Assignment 5_AN

April 7, 2023

[17]:

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import classification_report, confusion_matrix

#For this assignment, I chose to look at different RNA expression values to see␣
 ↪how training a model based on them would help us predict the type of tumor␣
 ↪within a patient. This data was found at https://archive.ics.uci.edu/ml/
 ↪datasets/gene%2Bexpression%2Bcancer%2BRNA-Seq. data.csv is a file with␣
 ↪patients in the rows and genes in the columns. Each patient has their own␣
 ↪RNA expression levels for each gene present in the data table. labels.csv is␣
 ↪a table of all the tumor types that each patient has. Thus, in the ML model,␣
 ↪X will be the RNA gene expression data and y will be the label data. This␣
 ↪code will use a Random Forest Classifier because it is best used for␣
 ↪classification problems such as this one.
```

[93]:

```
data = pd.read_csv("data.csv")
labels = pd.read_csv("labels.csv")

data_df = pd.DataFrame(data)
labels_df = pd.DataFrame(labels)

data_df = data_df.drop(columns = ["Unnamed: 0"])
labels_df = labels_df.drop(columns = ["Unnamed: 0"])
```

[94]:

```
print(data_df)
```

```
     gene_0    gene_1    gene_2    gene_3     gene_4  gene_5    gene_6  \
0       0.0  2.017209  3.265527  5.478487  10.431999     0.0  7.175175
1       0.0  0.592732  1.588421  7.586157   9.623011     0.0  6.816049
2       0.0  3.511759  4.327199  6.881787   9.870730     0.0  6.972130
3       0.0  3.663618  4.507649  6.659068  10.196184     0.0  7.843375
4       0.0  2.655741  2.821547  6.539454   9.738265     0.0  6.566967
..      …         …         …        …          …        …         …
796     0.0  1.865642  2.718197  7.350099  10.006003     0.0  6.764792
```

```
797     0.0  3.942955  4.453807  6.346597  10.056868     0.0  7.320331
798     0.0  3.249582  3.707492  8.185901   9.504082     0.0  7.536589
799     0.0  2.590339  2.787976  7.318624   9.987136     0.0  9.213464
800     0.0  2.325242  3.805932  6.530246   9.560367     0.0  7.957027

       gene_7  gene_8  gene_9  …  gene_20521  gene_20522  gene_20523  \
0    0.591871     0.0     0.0  …    4.926711    8.210257    9.723516
1    0.000000     0.0     0.0  …    4.593372    7.323865    9.740931
2    0.452595     0.0     0.0  …    5.125213    8.127123   10.908640
3    0.434882     0.0     0.0  …    6.076566    8.792959   10.141520
4    0.360982     0.0     0.0  …    5.996032    8.891425   10.373790
..        …     …     …  …         …         …         …
796  0.496922     0.0     0.0  …    6.088133    9.118313   10.004852
797  0.000000     0.0     0.0  …    6.371876    9.623335    9.823921
798  1.811101     0.0     0.0  …    5.719386    8.610704   10.485517
799  0.000000     0.0     0.0  …    5.785237    8.605387   11.004677
800  0.000000     0.0     0.0  …    6.403075    8.594354   10.243079

     gene_20524  gene_20525  gene_20526  gene_20527  gene_20528  gene_20529  \
0      7.220030    9.119813   12.003135    9.650743    8.921326    5.286759
1      6.256586    8.381612   12.674552   10.517059    9.397854    2.094168
2      5.401607    9.911597    9.045255    9.788359   10.090470    1.683023
3      8.942805    9.601208   11.392682    9.694814    9.684365    3.292001
4      7.181162    9.846910   11.922439    9.217749    9.461191    5.110372
..          …         …         …         …         …         …
796    4.484415    9.614701   12.031267    9.813063   10.092770    8.819269
797    6.555327    9.064002   11.633422   10.317266    8.745983    9.659081
798    3.589763    9.350636   12.180944   10.681194    9.466711    4.677458
799    4.745888    9.626383   11.198279   10.335513   10.400581    5.718751
800    9.139459   10.102934   11.641081   10.607358    9.844794    4.550716

     gene_20530
0      0.000000
1      0.000000
2      0.000000
3      0.000000
4      0.000000
..          …
796    0.000000
797    0.000000
798    0.586693
799    0.000000
800    0.000000

