Classification (1) – an issue with distance measures, and an implementation of Nearest Neighbour classification

Introduction

In this notebook we will expand on some of the concepts of classification, starting with an experiment with distance measures on data, then looking into the k-Nearest Neighbour algorithm.

1) Distance measures for high-dimensionality data

Algorithms such as k-Nearest Neighbour are conceptually very simple -- we predict the class value of an unlabelled *query* data point we are given by looking at all the labelled data point(s) in our data set, and predicting that our query will have the same class as the most similar data point(s) in the training set. So, all we need is a way of measuring similarity. The well-known *Euclidean distance measure* would seem to be a good choice. However, while we are very familiar with Euclidean distance in 2 and 3-dimensions, there was a warning that in high-dimensions there is a problem – what was this problem ?

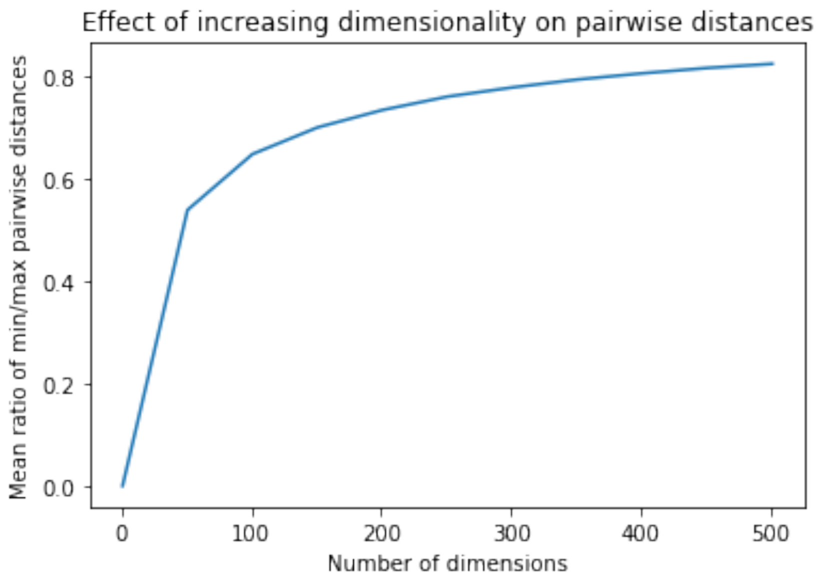
Pairwise distances in high-dimensional spaces

Answer: in high-dimensional spaces everything is far away from everything else, and so pairwise distances become uninformative.

But what does this actually mean ? There is a mathematical argument to show that this is a true statement, but an alternative approach is simply to simulate what happens. One approach is to randomly generate N points inside a d-dimensional cube centred around zero, such as $[-0.5, 0.5]^d$. Now we calculate the pairwise distances among the N points. After that for every data point we calculate the ratio of the minimum distance to the maximum distance to all of the other data points. The mean ratio represents the average range of pairwise distances there are in that dimensionality. We run the simulation from 1 dimension to 1000 dimensions and the ratios will be plotted on a line chart using the `matplotlib` library.

You should use the `numpy` library for this, and in particular the linear algebra methods to calculate distances such as the [L2 norm (https://docs.scipy.org/doc/numpy-1.13.0/reference/generated/numpy.linalg.norm.html#numpy.linalg.norm)](https://docs.scipy.org/doc/numpy-1.13.0/reference/generated/numpy.linalg.norm.html#numpy.linalg.norm).

