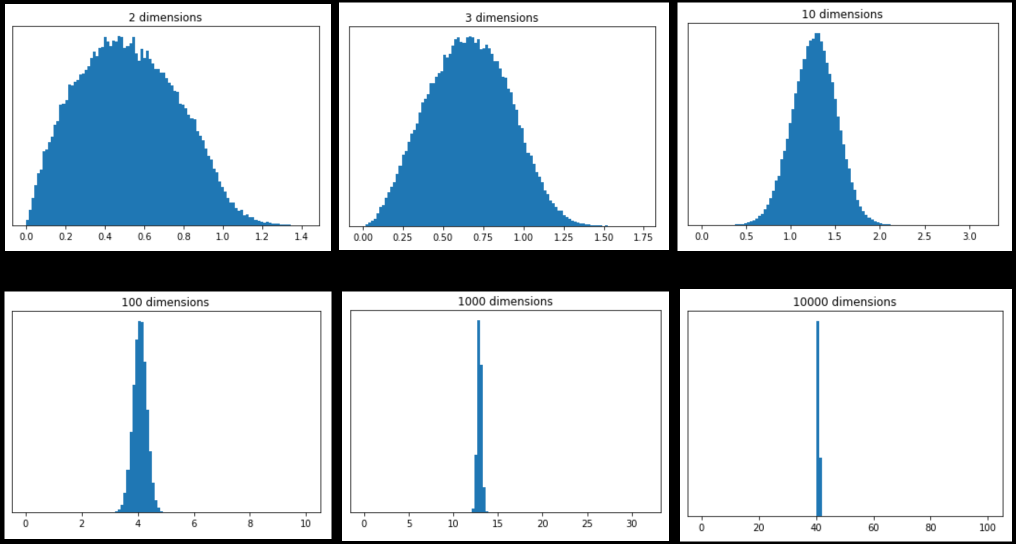
Customer Representation									
Cluster	Young Parents	College Athlete	Auto Enthusiast	Knitter	Steelers Fan	Shakespeare Reader	Sci-Fi Fan	Plumber	...
Distance	0.02	2.3	1.4	8.4	2.2	14.9	3.3	0.8	...

We have now accomplished two things:

- we have compressed our data
- learned something about our customers (who to send a dashcam promo to).

Curse of Dimensionality

This is a good time to point out how our intuition can lead us astray as we increase the dimensionality of our problems - which we will certainly be doing - and to a great degree. There are several related aspects to this phenomenon, often referred to as the *Curse of Dimensionality*. One root cause of confusion is that our notion of Euclidian distance starts to fail in higher dimensions.



These plots show the distributions of pairwise distances between randomly distributed points within differently dimensioned unit hypercubes. Notice how all the points start to be about the same distance apart.

Once can imagine this makes life harder on a clustering algorithm!

There are other surprising effects: random vectors are almost all orthogonal; the unit sphere takes almost no volume in the unit square. These cause all kinds of problems when generalizing algorithms from our lowly 3D world.

Metrics

Even the definition of distance (the *metric*) can vary based upon application. If you are solving chess problems, you might find the Manhattan distance (or taxicab metric) to be most useful.