[801 rows x 20531 columns]
```

[95]:

```
print(labels_df)
```

```
    Class
0    PRAD
1    LUAD
2    PRAD
3    PRAD
4    BRCA
..    …
796  BRCA
797  LUAD
798  COAD
799  PRAD
800  PRAD

[801 rows x 1 columns]
```

[96]:
```
data_df.shape #seeing the shape of our dataframes to make sure that the number␣
↪of samples (first number) matches in both
```

[96]:
```
(801, 20531)
```

[97]:
```
# The data_df dataframe has 20,531 genes. This is a lot of features to train by.
# So, let's choose a more reasonable number of genes, like 10 (arbitrary number␣
↪chosen). Because all of these genes
# are unknown, it may be interesting to see how the model works if the genes␣
↪are chosen at random.
# So, we can implement the following code:

data_df = data_df.sample(n=10, axis='columns')
data_df.shape
```

[97]:
```
(801, 10)
```

[98]:
```
labels_df.shape
```

[98]:
```
(801, 1)
```

[99]:
```
#Now we have to convert all the labels from categorical to numerical

labels_df["Class"].replace(['BRCA', 'KIRC', 'COAD', 'LUAD', 'PRAD'], [1, 2, 3,␣
↪4, 5], inplace = True)
print(labels_df)
```

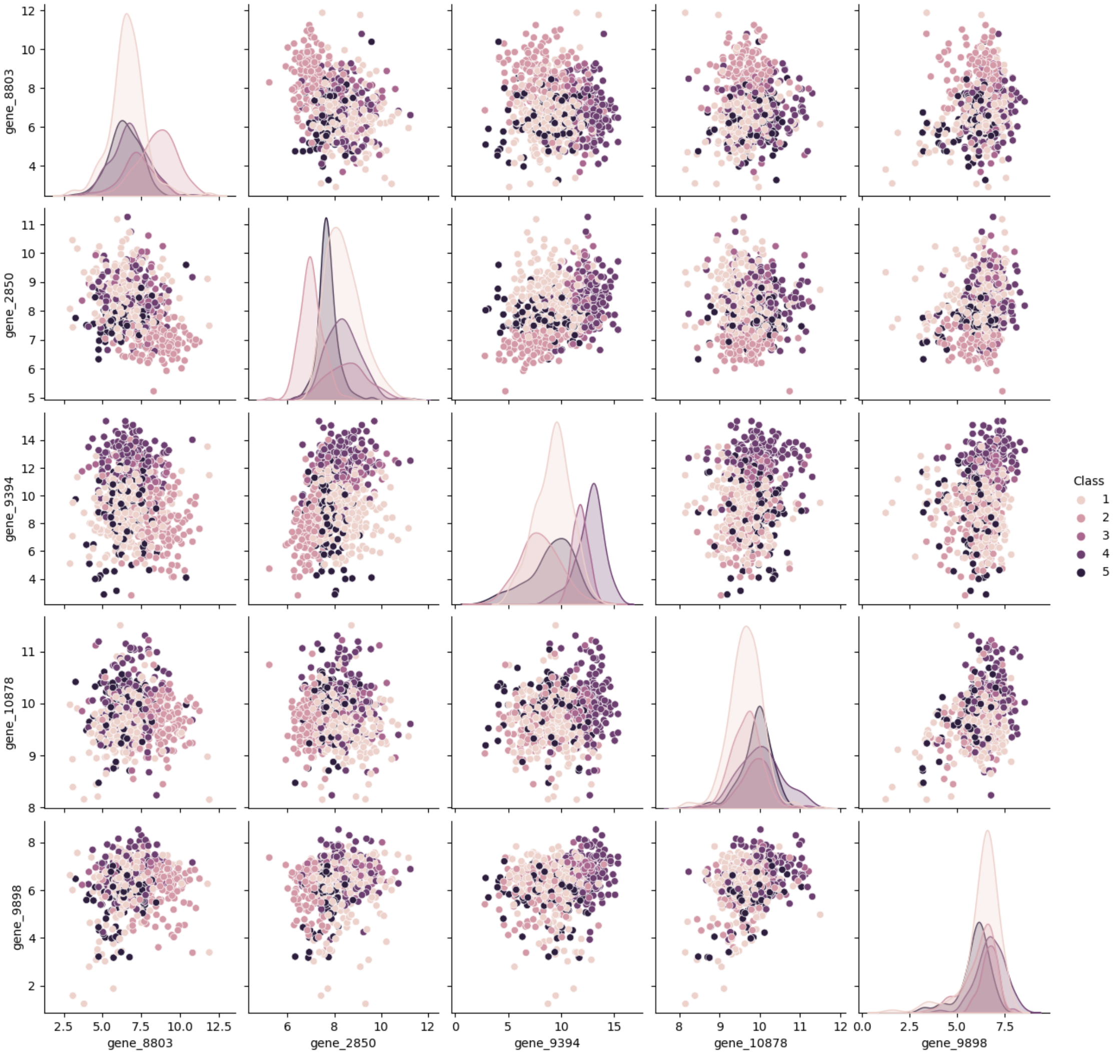
```
     Class
0        5
1        4
2        5
3        5
4        1
```