In [10]:
```
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt

def run_d_n(dim,N_pts,L):
    pts=np.random.rand(N_pts,dim)-0.5 # simulate N_pts points on di
    ratio_list=[]
    for i in range(N_pts):
        # ignore the data point itself
        selected_pts=np.array([j for j in range(N_pts) if j!=i])
        # calculate the L2 or L1 distance with other points
        dist=np.linalg.norm(pts[selected_pts]-pts[i],L,axis=1)
        # calculate the ratio of the min. distance to the max. dist
        ratio=np.min(dist)/np.max(dist)
        ratio_list.append(ratio)
    # output the mean ratio
    return np.mean(ratio_list)

# Initialise the N_pts, the number of points we simulate
N_pts=1000
# Setting l=2 to calculate the L2 distance
l=1
# Setting the number of dimensions we simulate
check_dim=range(1,550,50)
# Calculate the mean ratio on that dimension
ratio_list=[ run_d_n(dim,N_pts,l) for dim in check_dim]
# Plot the ratio with its corresponding dimension
plt.plot(check_dim,ratio_list)
plt.ylabel("Mean ratio of min/max pairwise distances")
plt.xlabel("Number of dimensions")
plt.title("Effect of increasing dimensionality on pairwise distance
plt.xticks(np.arange(0, 600, step=100))
plt.show()
```



Question: how can this plot be interpreted ? How else could you visualize this effect ?

We can interpret this as showing that as dimensionality increases the min. and max. distances from any point to any other point become more similar. Something this plot doesn't show is the distribution of the actual distances. To see this you could try plotting histograms of the distribution of all pairwise distances for a set of points of low, then higher dimensionality. If you do this, first think about how you would expect it to look.

2) Implement Nearest Neighbour from scratch

The following will give some practise in implementing a simple classifier, the k-Nearest Neighbour (kNN) algorithm. It should help us to write a kNN package from scratch. Most machine learning methods include two main steps, namely training (fitting to a model to the training data) and prediction (running the model on input data to generate output). However, in the kNN algorithm, since there is no explicit model-building step, we only require implementation of the prediction step without a training step.

In [11]:
```
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
```

Data Creation

In [38]:
```
mean_01 = np.array([1, 0.5])
cov_01 = np.array([[1, 0.1], [0.1, 1.2]])

mean_02 = np.array([4, 5])
cov_02 = np.array([[1, 0.1], [0.1, 1.2]])

dist_01 = np.random.multivariate_normal(mean_01, cov_01, 500)
dist_02 = np.random.multivariate_normal(mean_02, cov_02, 500)
print(dist_01.shape, dist_02.shape)
```

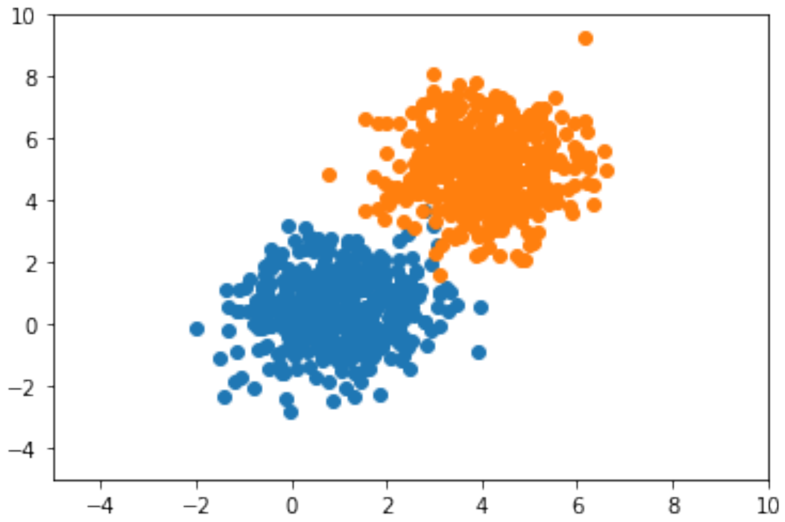
```
(500, 2) (500, 2)
```

We have created two 2-dimensional normal distributions of data points with the same covariance but different means.

Plotting the created Data

What does the data look like ? Notice the 2 unique clusters being formed.

In [13]:
```
plt.figure(0)
plt.xlim(-5, 10)
plt.ylim(-5, 10)

plt.scatter(dist_01[:, 0], dist_01[:, 1])
plt.scatter(dist_02[:, 0], dist_02[:, 1])#, color='red')
plt.show()
```



Let us now represent it in a tabular way. We will have dist_01 getting label 1.