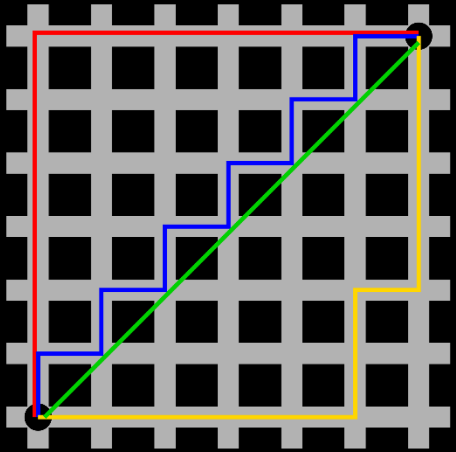


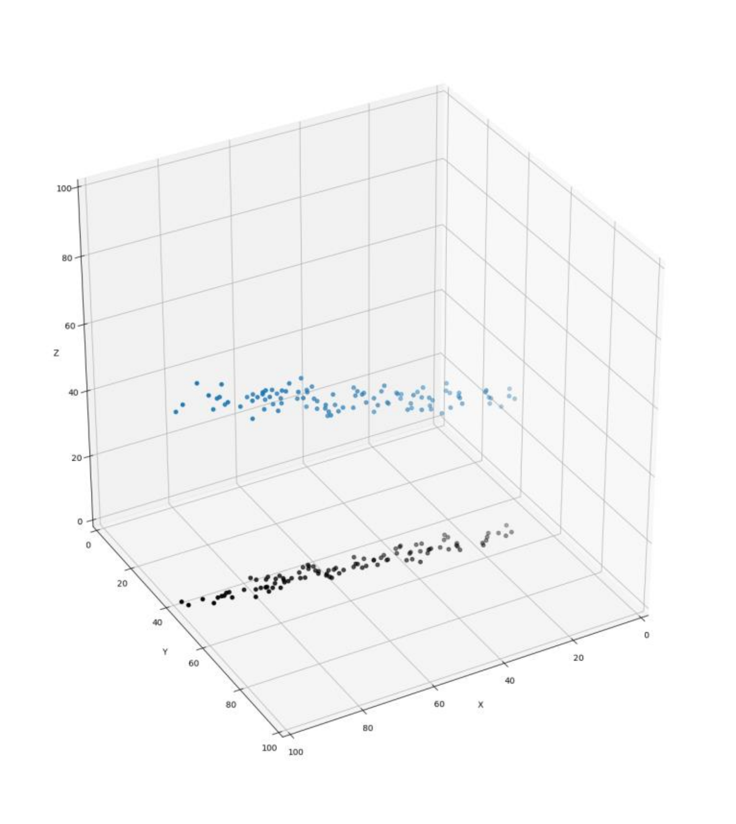
Image Source: Wikipedia

For comparing text strings, we might choose one of dozens of different metrics. For spell checking you might want one that is good for phonetic distance, or maybe edit distance. For natural language processing (NLP), you probably care more about tokens.

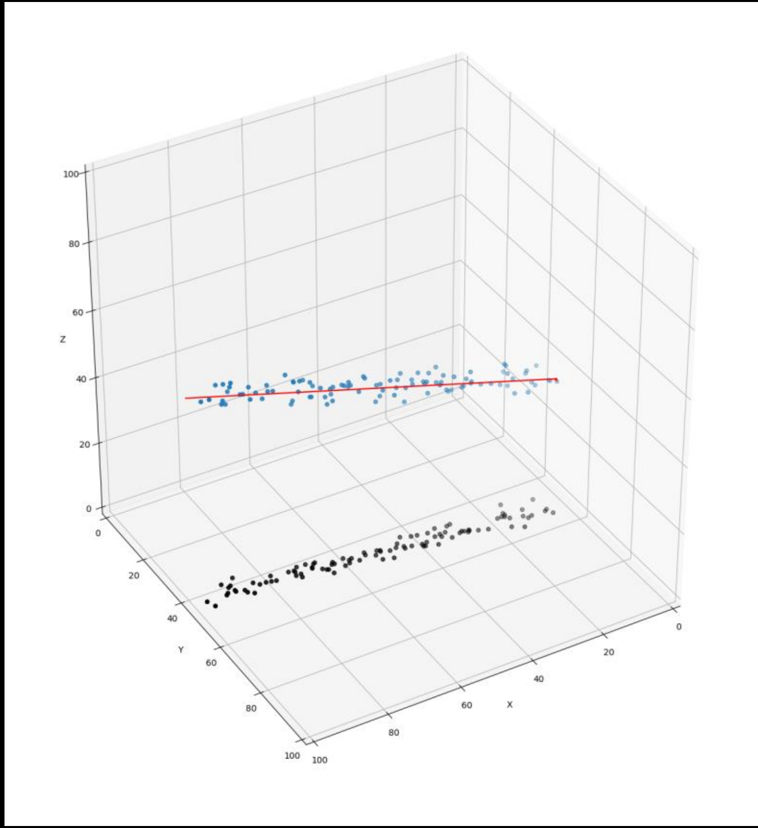
For genomics, you might care more about string sequences.

Some useful measures don't even qualify as metrics (usually because they fail the triangle inequality: $a + b \geq c$).