```
..      ...
796       1
797       4
798       3
799       5
800       5

[801 rows x 1 columns]
```

[100]:
```
#Combining data and labels to use in a pair plot to examine data just for the first five genes

combined_df = pd.concat([data_df, labels_df], axis=1, join='inner')
column_names = list(combined_df.columns)
sns.pairplot(combined_df, hue = "Class", vars = (column_names[0:5]))
plt.show()
```



[101]:

```python
#finding how many instances of each tumor type are in the labels

combined_df['Class'].value_counts()

#from here, we see that we have 300 BRCA, 146 KIRC, 141 LUAD, 136 PRAD, and 78 COAD instances
```

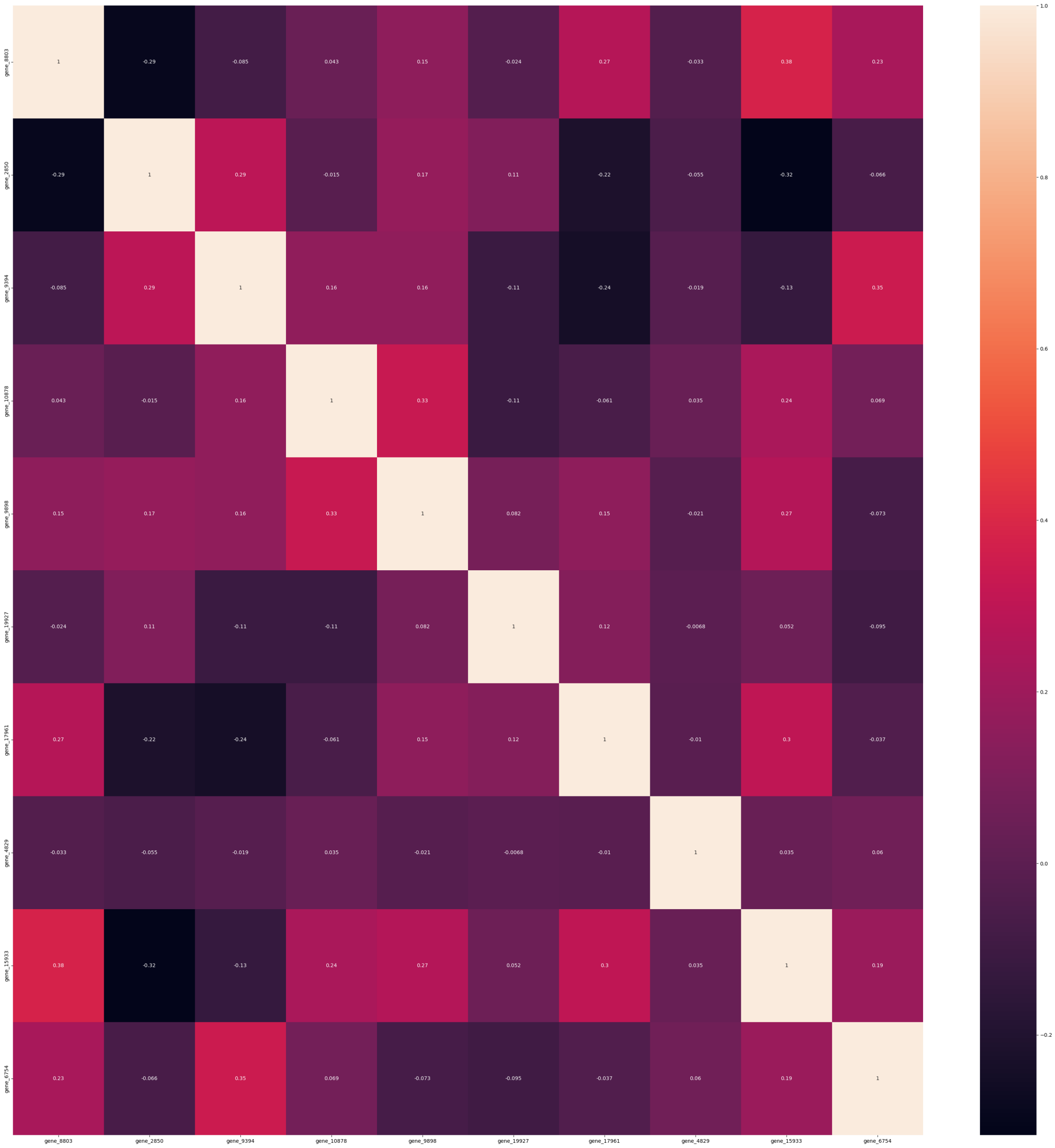
[101]:

```
1    300
2    146
4    141
5    136
3     78
Name: Class, dtype: int64
```

[102]:

```python
#Now let's check the correlation of the genes to complete Feature Reduction

plt.figure(figsize=(40,40))
sns.heatmap(data_df.corr(), annot=True)
plt.show()
```



[103]:

```
# As can be seen by the heatmap, there is no need for feature reduction with␣
↪this cleaned dataset
# as the genes do not correlate with one another that much. We can now train␣
↪the ML model on this data

X_train, X_test, y_train, y_test = train_test_split(data_df, labels_df,␣
↪test_size = 0.2, random_state = 20)
print ('The size of our training "X" (input features) is', X_train.shape)
print ('\n')
print ('The size of our testing "X" (input features) is', X_test.shape)
print ('\n')
print ('The size of our training "y" (output feature) is', y_train.shape)
print ('\n')
print ('The size of our testing "y" (output features) is', y_test.shape)
```

```
The size of our training "X" (input features) is (640, 10)


The size of our testing "X" (input features) is (161, 10)


The size of our training "y" (output feature) is (640, 1)


The size of our testing "y" (output features) is (161, 1)
```

[104]:

```
#introducing the classifier and fitting the ML model to the training data
classifier = RandomForestClassifier(n_estimators = 10, criterion = 'entropy',␣
 ↪random_state = 0)
classifier.fit(X_train, y_train)
```

```
/var/folders/z2/z4rmk799631_trmcdlb01zsw0000gn/T/ipykernel_74795/2146352827.py:2
: DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples,), for example using
ravel().
  classifier.fit(X_train, y_train)
```

[104]:

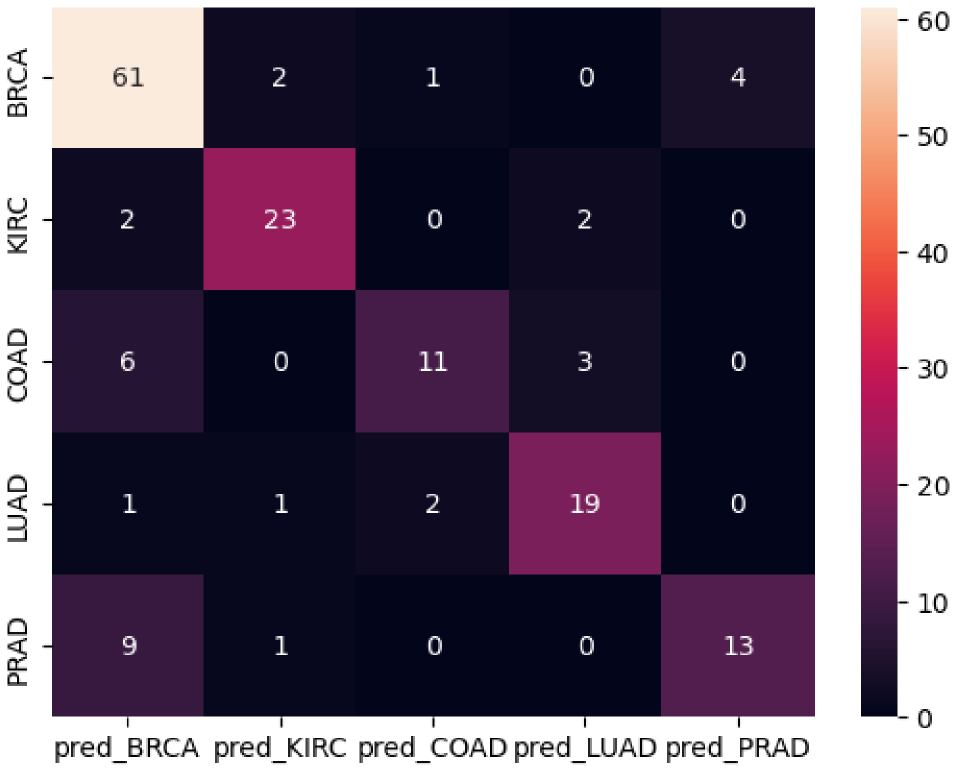
```
RandomForestClassifier(criterion='entropy', n_estimators=10, random_state=0)
```

[105]:

```
#using the trained model to predict the values given the test data
y_predict = classifier.predict(X_test)
```

[106]:

```
#setting up a visual to understand how many matches and mismatches there are␣
 ↪between the real data and predicted data
cm = np.array(confusion_matrix(y_test, y_predict, labels=[1,2,3,4,5]))
confusion = pd.DataFrame(cm, index=['BRCA', 'KIRC', 'COAD', 'LUAD', 'PRAD'],
                         columns=['pred_BRCA', 'pred_KIRC', 'pred_COAD',␣
 ↪'pred_LUAD', 'pred_PRAD'])
sns.heatmap(confusion, annot=True)
plt.show()
```



[107]:
```
print(classification_report(y_test, y_predict)) #these stats are not terrible
 ↪but let's see if we can do better
# There are two ways we can do this with this data. The first is by potentially
 ↪improving our model by normalizing our data
# and the second is by increasing the number of genes that we use to train the
 ↪data.
```

```
              precision    recall  f1-score   support

           1       0.77      0.90      0.83        68
           2       0.85      0.85      0.85        27
           3       0.79      0.55      0.65        20
           4       0.79      0.83      0.81        23
           5       0.76      0.57      0.65        23

    accuracy                           0.79       161
   macro avg       0.79      0.74      0.76       161
weighted avg       0.79      0.79      0.78       161
```

[112]:
```
#normalizing training data
```

```
X_train_min = X_train.min()
X_train_max = X_train.max()
X_train_range = (X_train_max - X_train_min)
X_train_scaled = (X_train - X_train_min)/(X_train_range)
print(X_train_scaled.head())
```

```
     gene_8803  gene_2850  gene_9394  gene_10878  gene_9898  gene_19927  \
211   0.423437   0.656435   0.458140    0.463808   0.783873    0.195302
708   0.469936   0.481567   0.609731    0.349199   0.759078    0.110130
225   0.544171   0.462359   0.494809    0.482953   0.790569    0.094362
191   0.739835   0.260766   0.685172    0.453420   0.798680    0.000000
57    0.460419   0.647779   0.711904    0.429402   0.795385    0.094243

     gene_17961  gene_4829  gene_15933  gene_6754
211    0.454850        0.0    0.484048   0.233592
708    0.479278        0.0    0.513701   0.629173
225    0.480363        0.0    0.656618   0.604435
191    0.602618        0.0    0.600246   0.732475
57     0.354689        0.0    0.403592   0.596182
(640, 10)
```

[109]:

```
#normalizing testing data

X_test_min = X_test.min()
X_test_max = X_test.max()
X_test_range = (X_test_max - X_test_min)
X_test_scaled = (X_test - X_test_min)/X_test_range
print(X_test_scaled.head())
```

```
     gene_8803  gene_2850  gene_9394  gene_10878  gene_9898  gene_19927  \
507   0.183232   0.879717   1.000000    0.519278   0.874427    0.000000
327   0.814372   0.275064   0.208080    0.532112   0.552825    0.000000
647   0.604977   0.185269   0.434592    0.715250   0.691257    0.215448
738   0.625158   0.508412   0.735127    0.701442   0.746648    0.000000
172   0.462398   0.658249   0.262070    0.656363   0.552696    0.303693

     gene_17961  gene_4829  gene_15933  gene_6754
507    0.305640        0.0    0.027677   0.788548
327    0.442585        0.0    0.719350   0.547335
647    0.354742        0.0    0.656915   0.559842
738    0.500595        0.0    0.708403   0.559404
172    0.711316        0.0    0.670659   0.299384
```

[113]:

```
#refitting the classifier with normalized data

classifier = RandomForestClassifier(n_estimators = 10, criterion = 'entropy',␣
 ↪random_state = 0)
```

```
classifier.fit(X_train_scaled, y_train)
```

```
/var/folders/z2/z4rmk799631_trmcdlb01zsw0000gn/T/ipykernel_74795/1531128739.py:2
: DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples,), for example using
ravel().
  classifier.fit(X_train_scaled, y_train)
```

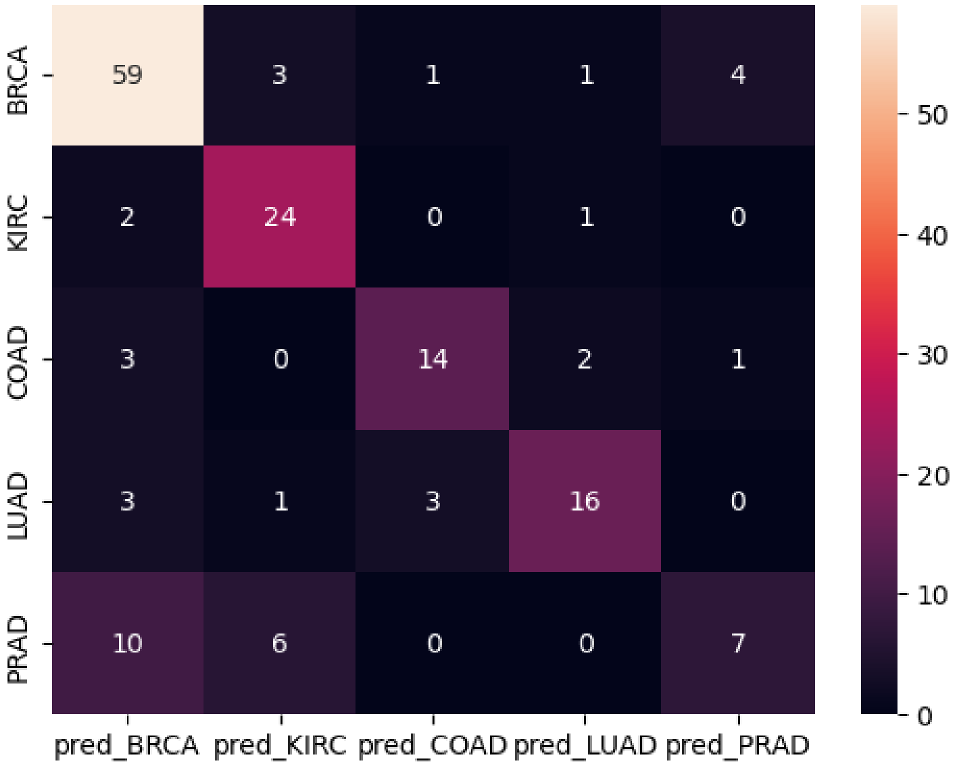
```
[113]: RandomForestClassifier(criterion='entropy', n_estimators=10, random_state=0)
```

```
[114]: #re-predicting with the normalized test data

y_predict_scaled = classifier.predict(X_test_scaled)
```

```
[115]: #using a heatmap to show the matches and mismatches with the normalized data

cm = np.array(confusion_matrix(y_test, y_predict_scaled, labels=[1,2,3,4,5]))
confusion = pd.DataFrame(cm, index=['BRCA', 'KIRC', 'COAD', 'LUAD', 'PRAD'],
                         columns=['pred_BRCA', 'pred_KIRC', 'pred_COAD',␣
 ↪'pred_LUAD', 'pred_PRAD'])
sns.heatmap(confusion, annot=True)
plt.show()
```



[116]:
```
print(classification_report(y_test,y_predict))
# Well that didn't exactly go according to plan. I normalized the data and our␣
 ↪accuracy and precision all decreased.
# Then, instead of normalizing the data, what if I looked at increasing the␣
 ↪number of factors in use by
#using all the data that was accessible to me?
```

```
              precision    recall  f1-score   support

           1       0.77      0.87      0.81        68
           2       0.71      0.89      0.79        27
           3       0.78      0.70      0.74        20
           4       0.80      0.70      0.74        23
           5       0.58      0.30      0.40        23

    accuracy                           0.75       161
   macro avg       0.73      0.69      0.70       161
weighted avg       0.74      0.75      0.73       161
```

[156]:
```
# To do that, I will increase the amount of genes included to a larger amount␣
 ↪and see if the classifer is able to run
# with a higher accuracy and/or precision:

data_df = pd.DataFrame(data)
data_df = data_df.drop(columns = ["Unnamed: 0"])

data_df = data_df.sample(n=500, axis='columns')
data_df.shape
```

[156]:
```
(801, 500)
```

[157]:
```
#this means retraining our data on the now 500 genes that we're using instead␣
 ↪of 10.

X_train, X_test, y_train, y_test = train_test_split(data_df, labels_df,␣
 ↪test_size = 0.2, random_state = 20)
print ('The size of our training "X" (input features) is', X_train.shape)
print ('\n')
print ('The size of our testing "X" (input features) is', X_test.shape)
print ('\n')
print ('The size of our training "y" (output feature) is', y_train.shape)
print ('\n')
print ('The size of our testing "y" (output features) is', y_test.shape)
```

```
The size of our training "X" (input features) is (640, 500)
The size of our testing "X" (input features) is (161, 500)


The size of our training "y" (output feature) is (640, 1)


The size of our testing "y" (output features) is (161, 1)
```

[158]:

```
#then we retrain the ML model on the 500 gene data points we have for each␣
 ↪patient.

classifier = RandomForestClassifier(n_estimators = 500, criterion = 'entropy',␣
 ↪random_state = 0)
classifier.fit(X_train, y_train)
```

```
/var/folders/z2/z4rmk79963l_trmcdlb01zsw0000gn/T/ipykernel_74795/2634136648.py:2
: DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples,), for example using
ravel().
  classifier.fit(X_train, y_train)
```

[158]:

```
RandomForestClassifier(criterion='entropy', n_estimators=500, random_state=0)
```

[159]:

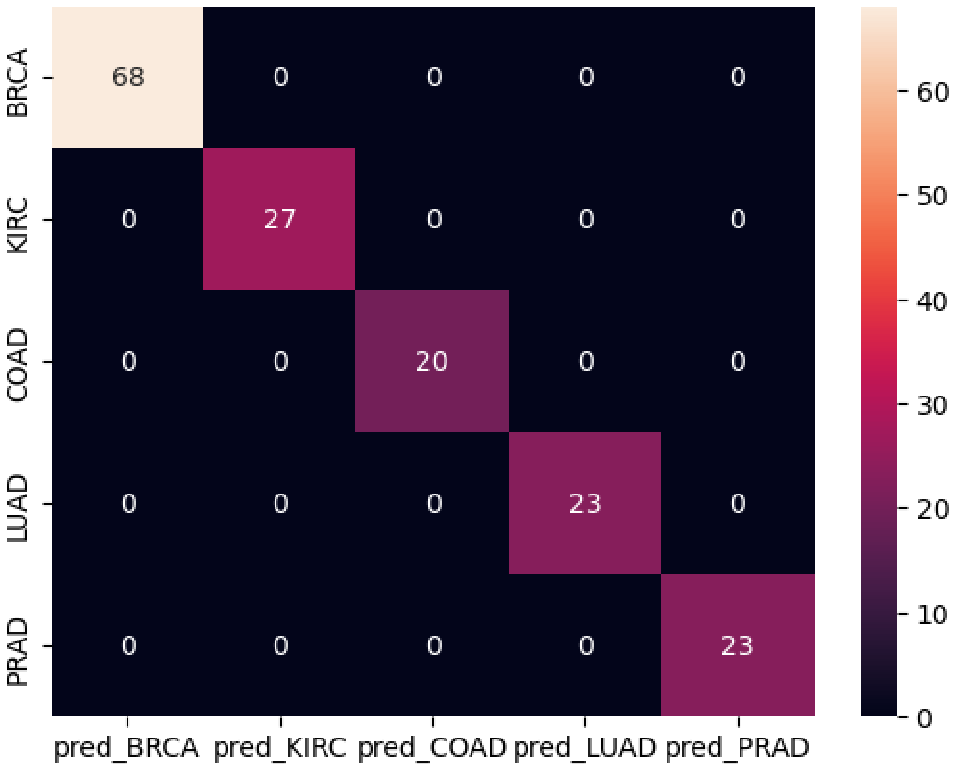
```
#we then use the new ML model to predict the classifications of the test data.
y_predict = classifier.predict(X_test)
```

[161]:

```
#also, we use a heatmap to visualize how many matches and mismatches we have

cm = np.array(confusion_matrix(y_test, y_predict, labels=[1,2,3,4,5]))
confusion = pd.DataFrame(cm, index=['BRCA', 'KIRC', 'COAD', 'LUAD', 'PRAD'],
                         columns=['pred_BRCA', 'pred_KIRC', 'pred_COAD',␣
 ↪'pred_LUAD', 'pred_PRAD'])
sns.heatmap(confusion, annot=True)
plt.show()

#seems like we don't have very many mismatches!
```



[160]:

```
print(classification_report(y_test,y_predict))

#using more factors to train our model on shows us that, in this case, it is␣
↪helping us differentiate between
#the different tumor types
```

```
              precision    recall  f1-score   support

           1       1.00      1.00      1.00        68
           2       1.00      1.00      1.00        27
           3       1.00      1.00      1.00        20
           4       1.00      1.00      1.00        23
           5       1.00      1.00      1.00        23

    accuracy                           1.00       161
   macro avg       1.00      1.00      1.00       161
weighted avg       1.00      1.00      1.00       161
```

[182]:

```
# Thus, based on the sheer amount of data available, it seems like Random␣
↪Forest Classifier is a good
```

```python
# model to use to predict the type of tumor in a patient based on the RNA expression values of 500 randomly
# selected genes. Another astonishing fact is that the sampling data is random which means when the sampling
# code was run over and over again, I got similar accuracy and precision as what is indicated above. I ran the
# previous lines of code above a total of 50 times (see for loop below) and saw that 50/50 times, the accuracy
# was reported to be above 95%.
counter = 0
for x in range(50):
    data_df = pd.DataFrame(data)
    data_df = data_df.drop(columns = ["Unnamed: 0"])
    data_df = data_df.sample(n=500, axis='columns')

    X_train, X_test, y_train, y_test = train_test_split(data_df, labels_df, test_size = 0.2, random_state = 20)

    classifier = RandomForestClassifier(n_estimators = 500, criterion = 'entropy', random_state = 0)
    classifier.fit(X_train, y_train)

    y_predict = classifier.predict(X_test)

    rep = classification_report(y_test,y_predict).split("\n")
    for num in rep[8].split(" "):
        if "." in num and num > "0.95":
            counter = counter + 1
    print(counter)
print(counter)
```

```
/var/folders/z2/z4rmk79963l_trmcdlb01zsw0000gn/T/ipykernel_74795/1717679701.py:1
6: DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples,), for example using
ravel().
  classifier.fit(X_train, y_train)
```

```
1
```

```
/var/folders/z2/z4rmk79963l_trmcdlb01zsw0000gn/T/ipykernel_74795/1717679701.py:1
6: DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples,), for example using
ravel().
  classifier.fit(X_train, y_train)
```

```
2
```

```
/var/folders/z2/z4rmk79963l_trmcdlb01zsw0000gn/T/ipykernel_74795/1717679701.py:1
6: DataConversionWarning: A column-vector y was passed when a 1d array was
```

```
expected. Please change the shape of y to (n_samples,), for example using
ravel().
  classifier.fit(X_train, y_train)

3

/var/folders/z2/z4rmk79963l_trmcdlb01zsw0000gn/T/ipykernel_74795/1717679701.py:1
6: DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples,), for example using
ravel().
  classifier.fit(X_train, y_train)

4

/var/folders/z2/z4rmk79963l_trmcdlb01zsw0000gn/T/ipykernel_74795/1717679701.py:1
6: DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples,), for example using
ravel().
  classifier.fit(X_train, y_train)

5

/var/folders/z2/z4rmk79963l_trmcdlb01zsw0000gn/T/ipykernel_74795/1717679701.py:1
6: DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples,), for example using
ravel().
  classifier.fit(X_train, y_train)

6

/var/folders/z2/z4rmk79963l_trmcdlb01zsw0000gn/T/ipykernel_74795/1717679701.py:1
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