In [14]:
```
r = dist_01.shape[0] + dist_02.shape[0]
c = dist_01.shape[1] + 1
data = np.zeros((r, c))
print(data.shape)

data[:dist_01.shape[0], :2] = dist_01
data[dist_01.shape[0]:, :2] = dist_02
data[dist_01.shape[0]:, -1] = 1.0

print(data.mean(axis=0))
```

```
(1000, 3)
[2.51648405 2.80105178 0.5       ]
```

Now shuffle the data and check by printing the first 10 rows.

In [15]:
```
np.random.shuffle(data)
print(data[:10])
```

```
[[-1.37710159  1.0943182   0.        ]
 [ 2.52389784  4.72684665  1.        ]
 [ 1.3890666   0.51780868  0.        ]
 [ 5.12792458  6.02518813  1.        ]
 [ 3.18550696  5.773212    1.        ]
 [ 1.5174317   1.19611605  0.        ]
 [ 3.29858777  2.89595293  1.        ]
 [ 4.128707    6.32898592  1.        ]
 [ 2.32702071  4.33926419  1.        ]
 [ 0.8326591  -0.63006695  0.        ]]
```

Implementation. Next, we implement our KNN algorithm. There are many ways to do this, but a basic approach will require a pairwise distance measure for instances, and a way to take a "training" dataset of classified instances and make a prediction for a "test" data instance. Here is a top-level outline:

In [39]:
```
def distance(x1, x2):
    d = np.sqrt(((x1-x2)**2).sum())
    return d

def knn(X_train, y_train, xt, k=7):
    vals = []
    for ix in range(X_train.shape[0]):
        d = distance(X_train[ix], xt)
        vals.append([d, y_train[ix]])
    sorted_labels = sorted(vals, key=lambda z: z[0])
    neighbours = np.asarray(sorted_labels)[:k, -1]

    freq = np.unique(neighbours, return_counts=True)

    return freq[0][freq[1].argmax()]
```

Now check to see if we can make a prediction.

In [40]:
```
test_point = np.array([8, -4])

# Un-comment the line below and check if it comes out as 0.0
print(knn(data[:, :2], data[:, -1], test_point))
```

```
0.0
```

Create a train and test split of the data

In [18]:
```
np.random.shuffle(data)
split = int(0.75 * data.shape[0])
# print split
train_data_X = data[:split, :2]
train_data_y = data[:split, -1]
test_data_X = data[split:, :2]
test_data_y = data[split:, -1]

print(train_data_X.shape, train_data_y.shape)
print(test_data_X.shape, test_data_y.shape)
```

```
(750, 2) (750,)
(250, 2) (250,)
```

Implementation. Next we need to implement some way to run our KNN classifier on all the test data and get the results.

In [41]:
```
def get_acc(kx):
    preds = []
    # print kx
    for ix in range(test_data_X.shape[0]):
        preds.append(knn(train_data_X, train_data_y, test_data_X[ix
    preds = np.asarray(preds)

    # print preds.shape
    return 100*float((test_data_y == preds).sum())/preds.shape[0]

print(get_acc(7))
```

```
99.2
```

What accuracy did you get ? You should get around 99 percent on this dataset.

Let's try different values of K.

In [42]:
```
for ix in range(2, 20):
    print ("k:", ix, "| Acc:", get_acc(ix))
```

```
k: 2 | Acc: 98.4
k: 3 | Acc: 99.2
k: 4 | Acc: 99.2
k: 5 | Acc: 99.2
k: 6 | Acc: 99.2
k: 7 | Acc: 99.2
k: 8 | Acc: 99.2
k: 9 | Acc: 99.2
k: 10 | Acc: 99.2
k: 11 | Acc: 99.2
k: 12 | Acc: 99.2
k: 13 | Acc: 99.2
k: 14 | Acc: 99.2
k: 15 | Acc: 99.2
k: 16 | Acc: 99.2
k: 17 | Acc: 99.2
k: 18 | Acc: 99.2
k: 19 | Acc: 99.2
```

Now let's try real data : MNIST

In [21]:
```
import pandas as pd
import datetime
```

Of course, MNIST is image data, but here we are using a CSV version where we can view the pixels as numbers (each row has the pixel data for an image of a digit, and the first column is the class of the digit, i.e., 0-9).