Alternative DR: Principal Component Analysis

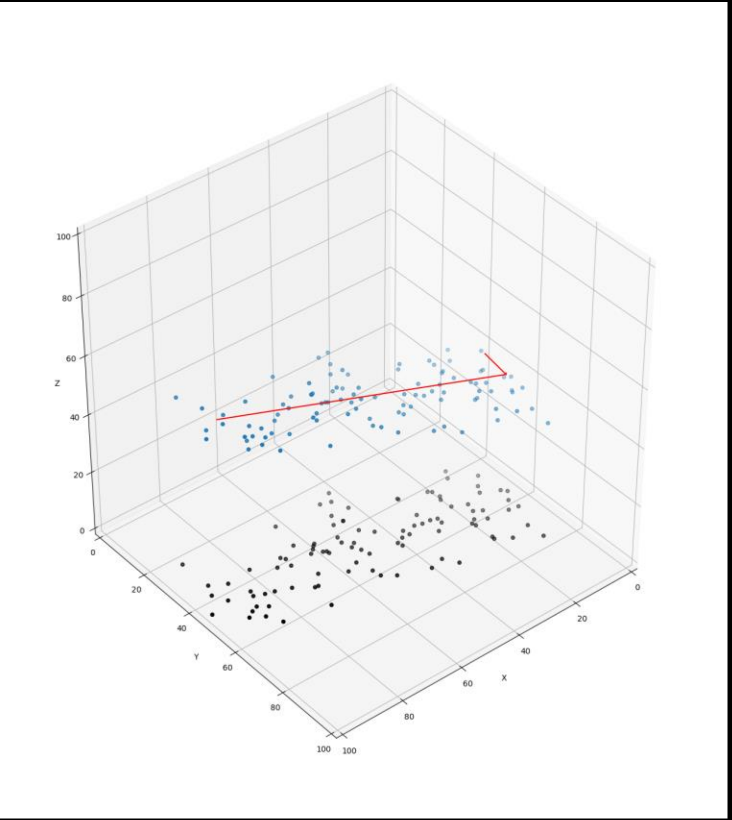


3D Data Set

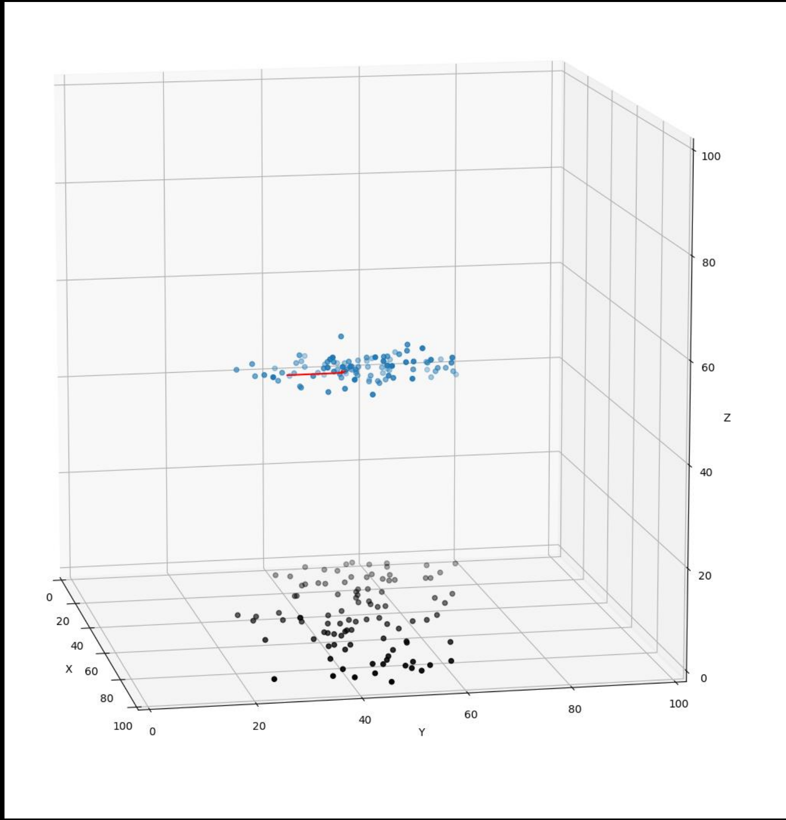


Maybe mostly 1D!

Alternative DR: Principal Component Analysis



Flatter 2D-ish Data Set



View down the 1st Princ. Comp.

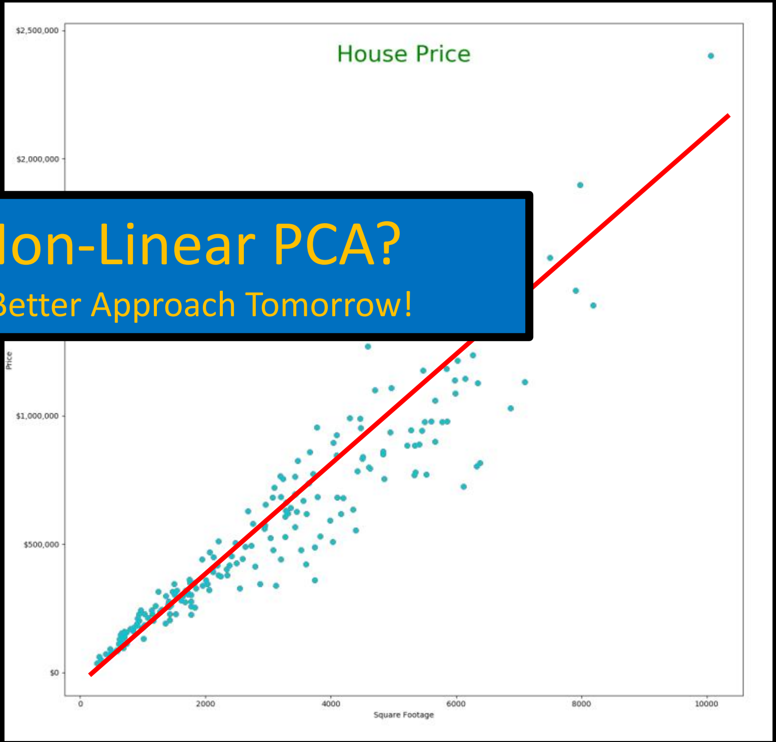
Why So Many Alternatives?

Let's look at one more example today. Suppose we are tying to do a Zillow type of analysis and predict home values based upon available factors. We may have an entry (vector) for each home that captures this kind of data:

Home Data	
Latitude	4833438 north
Longitude	630084 east
Last Sale Price	$ 480,000
Last Sale Year	1998
Width	62
Depth	40
Floors	3
Bedrooms	3
Bathrooms	2
Garage	2
Yard Width	84
Yard Depth	60
...	...

There may be some opportunities to reduce the dimension of the vector here. Perhaps clustering on the geographical coordinates...

Principal Component Analysis Fail



Non-Linear PCA?

A Better Approach Tomorrow!

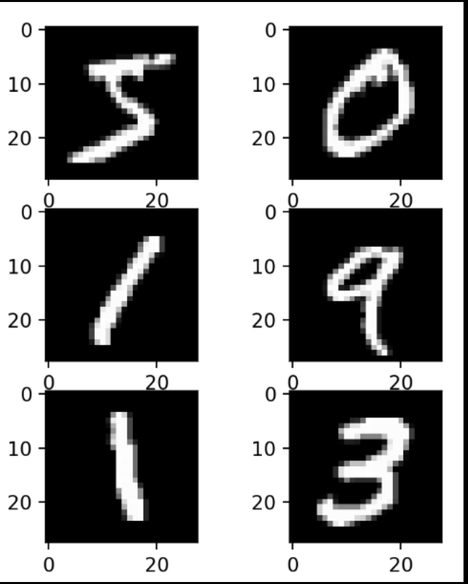
1st Component Off

Data Not Very Linear

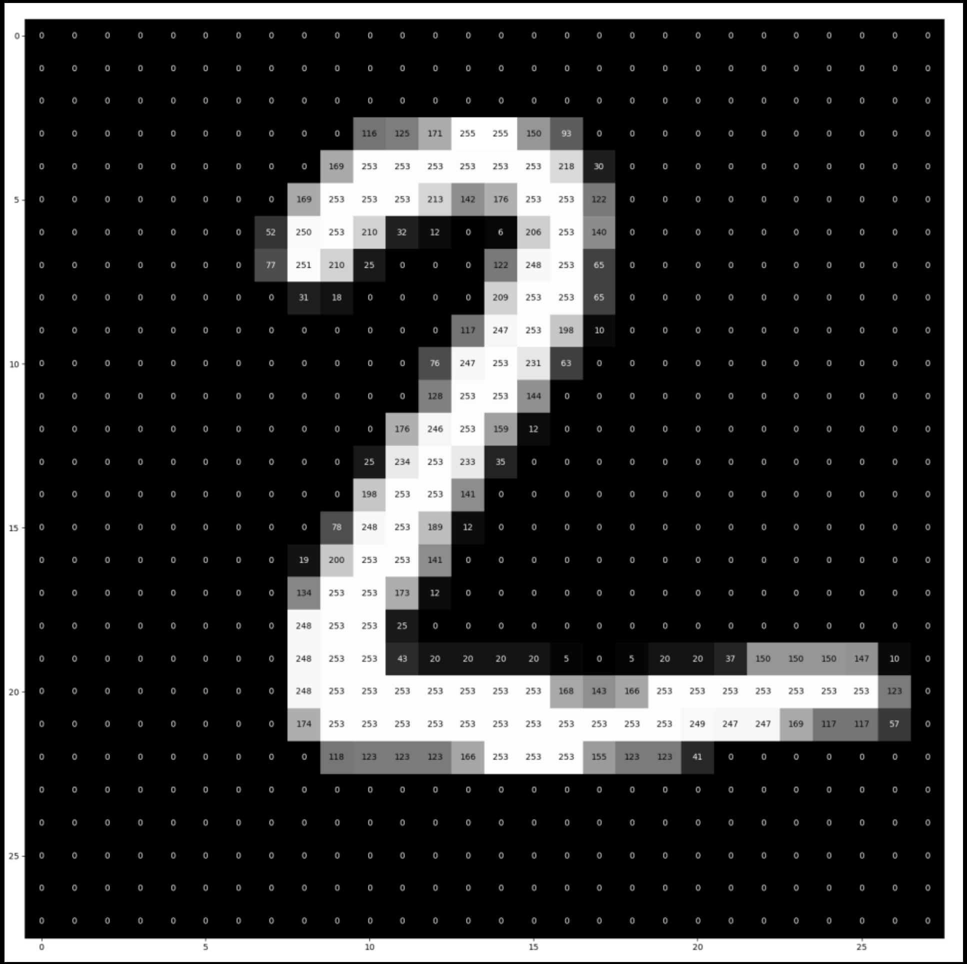
D x W Is Not Linear

But (DxW) Fits Well

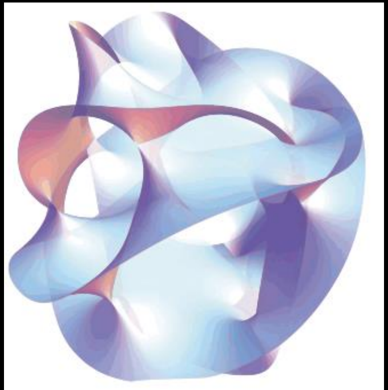
Why Would An Image Have 784 Dimensions?



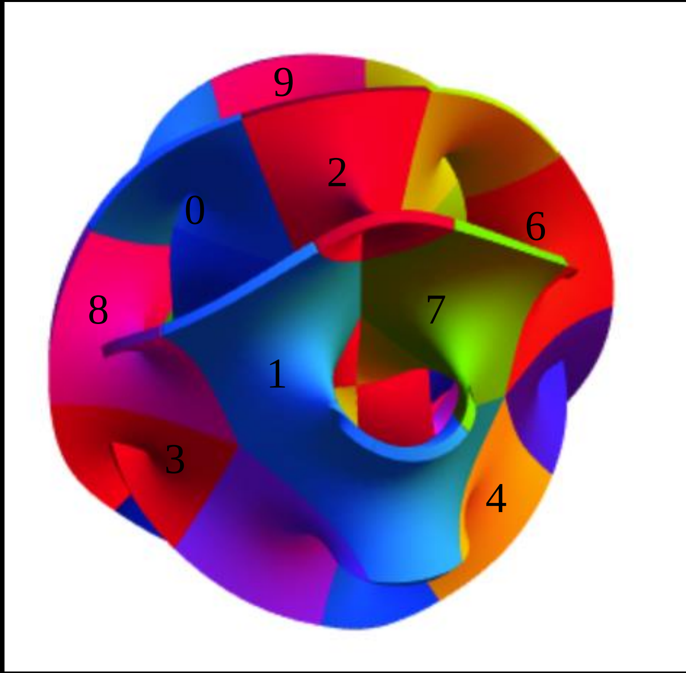
MNIST 28x28
greyscale images



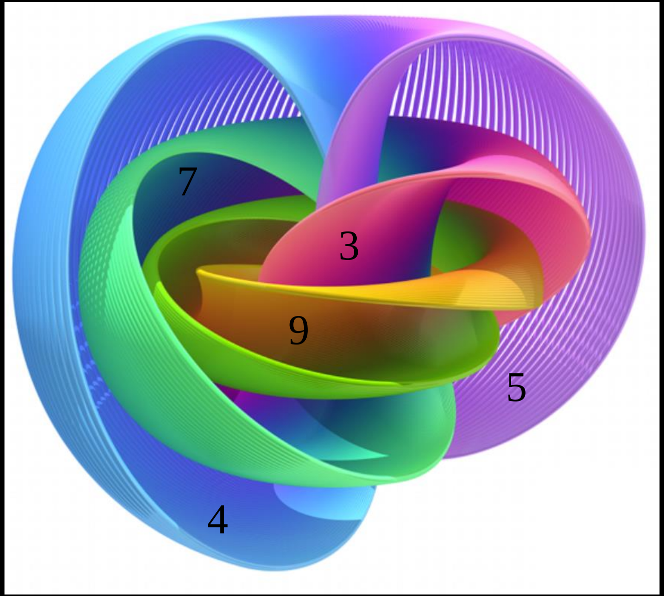
Central Hypothesis of Modern DL



Data Lives On
A Lower Dimensional
Manifold



Maybe Very Contiguous

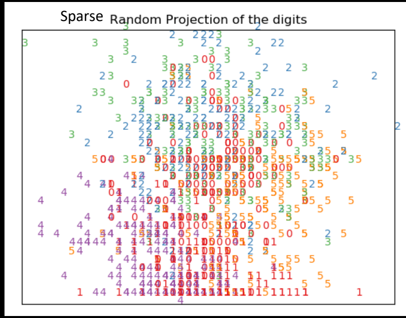


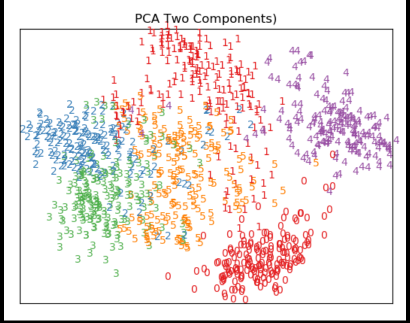
Maybe Less So

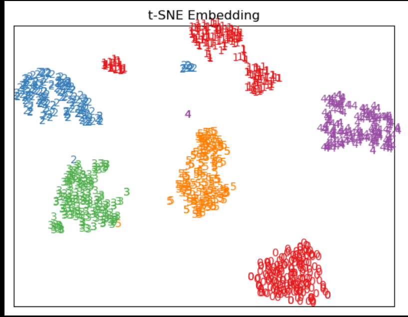
Images from Wikipedia

Testing These Ideas With Scikit-learn

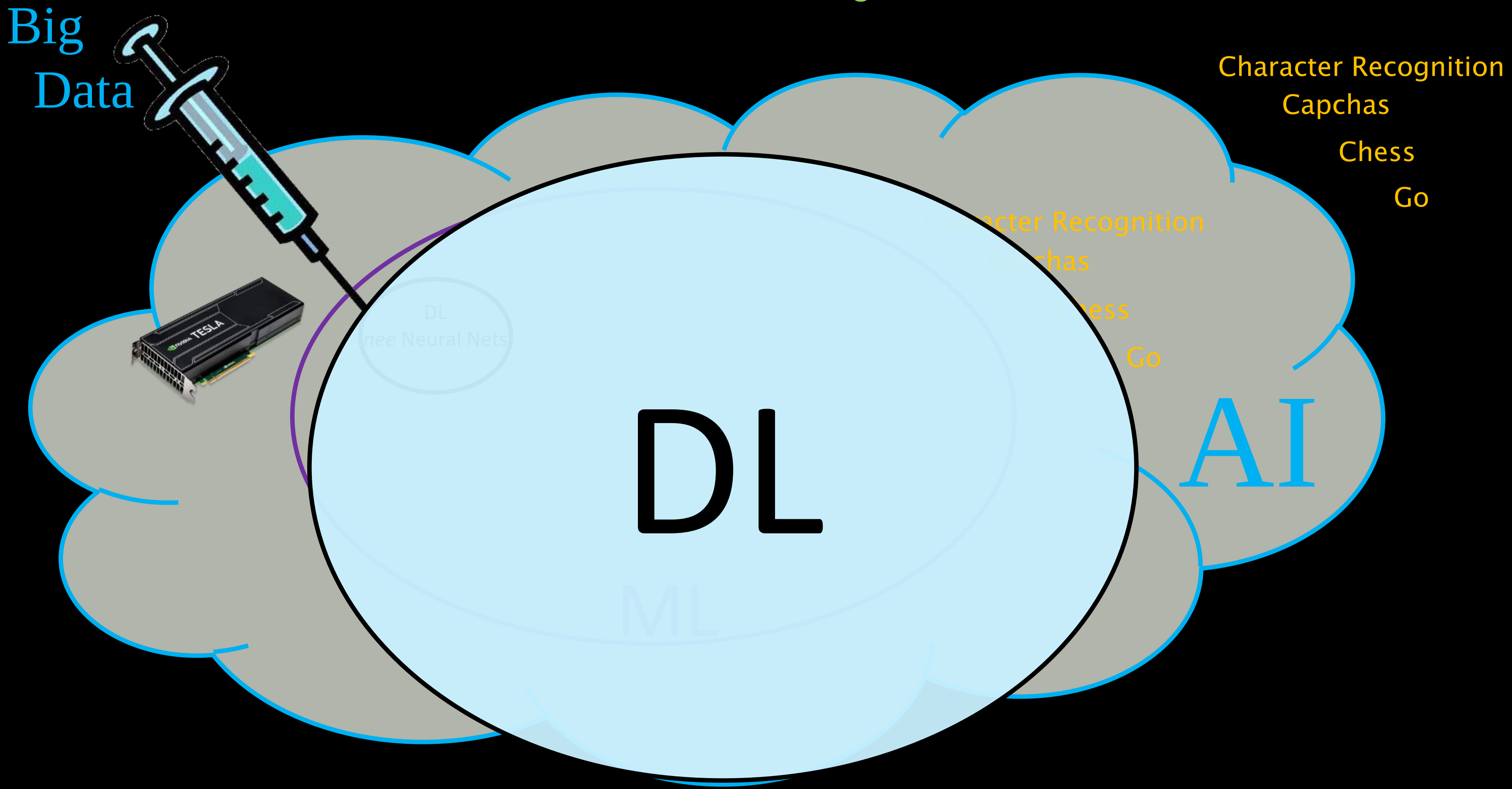
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn import (datasets, decomposition, manifold, random_projection)

def draw(X, title):
    plt.figure()
    plt.xlim(X.min(0)[0],X.max(0)[0]); plt.ylim(X.min(0)[1],X.max(0)[1])
    plt.xticks([]); plt.yticks([])
    plt.title(title)
    for i in range(X.shape[0]):
        plt.text(X[i, 0], X[i, 1], str(y[i]), color=plt.cm.Set1(y[i] / 10.) )

digits = datasets.load_digits(n_class=6)
X = digits.data
y = digits.target

rp = random_projection.SparseRandomProjection(n_components=2, random_state=42)
X_projected = rp.fit_transform(X)
draw(X_projected, "Sparse Random Projection of the digits")

X_pca = decomposition.PCA(n_components=2).fit_transform(X)
draw(X_pca, "PCA (Two Components)")

tsne = manifold.TSNE(n_components=2, init='pca', random_state=0)
X_tsne = tsne.fit_transform(X)
draw(X_tsne, "t-SNE Embedding")

plt.show()
```



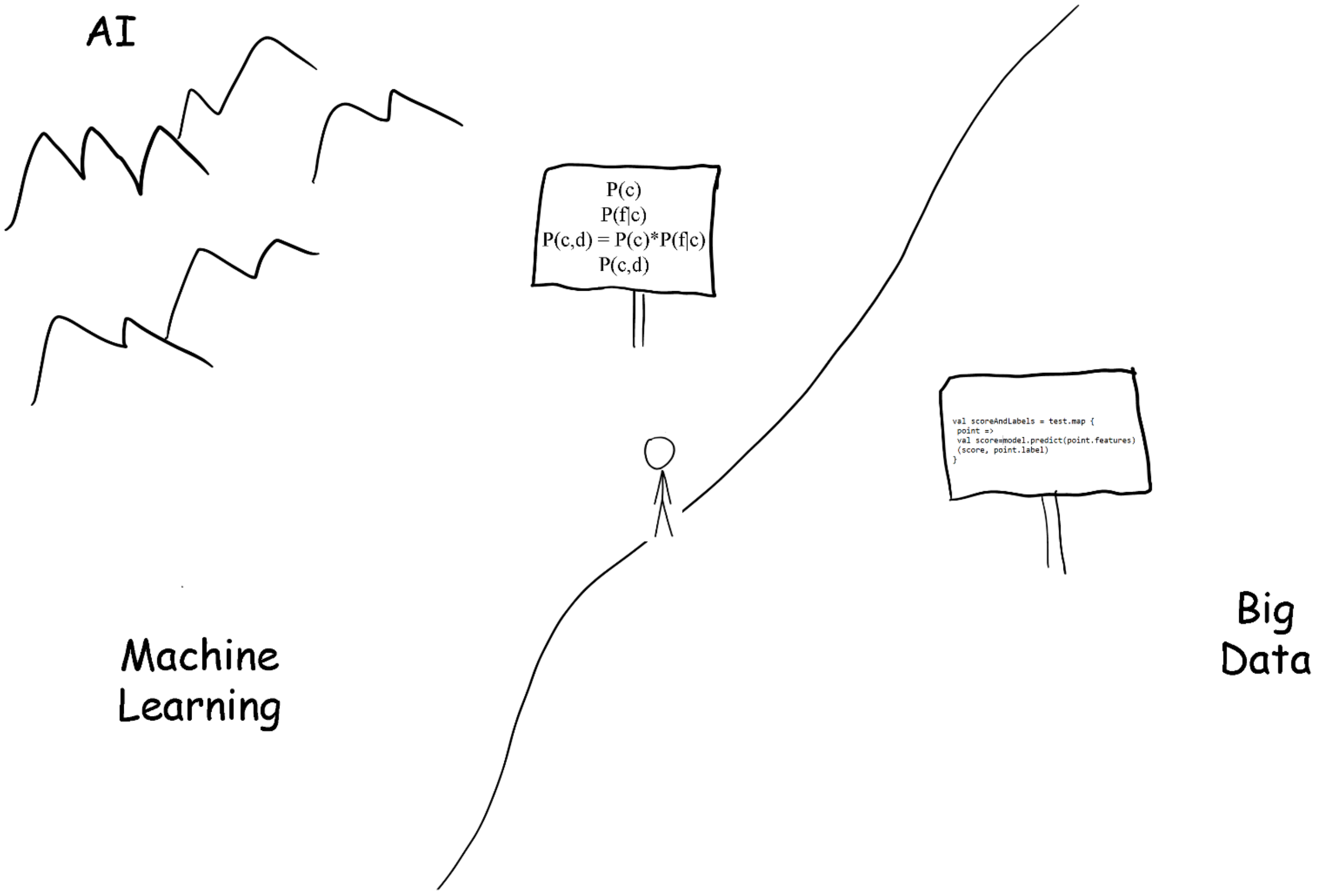




How does all this fit together?



The Journey Ahead



As the Data Scientist wanders across the ill-defined boundary between Data Science and Machine Learning, in search of the fabled land of Artificial Intelligence, they find that the language changes from programming to a creole of linear algebra and probablity and statistics.