L6_MLIntro_filled

February 4, 2019

```
In [1]: import numpy as np
        import matplotlib.pyplot as plt
        import pandas as pd
        %matplotlib inline
        # this is a new library you haven't seen before, what do you think it does?
        from sklearn.neighbors import KNeighborsClassifier
        from sklearn.model_selection import train_test_split
```

From this article in Scientific Reports

Read in the data

- elemental data: https://raw.githubusercontent.com/UWDIRECT/UWDIRECT.github.io/master/Wi18_content/DSMCER/atomsradii.csv
- testing data: https://raw.githubusercontent.com/UWDIRECT/UWDIRECT.github.io/master/Wi18_content/DSMCER/testing.csv

```
In [2]: d_train = pd.read_csv('https://raw.githubusercontent.com/UWDIRECT/UWDIRECT.github.io/ma
        d_test = pd.read_csv('https://raw.githubusercontent.com/UWDIRECT/UWDIRECT.github.io/mas
```

```
In [5]: d_test
```

Out[5]:

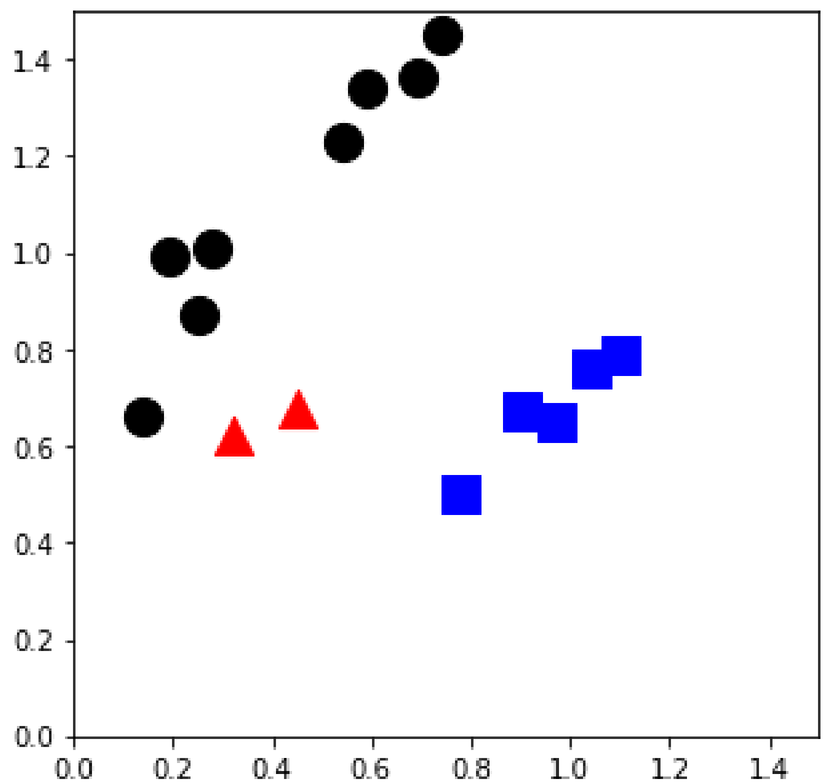
	rWC	rCh	Atom	Type
0	0.51	1.12	X1	Alk
1	0.37	0.77	X2	TM
2	0.62	0.35	X3	PT
3	0.62	0.62	X4	TM
4	0.62	0.93	X5	Alk

Take 1-2 min and look @ the data in elements using pandas and Python you and your partner decide what to do. E.g. you could recreate the above plot with plt.scatter(elements.rWC,elements.rCh)

```
In [3]: fig, ax = plt.subplots(figsize=(5, 5))
        colors = ['b', 'r', 'k']
        shape = ['s', '^', 'o']

        counter = 0
        for typ in d_train.Type.unique():
```

```
        ax.scatter(d_train[d_train['Type']==typ]['rWC'], d_train[d_train['Type']==typ]['rCh

        counter = counter + 1
    ax.set_xlim([0, 1.5])
    ax.set_ylim([0, 1.5])
```

Out[3]: (0, 1.5)



Now, let's make a new classifier object We'll use `KNeighborsClassifier(n_neighbors=k)` where `k` is the number of neighbors to use.

Then 'train' it using the `.fit` function on the object returned by the `KNeighborsClassifier` call.

In [7]:
```
inputs = ['rWC', 'rCh']
X_train = d_train[inputs]
y_train = d_train['Type']
X_test = d_test[inputs]
y_test = d_test['Type']
#X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.5)

KNNmodel = KNeighborsClassifier(n_neighbors=3)
KNNmodel.fit(X_train, y_train)
```

```
Out[7]: KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
                   metric_params=None, n_jobs=1, n_neighbors=3, p=2,
                   weights='uniform')
```

0.0.1 You can use the following function to see how your model is doing:

`knn.predict(X)`

As a function of K, you and your partner should determine:

- Testing error rate
- Training error rate

Need not be quantitative but spend (1/2 - 2/3 of remaining time exploring this)

```
In [8]: rate = KNNmodel.predict(X_train) == y_train
        print('Training Error Rate:', np.mean(rate))

        rate = KNNmodel.predict(X_test) == y_test
        print('Testing Error Rate:', np.mean(rate))
```

```
Training Error Rate: 1.0
Testing Error Rate: 0.6
```

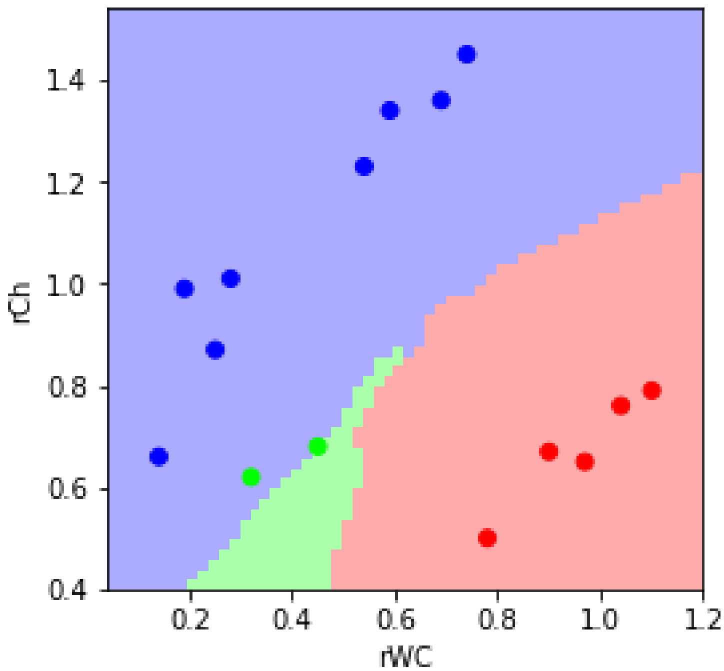
With remaining time go through the cell below and look at graphs of the decision boundary vs K.

- See if you can use the graph to determine your **testing** error rate
- Could you also use the graph to determine your **training** error rate? (*open ended*)

```
In [9]: # additional library we will use
        from matplotlib.colors import ListedColormap

        # just for convenience and similarity with sklearn tutorial
        # I am going to assign our X and Y data to specific vectors
        # this is not strictly needed and you could use elements df for the whole thing!
        d1 = d_train
        elements = d1
        X=elements[['rWC','rCh']]

        #this is a trick to turn our strings (type of element / class) into unique
        #numbers.  Play with this in a separate cell and make sure you know wth is
        #going on!
        levels,labels=pd.factorize(elements.Type)
        y=levels

        #This determines levelspacing for our color map and the colors themselves
```

```
h=0.02
cmap_light = ListedColormap(['#FFAAAA', '#AAFFAA', '#AAAAFF'])
cmap_bold = ListedColormap(['#FF0000', '#00FF00', '#0000FF'])

# in the sklearn tutorial two different weights are compared
# the decision between "uniform" and "distance" determines the probability
# weight.  "uniform" is the version presented in class, you can change to
# distance
weights='uniform'

# I am actually refitting the KNN here. If you had a big data set you would
# not do this, but I want you to have the convenience of changing K or
# weights here in this cell. Large training sets with many features can take
# awhile for KNN training!

K=5
clf = KNeighborsClassifier(n_neighbors=5, weights=weights)
clf.fit(X,y)

# Straight from the tutorial - quickly read and see if you know what these
# things are going - if you are < 5 min until end then you should skip this part

# Plot the decision boundary. For that, we will assign a color to each
# point in the mesh [x_min, x_max]x[y_min, y_max].
x_min, x_max = elements.rWC.min() - 0.1   , elements.rWC.max() + 0.1
y_min, y_max = elements.rCh.min() - 0.1   , elements.rCh.max() + 0.1
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))
Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])

# Put the result into a color plot
Z = Z.reshape(xx.shape)
plt.figure(figsize=(4,4));
plt.pcolormesh(xx, yy, Z, cmap=cmap_light)

# Plot also the training points
# This may be the 1st time you have seen how to color points by a 3rd vector
# In this case y ( see c=y in below statement ). This is very useful!
plt.scatter(X.rWC, X.rCh, c=y, cmap=cmap_bold)

# Set limits and lebels
plt.xlim(xx.min(), xx.max())
plt.ylim(yy.min(), yy.max())
plt.xlabel('rWC')
plt.ylabel('rCh')
```

```
Out[9]: Text(0,0.5,'rCh')
```



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