In [27]:
```
df = pd.read_csv('train.csv')
df.head()
```

Out[27]:

	5	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	...	0.608	0.609	0.610	0.611	0.612	0.613
0	0	0	0	0	0	0	0	0	0	0	...	0	0	0	0	0	0
1	4	0	0	0	0	0	0	0	0	0	...	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0	0	...	0	0	0	0	0	0
3	9	0	0	0	0	0	0	0	0	0	...	0	0	0	0	0	0
4	2	0	0	0	0	0	0	0	0	0	...	0	0	0	0	0	0

5 rows × 785 columns

Since the dataset is quite big, we will just use a subset.

In [28]:
```
data = df.values[:2000]
print (data.shape)
```

```
(2000, 785)
```

Make a train/test split of the data.

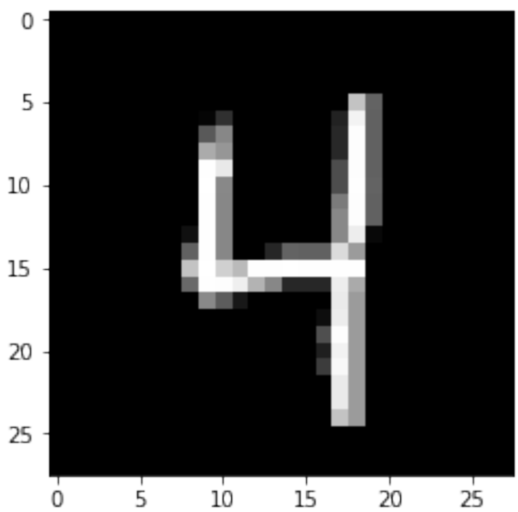
In [29]:
```
split = int(0.8 * data.shape[0])

X_train = data[:split, 1:]
X_test = data[split:, 1:]

y_train = data[:split, 0]
y_test = data[split:, 0]

print (X_train.shape, y_train.shape)
print (X_test.shape, y_test.shape)
```

```
(1600, 784) (1600,)
(400, 784) (400,)
```

Let us just check that our data really does represent images.

In [34]:
```
plt.figure(0)
plt.imshow(X_train[91].reshape((28, 28)), cmap='gray', interpolatio
print (y_train[91])
plt.show()
```

4



Implementation. Now code another `get_acc()` and try different values of K on our dataset.

In [47]:
```
def get_acc(kx):
    preds = []
    # print kx
    for ix in range(X_test.shape[0]):
        start = datetime.datetime.now()
        preds.append(knn(X_train, y_train, X_test[ix], k=kx))
        print("Test point: ", str(ix), " runtime: ", str(datetime.d
        # print(ix)
        # print(datetime.datetime.now() - start)
    preds = np.asarray(preds)

    # print preds.shape
    return 100*float((y_test == preds).sum())/preds.shape[0]

print("Result: ")
# print(get_acc(5))  # k=5 nearest neighbours
print(get_acc(20))  # k=20 nearest neighbours
```

```
Result:
Test point:  0  runtime:  0:00:00.034480
Test point:  1  runtime:  0:00:00.033142
Test point:  2  runtime:  0:00:00.032091
Test point:  3  runtime:  0:00:00.030807
Test point:  4  runtime:  0:00:00.029516
Test point:  5  runtime:  0:00:00.029437
Test point:  6  runtime:  0:00:00.030257
Test point:  7  runtime:  0:00:00.029595
Test point:  8  runtime:  0:00:00.029861
Test point:  9  runtime:  0:00:00.029216
Test point:  10  runtime:  0:00:00.028712
Test point:  11  runtime:  0:00:00.028461
Test point:  12  runtime:  0:00:00.029688
Test point:  13  runtime:  0:00:00.029761
Test point:  14  runtime:  0:00:00.030555
Test point:  15  runtime:  0:00:00.031027
Test point:  16  runtime:  0:00:00.032470
Test point:  17  runtime:  0:00:00.032462
Test point:  18  runtime:  0:00:00.031450
```

In [ ]: