MSEN660 HW2

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1 Assignment1

1.1 (a)

The mean and covariance matrices are

$$\Sigma_0 = \Sigma_1 = \sigma^2 \begin{pmatrix} 1 & 0.2 \\ 0.2 & 1 \end{pmatrix}$$

$$\mu_0 = \begin{pmatrix} 0 & 0 \end{pmatrix}$$

$$\mu_1 = \begin{pmatrix} 1 & 1 \end{pmatrix}$$

The prior probabilities P(Y=0) and P(Y=1)=.5. We simulate two QSPRs X1 and X2 and a property Y, using a Gaussian model. The optimal classifier in the Gaussian equal variance case is a hyperplane.

- Now we generate a 1000 synthetic training data sets for each sample size n = 20 to n = 100, in steps of 10, with $\sigma = 1$.
- \bullet For each training set and sample size we generate a corresponding independent test set of size L = 400
- Next we plot the average classification errors of the LDA, 3NN, and linear SVM classication rules, estimated with the test sets, as a function of n.

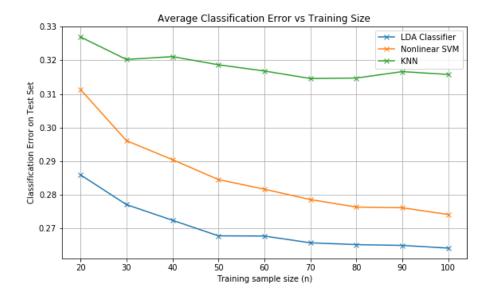


Figure 1: Average Classification Error on Test Set for different classifiers $\sigma=1$

• Next we plot the average classification errors of the LDA, 3NN, and linear SVM classication rules, estimated with the test sets, as a function of n with σ =2.

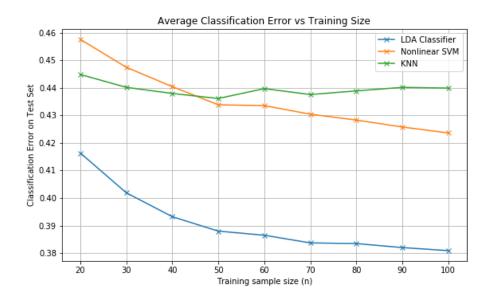


Figure 2: Average Classification Error on Test Set for different classifiers $\sigma=2$

1.2 (b)

- Now we use the same synthetic training data to obtain the average apparent error, leave one-out, and 5-fold cross-validation error error estimates for the LDA, 3NN, and linear SVM classication rules as a function of n.
- We have three plots, one for each classication rule. Each plot includes average classification error and the average error estimates.
- First we have $\sigma=1$.

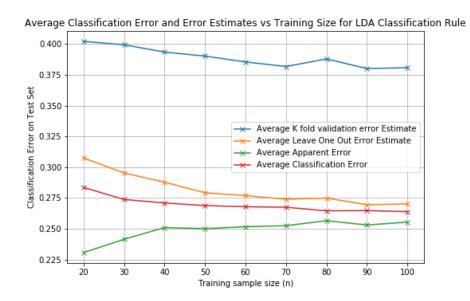


Figure 3: Average Error Estimates and Average Classification Error on Test Set for LDA $\sigma{=}1$

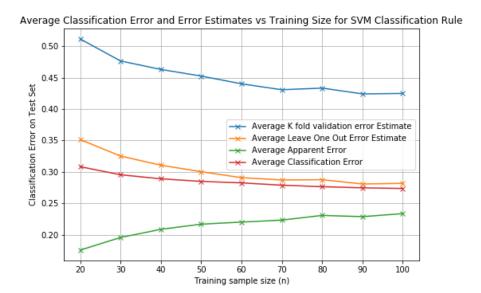


Figure 4: Average Error Estimates and Average Classification Error on Test Set for KNN $\sigma{=}1$

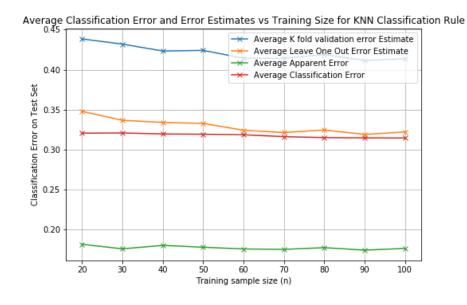


Figure 5: Average Error Estimates and Average Classification Error on Test Set for SVM $\sigma{=}1$

^{*} the Y axis label is supposed to be just "Classification Error"

• Now we have σ =2. We can expect to see higher error rates due to a lower ease of separability.

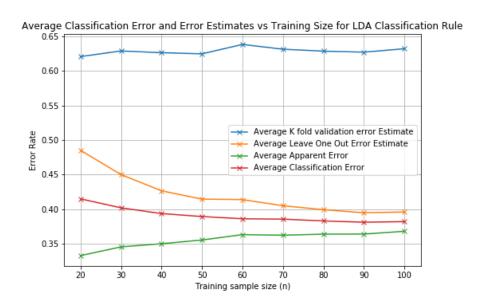
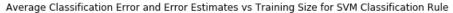


Figure 6: Average Error Estimates and Average Classification Error on Test Set for LDA $\sigma{=}2$



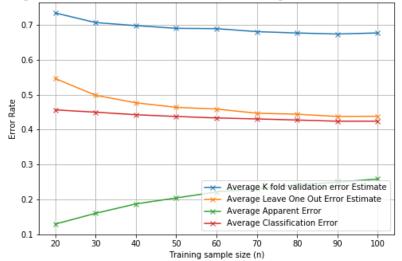


Figure 7: Average Error Estimates and Average Classification Error on Test Set for KNN $\sigma{=}2$

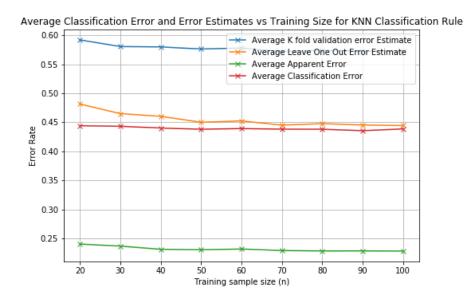


Figure 8: Average Error Estimates and Average Classification Error on Test Set for SVM $\sigma{=}2$

^{*} the Y axis label is supposed to be just "Classification Error"

- Explain what you see in terms of error estimation bias: We can see that since we are averaging over a large training sample set of m=1000 the trends are much more clear than what we observed in the first assignment. As such, as the training size increases we see the error rates decreasing continuously in most of the cases.
- With an increased σ we have a rise in estimated error for all types of error. This makes sense as the two distributions would become more spread out and difficult to separate. When distributions have far apart means and small σ we can easily separate them.
- In most of the cases we have observed an increasing apparent error. It is expected that as the training size n increases, the bias should decrease. And as the bias decreases the apparent error should slowly approach the true error or Bayesian error.
- Which error estimators are optimistic, and which are pessimistic?:
- From the plots we can see that KFold cross validation seems to be consistently pessimistic. It gives a conservative error compared to the other errors. This might be partly explained by the fact that a smaller set of data n is used for training. Generally, if we are able to have more training data we can create a better fit.
- Leave one out error and average classification error appear to be close to each other in most cases. This could be partly explained by the fact that their training set sizes n are almost the same.
- Finally, the apparent error is consistently lower than all the other error estimates. It is more optimistic than the rest. We can say that it is biased as we are computing the error from the same data that we use to train.
- Which error estimator would you would choose for each classication rule, based on these results?:
- I would prefer to use average classification error wherever possible. But that would require a wealth of data. Another good option would be Leave One Out Error as this gives an estimate close to classification error. And it uses as much of the data as possible for training. Of course it is susceptible to increased variance as we have only a single test sample.

2 Assignment2

- We consider LDA and 3NN as classication rules, and wrapper feature selection, with the apparent error estimate of the designed classifier as the criterion.
- We employ two simple feature selection methods: exhaustive search (for 1 to 5 variables) and sequential forward search (for 1 to 5 variables).
- First we have exhaustive search results in a table form.

	Categories	1 Feature	2 Features	3 Features	4 Features	5 Features
0	LDA Based Features	(Fe,)	(C, Fe)	(C, Ni, Fe)	(C, N, Fe, Mn)	(N, Ni, Fe, Si, Cr)
1	LDA best apparent Error	0.12	0.04	0.04	0.04	0
2	LDA test Error	[0.1428571428571429]	[0.12244897959183676]	[0.061224489795918324]	[0.11224489795918369]	[0.16326530612244894]
3	KNN Based Features	(Ni,)	(N, Ni)	(C, Ni, Fe)	(C, N, Ni, Si)	(C, Fe, Mn, Si, Cr)
4	KNN apparent Error	0.122449	0.0714286	0.0612245	0.0510204	0.0408163
5	KNN test Error	[0.2551020408163265]	[0.23469387755102045]	[0.23469387755102045]	[0.061224489795918324]	[0.061224489795918324]

Figure 9: Exhaustive Search with Feature Sets and Errors

• Now we have sequential forward search results in a table form.

	Categories	1 Feature	2 Features	3 Features	4 Features	5 Features
0	LDA Based Features	[Fe]	[Fe, C]	[Fe, C, Ni]	[Fe, C, Ni, Mn]	[Fe, C, Ni, Mn, N]
1	LDA best apparent Error	0.12	0.04	0.04	0.04	0.04
2	LDA test Error	[0.1428571428571429]	[0.12244897959183676]	[0.061224489795918324]	[0.061224489795918324]	[0.09183673469387754]
3	KNN Based Features	[Mn]	[Mn, C]	[Mn, C, N]	[Mn, C, N, Si]	[Mn, C, N, Si, Ni]
4	KNN best apparent Error	0.04	0.04	0.04	0.04	0.08
5	KNN_test Error	[0.2551020408163265]	[0.23469387755102045]	[0.23469387755102045]	[0.22448979591836737]	[0.09183673469387754]

Figure 10: Sequential Forward Search with Feature Sets and Errors

I observed that the error rates were very small. I wanted to confirm that the training data was so well separated and created a pair plot for help. This can help show that even with just considering pairs of predictors we can find some that are easily separable.

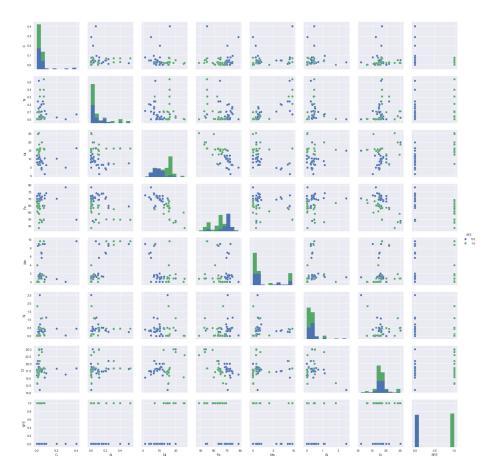


Figure 11: Pair Plot with High and Low SFE

Here is the t test statistics for the predictors from the first assignment.

```
[Ttest_indResult(statistic=-3.6652244046944773, pvalue=0.0013486369196097205), 'Ni']
[Ttest_indResult(statistic=2.359906793878512, pvalue=0.027438300016957032), 'Fe']
[Ttest_indResult(statistic=2.1848241668704795, pvalue=0.04179478729923675), 'Si']
[Ttest_indResult(statistic=1.4943828075999175, pvalue=0.15926508688174165), 'C']
[Ttest_indResult(statistic=-1.0278205792662476, pvalue=0.31477403802244214), 'Cr']
[Ttest_indResult(statistic=0.80913241119481, pvalue=0.4267305733623522), 'Mn']
[Ttest_indResult(statistic=0.2829267844867566, pvalue=0.7800377202267232), 'N']
```

Figure 12: Sorted Table with t-test statistics

• How do you compare the results against each other and against the results obtained with the simple filter feature selection used in Project 1? : It is important to note that in the first project we simply looked at the pair wise t test statistics to choose the best features. We ignored the multivariate

relationships. Here with exhaustive selection, we consider that as well and so we can see a lower test error.

- How do you compare the error estimators and feature selection methods used based on the variable sets found and the estimates of the true error?
 From what we can see it is observed that exhaustive search yields a somewhat clear decreasing error as compared to sequential forward search. This could be explained by the possibility of sequential search choosing a wrong feature early on and then its inability to drop that feature for a better one. On the other hand with exhaustive search we consider all possible combinations.
- How do you think the results might change if there were more training points available? : If we had more samples we would have clearer trends and lower variance in the errors. It would be easier to make comparisons between the two methods of feature selection. Sequential forward search especially may have improved performance as there would be more data to handle ties.

3 Code

The python code for all the problems is included below (as jupyter notebook pdf).

HW2_1

October 30, 2018

```
In [68]: import numpy as np
         import matplotlib.pyplot as plt
         from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
         from sklearn.svm import SVC
         from sklearn.metrics import confusion_matrix
         from sklearn.neighbors import KNeighborsClassifier
         #part1a
         sigma=1
         rho=0.2
         u1=np.array([0,0])
         u2=np.array([1,1])
         cov=np.array([[sigma**2,rho*sigma**2],[rho*sigma**2,sigma**2]])
         print('cov',cov)
         nlist=np.linspace(20,100,num=9)
         test_error=np.zeros(len(nlist))
         err_lda=np.zeros(len(nlist))
         count=0
         score_avg=np.zeros([len(nlist),3])
         for train_n in range(0,len(nlist)) :
             score=[0,0,0]
             conf_matrix=np.float64(([0,0],[0,0])*3)
             for rep_i in range(0,1000):
                 #import pdb; pdb.set_trace()
                 #create sample two guassian distributions for each mean training data
                 x1_train=np.random.multivariate_normal(u1,cov,int(nlist[train_n]/2))
                 y1_train=np.zeros(int(nlist[train_n]/2))
                 for i in range (0,int(nlist[train_n]/2)):
                     v1 train[i]=0
                 x2_train=np.random.multivariate_normal(u2,cov,int(nlist[train_n]/2))
                 y2_train=np.zeros(int(nlist[train_n]/2))
                 for i in range (0,int(nlist[train_n]/2)):
                     y2_train[i]=1
```

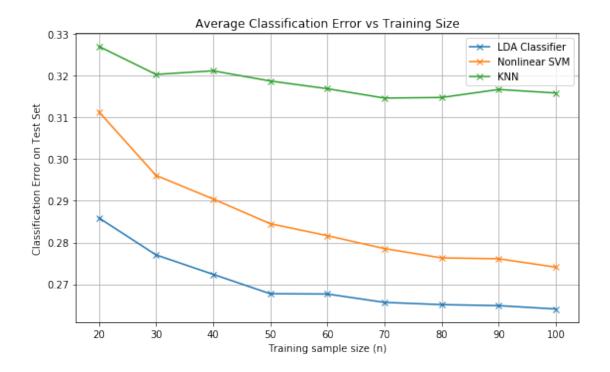
```
X_train=np.concatenate((x1_train,x2_train),axis=0)
Y_train=np.concatenate((y1_train,y2_train),axis=0)
# generate test set
x1_test=np.random.multivariate_normal(u1,cov,200)
y1 test=np.zeros(200)
for i in range (0,200):
    v1 test[i]=0
x2_test=np.random.multivariate_normal(u2,cov,200)
y2_test=np.zeros(200)
for i in range (0,200):
    y2_test[i]=1
X_test=np.concatenate((x1_test,x2_test),axis=0)
Y_test=np.concatenate((y1_test,y2_test),axis=0)
#model1
model1 = LinearDiscriminantAnalysis()
model1.fit(X train, Y train)
LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None,
solver='svd', store covariance=False, tol=0.0001)
Y_pred1=model1.predict(X_test)
#model2
model2 = SVC(gamma='auto')
model2.fit(X_train, Y_train)
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
max_iter=-1, probability=False, random_state=None, shrinking=True,
tol=0.001, verbose=False)
Y_pred2=model2.predict(X_test)
#model2
model3 = KNeighborsClassifier(n neighbors=3)
model3.fit(X_train, Y_train)
KNeighborsClassifier(...)
Y_pred3=model3.predict(X_test)
#acccuracy for this iteration
score[0]+=model1.score(X_test,Y_test)
score[1]+=model2.score(X_test,Y_test)
score[2] +=model3.score(X_test,Y_test)
conf_matrix[0:2][0:2]+=np.divide(confusion_matrix(Y_test, Y_pred1),200)
conf_matrix[2:4][0:2]+=np.divide(confusion_matrix(Y_test, Y_pred2),200)
conf_matrix[4:6][0:2]+=np.divide(confusion_matrix(Y_test, Y_pred3),200)
```

```
#average the accuracy and conf matrix
            for modelcount in range (0,3):
                print(score)
                score_avg[count,modelcount]=score[modelcount]/1000
                print('scoreavg', modelcount, score_avg[count, modelcount])
             count+=1
                #np.append(conf_matrix_avg[modelcount],np.divide(conf_matrix[modelcount],1000
cov [[1. 0.2]
 [0.2 1.]]
[714.084999999974, 688.665000000003, 673.032499999997]
scoreavg 0 0.714084999999974
[714.084999999974, 688.665000000003, 673.0324999999997]
scoreavg 1 0.6886650000000003
[714.084999999974, 688.665000000003, 673.0324999999997]
scoreavg 2 0.673032499999997
[722.9525000000006, 703.920000000001, 679.7474999999995]
scoreavg 0 0.7229525000000006
[722.9525000000006, 703.920000000001, 679.7474999999995]
scoreavg 1 0.703920000000001
[722.952500000006, 703.920000000001, 679.7474999999995]
scoreavg 2 0.679747499999995
[727.604999999984, 709.559999999994, 678.8874999999991]
scoreavg 0 0.727604999999984
[727.604999999984, 709.559999999994, 678.8874999999991]
scoreavg 1 0.709559999999994
[727.604999999984, 709.559999999994, 678.8874999999991]
scoreavg 2 0.678887499999991
[732.2525000000014, 715.495000000007, 681.3250000000003]
scoreavg 0 0.7322525000000014
[732.2525000000014, 715.495000000007, 681.3250000000003]
scoreavg 1 0.7154950000000007
[732.2525000000014, 715.495000000007, 681.3250000000003]
scoreavg 2 0.6813250000000003
[732.3200000000002, 718.360000000005, 683.169999999997]
scoreavg 0 0.7323200000000002
[732.3200000000002, 718.360000000005, 683.169999999997]
scoreavg 1 0.7183600000000004
[732.3200000000002, 718.360000000005, 683.169999999997]
scoreavg 2 0.683169999999997
[734.3250000000002, 721.4550000000013, 685.4149999999996]
scoreavg 0 0.734325000000001
[734.3250000000002, 721.4550000000013, 685.4149999999996]
scoreavg 1 0.7214550000000013
[734.3250000000002, 721.4550000000013, 685.4149999999996]
scoreavg 2 0.685414999999997
[734.860000000004, 723.68, 685.2775]
```

```
scoreavg 0 0.7348600000000004
[734.860000000004, 723.68, 685.2775]
scoreavg 1 0.72368
[734.860000000004, 723.68, 685.2775]
scoreavg 2 0.6852775
[735.102499999997, 723.887499999998, 683.3574999999998]
scoreavg 0 0.735102499999998
[735.102499999997, 723.887499999998, 683.3574999999998]
scoreavg 1 0.723887499999998
[735.102499999997, 723.887499999998, 683.3574999999998]
scoreavg 2 0.683357499999998
[735.907499999998, 725.902499999997, 684.205]
scoreavg 0 0.735907499999998
[735.907499999998, 725.902499999997, 684.205]
scoreavg 1 0.7259024999999997
[735.907499999998, 725.902499999997, 684.205]
scoreavg 2 0.6842050000000001
In [67]: conf_matrix=np.float64(([0,0],[0,0])*3)
         score_avg.shape
Out[67]: (9, 3)
In [69]: #plot error vs n
        fig, ax = plt.subplots(figsize=[8,5])
        plt.plot(nlist,1-score_avg[:,0],marker='x',label='LDA Classifier')
        plt.plot(nlist,1-score_avg[:,1],marker='x',label='Nonlinear SVM')
        plt.plot(nlist,1-score_avg[:,2],marker='x',label='KNN')
        plt.hold(True)
        plt.title('Average Classification Error vs Training Size')
        plt.ylabel('Classification Error on Test Set')
        plt.xlabel('Training sample size (n)')
        fig.tight_layout()
        ax.legend()
        plt.grid(True)
        plt.show
        fig.savefig('hw2_1a.png')
C:\Users\aksha\Anaconda3\lib\site-packages\ipykernel_launcher.py:6: MatplotlibDeprecationWarni
    Future behavior will be consistent with the long-time default:
   plot commands add elements without first clearing the
   Axes and/or Figure.
C:\Users\aksha\Anaconda3\lib\site-packages\matplotlib\__init__.py:911: MatplotlibDeprecationWa
 mplDeprecation)
```

mplDeprecation)

C:\Users\aksha\Anaconda3\lib\site-packages\matplotlib\rcsetup.py:156: MatplotlibDeprecationWar



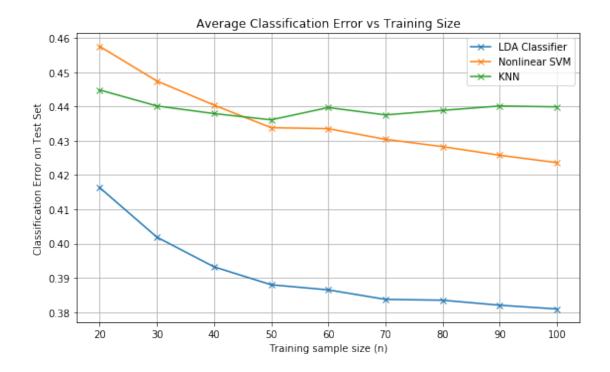
```
In [70]: #part1a
         sigma=2
         rho=0.2
         u1=np.array([0,0])
         u2=np.array([1,1])
         cov=np.array([[sigma**2,rho*sigma**2],[rho*sigma**2,sigma**2]])
         print('cov',cov)
         nlist=np.linspace(20,100,num=9)
         test_error=np.zeros(len(nlist))
         err_lda=np.zeros(len(nlist))
         score_avg=np.zeros([len(nlist),3])
         for train_n in range(0,len(nlist)) :
             score=[0,0,0]
             conf_matrix=np.float64(([0,0],[0,0])*3)
             for rep_i in range(0,1000):
                 #import pdb; pdb.set_trace()
                 #create sample two guassian distributions for each mean training data
                 x1_train=np.random.multivariate_normal(u1,cov,int(nlist[train_n]/2))
                 y1_train=np.zeros(int(nlist[train_n]/2))
                 for i in range (0,int(nlist[train_n]/2)):
```

```
y1_train[i]=0
x2_train=np.random.multivariate_normal(u2,cov,int(nlist[train_n]/2))
y2_train=np.zeros(int(nlist[train_n]/2))
for i in range (0,int(nlist[train_n]/2)):
    y2_train[i]=1
X_train=np.concatenate((x1_train,x2_train),axis=0)
Y_train=np.concatenate((y1_train,y2_train),axis=0)
# generate test set
x1_test=np.random.multivariate_normal(u1,cov,200)
y1_test=np.zeros(200)
for i in range (0,200):
    y1_test[i]=0
x2_test=np.random.multivariate_normal(u2,cov,200)
y2_test=np.zeros(200)
for i in range (0,200):
    y2_test[i]=1
X_test=np.concatenate((x1_test,x2_test),axis=0)
Y_test=np.concatenate((y1_test,y2_test),axis=0)
model1 = LinearDiscriminantAnalysis()
model1.fit(X_train, Y_train)
LinearDiscriminantAnalysis(n components=None, priors=None, shrinkage=None,
solver='svd', store_covariance=False, tol=0.0001)
Y_pred1=model1.predict(X_test)
#model2
model2 = SVC(gamma='auto')
model2.fit(X_train, Y_train)
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
max_iter=-1, probability=False, random_state=None, shrinking=True,
tol=0.001, verbose=False)
Y_pred2=model2.predict(X_test)
#model2
model3 = KNeighborsClassifier(n_neighbors=3)
model3.fit(X_train, Y_train)
KNeighborsClassifier(...)
Y_pred3=model3.predict(X_test)
#acccuracy for this iteration
score[0]+=model1.score(X_test,Y_test)
score[1]+=model2.score(X_test,Y_test)
```

```
score[2] +=model3.score(X_test,Y_test)
                 conf_matrix[0:2][0:2]+=np.divide(confusion_matrix(Y_test, Y_pred1),200)
                 conf matrix[2:4][0:2]+=np.divide(confusion_matrix(Y_test, Y_pred2),200)
                 conf_matrix[4:6][0:2]+=np.divide(confusion_matrix(Y_test, Y_pred3),200)
             #average the accuracy and conf matrix
             for modelcount in range (0,3):
                 print(score)
                 score avg[count,modelcount]=score[modelcount]/1000
                 print('scoreavg', modelcount, score_avg[count, modelcount])
             count+=1
                 #np.append(conf_matrix_avq[modelcount],np.divide(conf_matrix[modelcount],1000
cov [[4. 0.8]
 [0.8 4.]]
[583.6624999999991, 542.4375000000008, 555.1675]
scoreavg 0 0.5836624999999991
[583.662499999991, 542.4375000000008, 555.1675]
scoreavg 1 0.5424375000000008
[583.662499999991, 542.4375000000008, 555.1675]
scoreavg 2 0.5551675
[598.107499999998, 552.552499999999, 559.8300000000002]
scoreavg 0 0.598107499999998
[598.107499999998, 552.552499999999, 559.8300000000002]
scoreavg 1 0.5525524999999999
[598.107499999998, 552.552499999999, 559.8300000000002]
scoreavg 2 0.5598300000000002
[606.775, 559.579999999997, 562.049999999997]
scoreavg 0 0.606775
[606.775, 559.579999999997, 562.049999999997]
scoreavg 1 0.559579999999997
[606.775, 559.579999999997, 562.049999999997]
scoreavg 2 0.562049999999997
[612.007499999998, 566.1625000000001, 563.8750000000005]
scoreavg 0 0.612007499999998
[612.007499999998, 566.1625000000001, 563.8750000000005]
scoreavg 1 0.5661625000000001
[612.007499999998, 566.1625000000001, 563.8750000000005]
scoreavg 2 0.5638750000000005
[613.5049999999999, 566.4575, 560.2950000000003]
scoreavg 0 0.6135049999999999
[613.5049999999999, 566.4575, 560.2950000000003]
scoreavg 1 0.5664575
[613.5049999999999, 566.4575, 560.2950000000003]
scoreavg 2 0.5602950000000003
[616.275, 569.569999999999, 562.4374999999993]
scoreavg 0 0.616275
```

```
[616.275, 569.569999999999, 562.4374999999993]
scoreavg 1 0.5695699999999999
[616.275, 569.569999999999, 562.4374999999993]
scoreavg 2 0.5624374999999994
[616.519999999999, 571.7, 561.1224999999995]
scoreavg 0 0.616519999999998
[616.519999999999, 571.7, 561.1224999999995]
scoreavg 1 0.571700000000001
[616.519999999999, 571.7, 561.1224999999995]
scoreavg 2 0.561122499999995
[617.977499999993, 574.2150000000001, 559.8374999999993]
scoreavg 0 0.617977499999993
[617.977499999993, 574.215000000001, 559.837499999993]
scoreavg 1 0.5742150000000001
[617.977499999993, 574.215000000001, 559.837499999993]
scoreavg 2 0.5598374999999993
[619.0825000000006, 576.3650000000006, 560.0925000000001]
scoreavg 0 0.6190825000000005
[619.0825000000006, 576.3650000000006, 560.0925000000001]
scoreavg 1 0.5763650000000006
[619.0825000000006, 576.3650000000006, 560.0925000000001]
scoreavg 2 0.5600925000000001
In [71]: \#plot\ error\ vs\ n
        fig, ax = plt.subplots(figsize=[8,5])
        plt.plot(nlist,1-score_avg[:,0],marker='x',label='LDA Classifier')
        plt.plot(nlist,1-score_avg[:,1],marker='x',label='Nonlinear SVM')
        plt.plot(nlist,1-score_avg[:,2],marker='x',label='KNN')
        plt.hold(True)
        plt.title('Average Classification Error vs Training Size')
        plt.ylabel('Classification Error on Test Set')
        plt.xlabel('Training sample size (n)')
        fig.tight_layout()
        ax.legend()
        plt.grid(True)
        plt.show
        fig.savefig('hw2_11a.png')
C:\Users\aksha\Anaconda3\lib\site-packages\ipykernel_launcher.py:6: MatplotlibDeprecationWarni
    Future behavior will be consistent with the long-time default:
   plot commands add elements without first clearing the
   Axes and/or Figure.
C:\Users\aksha\Anaconda3\lib\site-packages\matplotlib\__init__.py:911: MatplotlibDeprecationWa
 mplDeprecation)
C:\Users\aksha\Anaconda3\lib\site-packages\matplotlib\rcsetup.py:156: MatplotlibDeprecationWar
```

mplDeprecation)



```
In [106]: from sklearn.model_selection import LeaveOneOut
          from sklearn.model_selection import KFold
          #part1a
          sigma=1
          rho=0.2
          u1=np.array([0,0])
          u2=np.array([1,1])
          cov=np.array([[sigma**2,rho*sigma**2],[rho*sigma**2,sigma**2]])
          print('cov',cov)
          nlist=np.linspace(20,100,num=9)
          test_error=np.zeros(len(nlist))
          err_lda=np.zeros(len(nlist))
          count=0
          score_avg=np.zeros([len(nlist),3])
          score_avgkf=np.zeros([len(nlist),3])
          score_avgloo=np.zeros([len(nlist),3])
          score_avgcl=np.zeros([len(nlist),3])
          for train_n in range(0,len(nlist)) :
              scorekf=[0,0,0]
              scoreloo=[0,0,0]
              score=[0,0,0]
```

```
score_cl=[0,0,0]
#import pdb; pdb.set_trace()
for rep_i in range(0,1000):
    #import pdb; pdb.set_trace()
    #create sample two guassian distributions for each mean training data
    x1_train=np.random.multivariate_normal(u1,cov,int(nlist[train_n]/2))
    y1_train=np.zeros(int(nlist[train_n]/2))
    for i in range (0,int(nlist[train_n]/2)):
        y1_train[i]=0
    x2_train=np.random.multivariate_normal(u2,cov,int(nlist[train_n]/2))
    y2_train=np.zeros(int(nlist[train_n]/2))
    for i in range (0,int(nlist[train_n]/2)):
        y2_train[i]=1
    X_train=np.concatenate((x1_train,x2_train),axis=0)
    Y_train=np.concatenate((y1_train,y2_train),axis=0)
    # generate test set
    x1_test=np.random.multivariate_normal(u1,cov,200)
    y1_test=np.zeros(200)
    for i in range (0,200):
        y1_test[i]=0
    x2_test=np.random.multivariate_normal(u2,cov,200)
    y2_test=np.zeros(200)
    for i in range (0,200):
        y2_test[i]=1
    X_test=np.concatenate((x1_test,x2_test),axis=0)
    Y_test=np.concatenate((y1_test,y2_test),axis=0)
    #kfold validation error estimate
   kf = KFold(n_splits=5)
    kf.get_n_splits(X_train)
    KFold(n_splits=5, random_state=None, shuffle=True)
    for train_index, test_index in kf.split(X_train):
        X_trainkf, X_testkf = X_train[train_index], X_train[test_index]
        Y_trainkf, Y_testkf = Y_train[train_index], Y_train[test_index]
        #model1
        model1 = LinearDiscriminantAnalysis()
        model1.fit(X_trainkf, Y_trainkf)
        LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None
        solver='svd', store_covariance=False, tol=0.0001)
        Y_pred1=model1.predict(X_testkf)
        #model2
        model2 = SVC(gamma='auto')
```

```
model2.fit(X_trainkf, Y_trainkf)
    SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)
    Y_pred2=model2.predict(X_testkf)
    #model2
    model3 = KNeighborsClassifier(n_neighbors=3)
    model3.fit(X_trainkf, Y_trainkf)
    KNeighborsClassifier(...)
    Y_pred3=model3.predict(X_testkf)
    #acccuracy for this iteration
    scorekf[0]+=model1.score(X_testkf,Y_testkf)
    scorekf[1]+=model2.score(X_testkf,Y_testkf)
    scorekf[2]+=model3.score(X_testkf,Y_testkf)
#import pdb; pdb.set_trace()
# leave one out error estimate
loo = LeaveOneOut()
loo.get_n_splits(X_train)
LeaveOneOut()
for train_index, test_index in loo.split(X_train):
    X_trainloo, X_testloo = X_train[train_index], X_train[test_index]
    Y_trainloo, Y_testloo = Y_train[train_index], Y_train[test_index]
    #model1
    model1 = LinearDiscriminantAnalysis()
    model1.fit(X_trainloo, Y_trainloo)
    LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None
    solver='svd', store_covariance=False, tol=0.0001)
    Y_pred1=model1.predict(X_testloo)
    #model2
    model2 = SVC(gamma='auto')
    model2.fit(X_trainloo, Y_trainloo)
    SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)
    Y_pred2=model2.predict(X_testloo)
    #model2
    model3 = KNeighborsClassifier(n_neighbors=3)
```

```
model3.fit(X_trainloo, Y_trainloo)
    KNeighborsClassifier(...)
    Y_pred3=model3.predict(X_testloo)
    #acccuracy for this iteration
    scoreloo[0]+=model1.score(X_testloo,Y_testloo)
    scoreloo[1]+=model2.score(X testloo,Y testloo)
    scoreloo[2]+=model3.score(X_testloo,Y_testloo)
# average apparent error
#model1
model1 = LinearDiscriminantAnalysis()
model1.fit(X_train, Y_train)
LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None,
solver='svd', store_covariance=False, tol=0.0001)
Y_pred1=model1.predict(X_test)
#model2
model2 = SVC(gamma='auto')
model2.fit(X_train, Y_train)
SVC(C=1.0, cache size=200, class weight=None, coef0=0.0,
decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
max_iter=-1, probability=False, random_state=None, shrinking=True,
tol=0.001, verbose=False)
Y_pred2=model2.predict(X_test)
#model2
model3 = KNeighborsClassifier(n_neighbors=3)
model3.fit(X_train, Y_train)
KNeighborsClassifier(...)
Y_pred3=model3.predict(X_test)
#acccuracy for this iteration
score[0]+=model1.score(X_train,Y_train)
score[1]+=model2.score(X_train,Y_train)
score[2]+=model3.score(X_train,Y_train)
# average classification error
#model1
model1 = LinearDiscriminantAnalysis()
model1.fit(X_train, Y_train)
LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None,
solver='svd', store_covariance=False, tol=0.0001)
Y_pred1=model1.predict(X_test)
```

#mode1.2

```
model2.fit(X_train, Y_train)
        SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
        decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
        max_iter=-1, probability=False, random_state=None, shrinking=True,
        tol=0.001, verbose=False)
        Y_pred2=model2.predict(X_test)
        #model2
        model3 = KNeighborsClassifier(n_neighbors=3)
        model3.fit(X_train, Y_train)
        KNeighborsClassifier(...)
        Y_pred3=model3.predict(X_test)
        #acccuracy for this iteration
        score_cl[0]+=model1.score(X_test,Y_test)
        score_cl[1]+=model2.score(X_test,Y_test)
        score_cl[2]+=model3.score(X_test,Y_test)
    #average across k folds
    scorekf=np.divide(scorekf,5)
    #average leave one out error estimate
    scoreloo=np.divide(scoreloo,int(nlist[train_n]))
    #average the accuracy for kf, loo, and average classification error
    for modelcount in range (0,3):
        score_avgkf[count,modelcount]=scorekf[modelcount]/1000
        score_avgloo(count, modelcount) = scoreloo(modelcount) / 1000
        score_avg[count,modelcount]=score[modelcount]/1000
        score_avgcl[count,modelcount]=score_cl[modelcount]/1000
    count+=1
    print ('count of n',count)
    print ('score kf',score_avgkf)
    print('score loo',score_avgloo)
    print('score avg',score_avg)
    print('score avg',score_avgcl)
#plot error curves for LDA
fig, ax = plt.subplots(figsize=[8,5])
plt.plot(nlist,1-score_avgkf[:,0],marker='x',label='Average K fold validation error
plt.plot(nlist,1-score_avgloo[:,0],marker='x',label='Average Leave One Out Error Est
plt.plot(nlist,1-score_avg[:,0],marker='x',label='Average Apparent Error')
plt.plot(nlist,1-score_avgcl[:,0],marker='x',label='Average Classification Error')
plt.title('Average Classification Error and Error Estimates vs Training Size for LDA
plt.ylabel('Error Rate')
plt.xlabel('Training sample size (n)')
```

model2 = SVC(gamma='auto')

```
ax.legend()
          plt.grid(True)
          plt.show
          fig.savefig('hw2_14b.png')
          #plot error curves for SVM
          fig, ax = plt.subplots(figsize=[8,5])
          plt.plot(nlist,1-score_avgkf[:,1],marker='x',label='Average K fold validation error
          plt.plot(nlist,1-score_avgloo[:,1],marker='x',label='Average Leave One Out Error Est
          plt.plot(nlist,1-score_avg[:,1],marker='x',label='Average Apparent Error')
          plt.plot(nlist,1-score_avgcl[:,1],marker='x',label='Average Classification Error')
          plt.title('Average Classification Error and Error Estimates vs Training Size for SVM
          plt.ylabel('Error Rate')
          plt.xlabel('Training sample size (n)')
          fig.tight_layout()
          ax.legend()
          plt.grid(True)
          plt.show
          fig.savefig('hw2_15b.png')
          #plot error curves for KNN
          fig, ax = plt.subplots(figsize=[8,5])
          plt.plot(nlist,1-score_avgkf[:,2],marker='x',label='Average K fold validation error
          plt.plot(nlist,1-score_avgloo[:,2],marker='x',label='Average Leave One Out Error Est
          plt.plot(nlist,1-score_avg[:,2],marker='x',label='Average Apparent Error')
          plt.plot(nlist,1-score_avgcl[:,2],marker='x',label='Average Classification Error')
          plt.title('Average Classification Error and Error Estimates vs Training Size for KNN
          plt.ylabel('Error Rate')
          plt.xlabel('Training sample size (n)')
          fig.tight_layout()
          ax.legend()
          plt.grid(True)
          plt.show
          fig.savefig('hw2_16b.png')
cov [[1. 0.2]
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count of n 1
score kf [[0.59785 0.48825 0.56155]
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fig.tight_layout()

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score loo [[0.6925 0.6485 0.6521]
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score avg [[0.76935 0.8246
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score avg [[0.716375
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count of n 2
score kf [[0.59785
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score loo [[0.6925
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score avg [[0.76935
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 [0.75853333 0.8045
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score avg [[0.716375 0.6917125 0.6794275]
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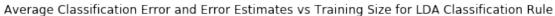
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score avg [[0.716375
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count of n 5
score kf [[0.59785
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              0.55973333 0.58565
                                      1
```

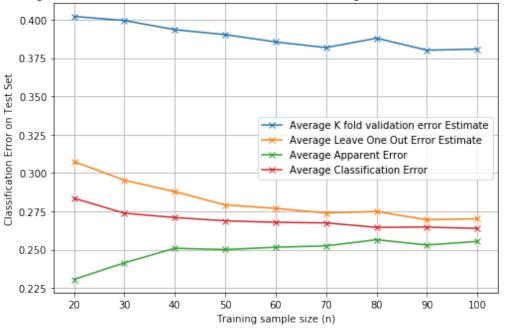
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              0.
                          0.
 [0.
              0.
                          0.
                                     ]]
score avg [[0.716375 0.6917125 0.6794275]
 [0.72618
             0.7045625 0.6791725]
 [0.729005 0.711005
                        0.680395 ]
 [0.7311475 0.71515
                        0.6807675]
 [0.7321125 0.7175
                        0.6814625]
 [0.
             0.
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 [0.
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 [0.
             0.
                        0.
count of n 6
score kf [[0.59785
                                    0.56155
                        0.48825
                                               ]
 [0.60053333 0.5233
                          0.568
                                     ]
 [0.6065
              0.536825
                          0.576625
                                    ]
 [0.60976
              0.5474
                          0.57588
 [0.6145
              0.55973333 0.58565
 [0.61821429 0.56921429 0.58587143]
 [0.
              0.
                          0.
 [0.
                                     ]
              0.
                          0.
 [0.
              0.
                          0.
                                     ]]
score loo [[0.6925
                                     0.6521
                                                ]
                         0.6485
 [0.70466667 0.67476667 0.6633
                                     ]
 [0.712125
              0.689325
                          0.66595
                                     ]
 [0.72078
              0.69972
                          0.66722
                                     ]
 [0.72305
              0.7092
                          0.67575
                                     ]
 [0.72601429 0.71288571 0.67862857]
 [0.
              0.
                          0.
                                     ]
```

```
[0.
              0.
                          0.
 [0.
              0.
                                    ]]
                          0.
score avg [[0.76935
                                    0.8184
                                               ]
                        0.8246
 [0.75853333 0.8045
                          0.82406667]
 [0.749025
                          0.819825
              0.7915
 [0.74988
              0.78326
                          0.82206
 [0.74835
              0.77993333 0.82425
 [0.7475
              0.77681429 0.82478571]
 [0.
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 ГО.
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              0.
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                                    ]]
score avg [[0.716375 0.6917125 0.6794275]
 [0.72618
            0.7045625 0.6791725]
 [0.729005 0.711005
                       0.680395 ]
 [0.7311475 0.71515
                        0.6807675]
 [0.7321125 0.7175
                        0.6814625]
 [0.7325075 0.721205
                       0.6837525]
 [0.
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             0.
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count of n 7
score kf [[0.59785
                                   0.56155
                                              ]
                       0.48825
 [0.60053333 0.5233
                          0.568
                                    ٦
 [0.6065
              0.536825
                          0.576625
                                    ]
 [0.60976
              0.5474
                          0.57588
                                    ٦
 [0.6145
              0.55973333 0.58565
 [0.61821429 0.56921429 0.58587143]
 [0.6120625
             0.5665875
                         0.5811
 [0.
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                                    ٦
              0.
 [0.
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                                    ]]
                                    0.6521
score loo [[0.6925
                        0.6485
                                               ٦
 [0.70466667 0.67476667 0.6633
                                    ]
 [0.712125
              0.689325
                          0.66595
                                    1
 [0.72078
              0.69972
                          0.66722
                                    ]
 [0.72305
              0.7092
                          0.67575
                                    ]
 [0.72601429 0.71288571 0.67862857]
 [0.7250625
             0.712475
                          0.67545
                                    ]
 ГО.
              0.
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                                    1
 [0.
              0.
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                                    ]]
score avg [[0.76935
                        0.8246
                                    0.8184
                                               ]
 [0.75853333 0.8045
                          0.82406667]
 [0.749025
              0.7915
                          0.819825
                                    ]
 [0.74988
              0.78326
                          0.82206
 [0.74835
              0.77993333 0.82425
                                    ٦
 [0.7475
              0.77681429 0.82478571]
 [0.74345
              0.7692875
                         0.8226
                                    ]
 [0.
              0.
                          0.
                                    1
 [0.
              0.
                          0.
                                    ]]
```

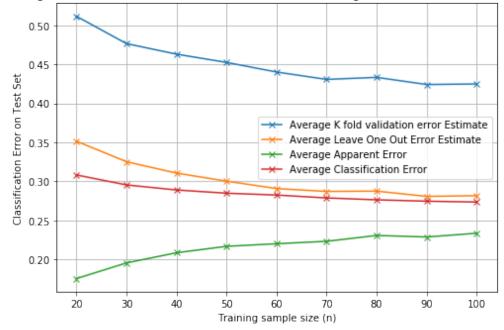
```
score avg [[0.716375 0.6917125 0.6794275]
            0.7045625 0.6791725]
 [0.72618
 [0.729005 0.711005 0.680395]
 [0.7311475 0.71515
                       0.6807675]
 [0.7321125 0.7175
                       0.6814625]
 [0.7325075 0.721205
                       0.6837525]
 [0.7354
            0.72361
                       0.6849825]
 ΓΟ.
            0.
                       0.
                                1
 ГО.
                                ]]
            0.
                       0.
count of n 8
score kf [[0.59785
                       0.48825
                                  0.56155
                                             1
 [0.60053333 0.5233
                         0.568
                                   ٦
 [0.6065
             0.536825
                         0.576625
                                   ]
 [0.60976
             0.5474
                         0.57588
 [0.6145
             0.55973333 0.58565
 [0.61821429 0.56921429 0.58587143]
 [0.6120625
             0.5665875 0.5811
 [0.61988889 0.57577778 0.58855556]
 [0.
             0.
                         0.
                                   ]]
score loo [[0.6925
                        0.6485
                                   0.6521
                                              1
 [0.70466667 0.67476667 0.6633
 [0.712125
             0.689325
                         0.66595
 [0.72078]
             0.69972
                         0.66722
                                   1
 [0.72305
             0.7092
                         0.67575
                                   ]
 [0.72601429 0.71288571 0.67862857]
 [0.7250625 0.712475
                         0.67545
 [0.73046667 0.71924444 0.68096667]
 [0.
             0.
                         0.
                                   ]]
score avg [[0.76935
                        0.8246
                                              ]
                                   0.8184
 [0.75853333 0.8045
                         0.82406667]
 [0.749025
             0.7915
                         0.819825
 [0.74988
             0.78326
                         0.82206
 [0.74835
             0.77993333 0.82425
 [0.7475
             0.77681429 0.82478571]
 [0.74345
             0.7692875 0.8226
 [0.74691111 0.77128889 0.8257
                                   1
 [0.
             0.
                         0.
                                   ]]
score avg [[0.716375 0.6917125 0.6794275]
 [0.72618
            0.7045625 0.6791725]
 [0.729005 0.711005 0.680395]
 [0.7311475 0.71515
                       0.6807675]
 [0.7321125 0.7175
                       0.6814625]
 [0.7325075 0.721205
                       0.6837525]
 [0.7354
                       0.6849825]
            0.72361
 [0.7352425 0.725385
                       0.685275 ]
 [0.
            0.
                       0.
                                ]]
count of n 9
score kf [[0.59785
                       0.48825
                                  0.56155
                                             1
```

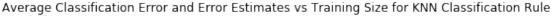
```
[0.60053333 0.5233
                        0.568
 [0.6065
             0.536825
                        0.576625
                                  ]
 [0.60976
             0.5474
                        0.57588
                                   ]
 [0.6145
             0.55973333 0.58565
                                  ]
 [0.61821429 0.56921429 0.58587143]
 [0.6120625
             0.5665875 0.5811
 [0.61988889 0.57577778 0.58855556]
 [0.61918
             0.57506
                        0.58643
                                   11
score loo [[0.6925
                       0.6485
                                   0.6521
                                             ]
 [0.70466667 0.67476667 0.6633
                                  ]
 [0.712125
             0.689325
                        0.66595
                                  ]
 [0.72078
             0.69972
                        0.66722
                                  1
 [0.72305
             0.7092
                        0.67575
                                  ]
 [0.72601429 0.71288571 0.67862857]
 [0.7250625
             0.712475
                        0.67545
 [0.73046667 0.71924444 0.68096667]
 [0.72978
             0.71831
                        0.67796
                                  ]]
                       0.8246
score avg [[0.76935
                                   0.8184
                                             ]
 [0.75853333 0.8045
                        0.82406667]
 [0.749025
             0.7915
                        0.819825
                                 1
 [0.74988
             0.78326
                        0.82206
 [0.74835
             0.77993333 0.82425
 Γ0.7475
             0.77681429 0.82478571]
 [0.74345
             0.7692875 0.8226
                                   1
 [0.74691111 0.77128889 0.8257
                                  ]
 [0.74458
             0.76644
                        0.82358
                                  ]]
score avg [[0.716375 0.6917125 0.6794275]
            0.7045625 0.6791725]
 [0.72618
 [0.729005 0.711005 0.680395]
 [0.7311475 0.71515
                      0.6807675]
 [0.7321125 0.7175
                      0.6814625]
 [0.7325075 0.721205 0.6837525]
 Γ0.7354
            0.72361
                      0.6849825]
 [0.7352425 0.725385 0.685275 ]
 [0.7360875 0.7264575 0.6854525]]
```

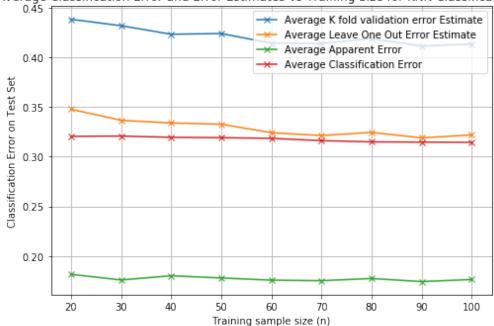




Average Classification Error and Error Estimates vs Training Size for SVM Classification Rule







```
In [107]: from sklearn.model_selection import LeaveOneOut
          from sklearn.model_selection import KFold
          #part1a
          sigma=2
          rho=0.2
          u1=np.array([0,0])
          u2=np.array([1,1])
          cov=np.array([[sigma**2,rho*sigma**2],[rho*sigma**2,sigma**2]])
          print('cov',cov)
          nlist=np.linspace(20,100,num=9)
          test_error=np.zeros(len(nlist))
          err_lda=np.zeros(len(nlist))
          count=0
          score_avg=np.zeros([len(nlist),3])
          score avgkf=np.zeros([len(nlist),3])
          score_avgloo=np.zeros([len(nlist),3])
          score_avgcl=np.zeros([len(nlist),3])
          for train_n in range(0,len(nlist)) :
              scorekf=[0,0,0]
              scoreloo=[0,0,0]
              score=[0,0,0]
```

```
score_cl=[0,0,0]
#import pdb; pdb.set_trace()
for rep_i in range(0,1000):
    #import pdb; pdb.set_trace()
    #create sample two guassian distributions for each mean training data
    x1_train=np.random.multivariate_normal(u1,cov,int(nlist[train_n]/2))
    y1_train=np.zeros(int(nlist[train_n]/2))
    for i in range (0,int(nlist[train_n]/2)):
        y1_train[i]=0
    x2_train=np.random.multivariate_normal(u2,cov,int(nlist[train_n]/2))
    y2_train=np.zeros(int(nlist[train_n]/2))
    for i in range (0,int(nlist[train_n]/2)):
        y2_train[i]=1
    X_train=np.concatenate((x1_train,x2_train),axis=0)
    Y_train=np.concatenate((y1_train,y2_train),axis=0)
    # generate test set
    x1_test=np.random.multivariate_normal(u1,cov,200)
    y1_test=np.zeros(200)
    for i in range (0,200):
        y1_test[i]=0
    x2_test=np.random.multivariate_normal(u2,cov,200)
    y2_test=np.zeros(200)
    for i in range (0,200):
        y2_test[i]=1
    X_test=np.concatenate((x1_test,x2_test),axis=0)
    Y_test=np.concatenate((y1_test,y2_test),axis=0)
    #kfold validation error estimate
   kf = KFold(n_splits=5)
    kf.get_n_splits(X_train)
    KFold(n_splits=5, random_state=None, shuffle=True)
    for train_index, test_index in kf.split(X_train):
        X_trainkf, X_testkf = X_train[train_index], X_train[test_index]
        Y_trainkf, Y_testkf = Y_train[train_index], Y_train[test_index]
        #model1
        model1 = LinearDiscriminantAnalysis()
        model1.fit(X_trainkf, Y_trainkf)
        LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None
        solver='svd', store_covariance=False, tol=0.0001)
        Y_pred1=model1.predict(X_testkf)
        #model2
        model2 = SVC(gamma='auto')
```

```
model2.fit(X_trainkf, Y_trainkf)
    SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)
    Y_pred2=model2.predict(X_testkf)
    #model2
    model3 = KNeighborsClassifier(n_neighbors=3)
    model3.fit(X_trainkf, Y_trainkf)
    KNeighborsClassifier(...)
    Y_pred3=model3.predict(X_testkf)
    #acccuracy for this iteration
    scorekf[0]+=model1.score(X_testkf,Y_testkf)
    scorekf[1]+=model2.score(X_testkf,Y_testkf)
    scorekf[2]+=model3.score(X_testkf,Y_testkf)
#import pdb; pdb.set_trace()
# leave one out error estimate
loo = LeaveOneOut()
loo.get_n_splits(X_train)
LeaveOneOut()
for train_index, test_index in loo.split(X_train):
    X_trainloo, X_testloo = X_train[train_index], X_train[test_index]
    Y_trainloo, Y_testloo = Y_train[train_index], Y_train[test_index]
    #model1
    model1 = LinearDiscriminantAnalysis()
    model1.fit(X_trainloo, Y_trainloo)
    LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None
    solver='svd', store_covariance=False, tol=0.0001)
    Y_pred1=model1.predict(X_testloo)
    #model2
    model2 = SVC(gamma='auto')
    model2.fit(X_trainloo, Y_trainloo)
    SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)
    Y_pred2=model2.predict(X_testloo)
    #model2
    model3 = KNeighborsClassifier(n_neighbors=3)
```

```
model3.fit(X_trainloo, Y_trainloo)
    KNeighborsClassifier(...)
    Y_pred3=model3.predict(X_testloo)
    #acccuracy for this iteration
    scoreloo[0]+=model1.score(X_testloo,Y_testloo)
    scoreloo[1]+=model2.score(X testloo,Y testloo)
    scoreloo[2]+=model3.score(X_testloo,Y_testloo)
# average apparent error
#model1
model1 = LinearDiscriminantAnalysis()
model1.fit(X_train, Y_train)
LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None,
solver='svd', store_covariance=False, tol=0.0001)
Y_pred1=model1.predict(X_test)
#model2
model2 = SVC(gamma='auto')
model2.fit(X_train, Y_train)
SVC(C=1.0, cache size=200, class weight=None, coef0=0.0,
decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
max_iter=-1, probability=False, random_state=None, shrinking=True,
tol=0.001, verbose=False)
Y_pred2=model2.predict(X_test)
#model2
model3 = KNeighborsClassifier(n_neighbors=3)
model3.fit(X_train, Y_train)
KNeighborsClassifier(...)
Y_pred3=model3.predict(X_test)
#acccuracy for this iteration
score[0]+=model1.score(X_train,Y_train)
score[1]+=model2.score(X_train,Y_train)
score[2]+=model3.score(X_train,Y_train)
# average classification error
#model1
model1 = LinearDiscriminantAnalysis()
model1.fit(X_train, Y_train)
LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None,
solver='svd', store_covariance=False, tol=0.0001)
Y_pred1=model1.predict(X_test)
```

#mode1.2

```
model2.fit(X_train, Y_train)
                  SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
                  decision_function_shape='ovr', degree=3, gamma='auto', kernel='rbf',
                  max_iter=-1, probability=False, random_state=None, shrinking=True,
                  tol=0.001, verbose=False)
                  Y pred2=model2.predict(X test)
                  #model2
                  model3 = KNeighborsClassifier(n_neighbors=3)
                  model3.fit(X_train, Y_train)
                  KNeighborsClassifier(...)
                  Y_pred3=model3.predict(X_test)
                  #acccuracy for this iteration
                  score_cl[0]+=model1.score(X_test,Y_test)
                  score_cl[1]+=model2.score(X_test,Y_test)
                  score_cl[2]+=model3.score(X_test,Y_test)
              #average across k folds
              scorekf=np.divide(scorekf,5)
              #average leave one out error estimate
              scoreloo=np.divide(scoreloo,int(nlist[train_n]))
              #average the accuracy for kf, loo, and average classification error
              for modelcount in range (0,3):
                  score_avgkf[count,modelcount]=scorekf[modelcount]/1000
                  score_avgloo[count,modelcount]=scoreloo[modelcount]/1000
                  score_avg[count,modelcount]=score[modelcount]/1000
                  score_avgcl[count,modelcount]=score_cl[modelcount]/1000
              count+=1
              print ('count of n',count)
              print ('score kf',score avgkf)
              print('score loo',score_avgloo)
              print('score avg',score avg)
              print('score avg',score_avgcl)
cov [[4. 0.8]
 [0.8 4.]]
count of n 1
score kf [[0.37915 0.2659 0.4081]
 [0.
                  0.
          0.
                         ]
 ГО.
          0.
                  0.
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 [0.
                  0.
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                  0.
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 [0.
          0.
                  0.
                         ]
```

model2 = SVC(gamma='auto')

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[0.
           0.
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 [0.
           0.
                     0.
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 [0.
           0.
                     0.
                             ]]
score loo [[0.51465 0.45365 0.51855]
 [0.
           0.
                     0.
                             ]
 [0.
           0.
                     0.
                             ]
 [0.
                             ]
           0.
                     0.
                             1
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 [0.
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                             ]
 [0.
           0.
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                             ]
 [0.
           0.
                     0.
                             ]]
score avg [[0.66725 0.87095 0.75975]
 [0.
           0.
                     0.
                             ]
                             ]
 [0.
           0.
                     0.
 [0.
           0.
                     0.
                             1
 [0.
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 [0.
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           0.
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                             ]
 [0.
                             ]]
           0.
                     0.
score avg [[0.5850225 0.5435975 0.5558825]
 [0.
              0.
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                                    ]
 [0.
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              0.
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 [0.
              0.
                          0.
                                    ]]
count of n 2
score kf [[0.37915
                          0.2659
                                       0.4081
                                                   ]
 [0.37093333 0.2935
                            0.41946667]
 [0.
                            0.
               0.
                                        ]
                                        ]
 [0.
               0.
                            0.
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               0.
                            0.
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                                        ]
 [0.
               0.
                            0.
                                        ]]
score loo [[0.51465
                           0.45365
                                        0.51855
                                                    ]
 [0.54993333 0.50176667 0.53506667]
 [0.
               0.
                            0.
                                        ]
 [0.
               0.
                            0.
 [0.
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 [0.
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```

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[0.
                           0.
                                      ]]
              0.
score avg [[0.66725
                          0.87095
                                      0.75975
                                                 ]
 [0.65463333 0.84006667 0.76326667]
 [0.
              0.
                           0.
 [0.
                                      ]
              0.
                           0.
 [0.
                                      ]
              0.
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 [0.
              0.
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 ГО.
              0.
                           0.
 [0.
              0.
                           0.
                                      1
 [0.
              0.
                           0.
                                      ]]
score avg [[0.5850225 0.5435975 0.5558825]
 [0.5980475 0.550245 0.556865 ]
 [0.
             0.
                         0.
 [0.
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                         0.
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             0.
                         0.
                                   ]
 ГО.
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count of n 3
score kf [[0.37915
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                                     0.4081
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 [0.37093333 0.2935
                           0.41946667]
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score loo [[0.51465
                          0.45365
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 [0.54993333 0.50176667 0.53506667]
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score avg [[0.66725
                          0.87095
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score avg [[0.5850225 0.5435975 0.5558825]
```

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[0.5980475 0.550245
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                        0.559835 ]
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count of n 4
score kf [[0.37915
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 [0.37093333 0.2935
                           0.41946667]
 [0.373475
              0.302225
                           0.42015
                                      ]
 [0.37512
                           0.42372
              0.31006
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score loo [[0.51465
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                          0.45365
                                      0.51855
 [0.54993333 0.50176667 0.53506667]
 [0.573375
              0.52335
                           0.539675
 [0.5855
              0.53636
                           0.54992
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score avg [[0.66725
                          0.87095
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 [0.65463333 0.84006667 0.76326667]
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score avg [[0.5850225 0.5435975 0.5558825]
 [0.5980475 0.550245 0.556865 ]
 [0.6064025 0.55752
                        0.559835 ]
 [0.610645 0.5624775 0.5620175]
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count of n 5
score kf [[0.37915
                        0.2659
                                     0.4081
                                                ]
 [0.37093333 0.2935
                           0.41946667]
```

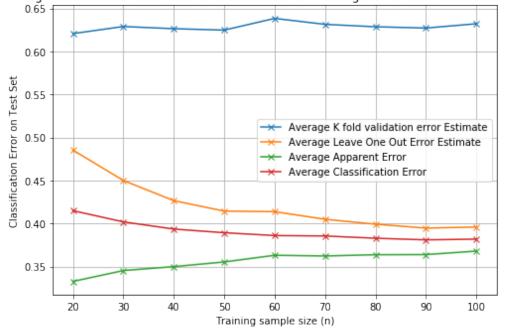
```
[0.373475
              0.302225
                          0.42015
 [0.37512
              0.31006
                          0.42372
                                     ]
 [0.3615
              0.31091667 0.42218333]
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score loo [[0.51465
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                                     0.51855
 [0.54993333 0.50176667 0.53506667]
 [0.573375
              0.52335
                          0.539675
                          0.54992
 [0.5855
              0.53636
 [0.58616667 0.5413
                          0.54758333]
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score avg [[0.66725
                         0.87095
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                                                ]
 [0.65463333 0.84006667 0.76326667]
 [0.65005
              0.8131
                          0.76875
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              0.79598
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                                     ]
 [0.63685
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score avg [[0.5850225 0.5435975 0.5558825]
 [0.5980475 0.550245 0.556865]
 [0.6064025 0.55752
                        0.559835 ]
 [0.610645 0.5624775 0.5620175]
 [0.6139225 0.566785
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count of n 6
score kf [[0.37915
                        0.2659
                                               ]
                                    0.4081
 [0.37093333 0.2935
                          0.41946667]
 [0.373475
              0.302225
                          0.42015
 [0.37512
              0.31006
                          0.42372
 [0.3615
              0.31091667 0.42218333]
 [0.36842857 0.31951429 0.42804286]
 [0.
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score loo [[0.51465
                         0.45365
                                     0.51855
                                                ]
 [0.54993333 0.50176667 0.53506667]
 [0.573375
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[0.58616667 0.5413
                         0.547583331
 [0.59504286 0.55318571 0.55492857]
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score avg [[0.66725
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score avg [[0.5850225 0.5435975 0.5558825]
 [0.5980475 0.550245 0.556865 ]
 [0.6064025 0.55752
                       0.559835 ]
 [0.610645 0.5624775 0.5620175]
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                       0.56079
 [0.6144275 0.569565
                       0.5618625]
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count of n 7
score kf [[0.37915
                       0.2659
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                                              1
 [0.37093333 0.2935
                         0.41946667]
             0.302225
                         0.42015
 [0.373475
 [0.37512
             0.31006
                         0.42372
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             0.31091667 0.42218333]
 [0.36842857 0.31951429 0.42804286]
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             0.3233625
                         0.4258625 ]
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score loo [[0.51465
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                                    0.51855
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 [0.54993333 0.50176667 0.53506667]
 [0.573375
             0.52335
                         0.539675
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              0.53636
                         0.54992
 [0.58616667 0.5413
                         0.547583331
 [0.59504286 0.55318571 0.55492857]
 [0.600725
             0.5561
                         0.5523125 ]
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score avg [[0.66725
                        0.87095
                                    0.75975
                                               ]
 [0.65463333 0.84006667 0.76326667]
 [0.65005
             0.8131
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 [0.64464
             0.79598
                         0.7696
 [0.63685
             0.77876667 0.76825
                                    ]
 [0.63767143 0.7699
                         0.7709
                                    1
```

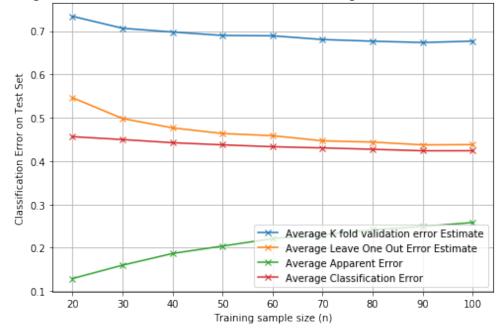
```
Γ0.6362
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score avg [[0.5850225 0.5435975 0.5558825]
 [0.5980475 0.550245 0.556865 ]
 [0.6064025 0.55752
                       0.559835 ]
 [0.610645 0.5624775 0.5620175]
 [0.6139225 0.566785
                      0.56079 1
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                      0.5618625]
 [0.6170375 0.57271
                       0.56194257
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count of n 8
score kf [[0.37915
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 [0.37093333 0.2935
                         0.41946667]
 [0.373475
             0.302225
                         0.42015
 [0.37512
             0.31006
                         0.42372
 [0.3615
             0.31091667 0.42218333]
 [0.36842857 0.31951429 0.42804286]
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             0.3233625 0.4258625 1
 [0.37271111 0.32636667 0.42763333]
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score loo [[0.51465
                        0.45365
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 [0.54993333 0.50176667 0.53506667]
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                         0.539675 ]
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             0.53636
                         0.54992
 [0.58616667 0.5413
                         0.54758333]
 [0.59504286 0.55318571 0.55492857]
 [0.600725
             0.5561
                         0.5523125 ]
 [0.60526667 0.5625
                         0.55468889]
 [0.
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                                   11
                         0.
score avg [[0.66725
                                   0.75975
                        0.87095
                                             ]
 [0.65463333 0.84006667 0.76326667]
 [0.65005
             0.8131
                         0.76875
                                   ]
 [0.64464
             0.79598
                         0.7696
                                   ]
 [0.63685
             0.77876667 0.76825
 [0.63767143 0.7699
                         0.7709
 Γ0.6362
             0.75865
                         0.771625
 [0.63604444 0.75071111 0.77153333]
 [0.
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score avg [[0.5850225 0.5435975 0.5558825]
 [0.5980475 0.550245 0.556865 ]
 [0.6064025 0.55752
                       0.559835 ]
 [0.610645 0.5624775 0.5620175]
 [0.6139225 0.566785 0.56079 ]
 [0.6144275 0.569565 0.5618625]
 [0.6170375 0.57271
                       0.5619425]
 Γ0.61893
            0.5761625 0.5644725]
```

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[0.
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count of n 9
score kf [[0.37915
                      0.2659
                                 0.4081
                                           1
 [0.37093333 0.2935
                        0.41946667]
             0.302225
                        0.42015
 [0.373475
                                  ]
 [0.37512
             0.31006
                        0.42372
 [0.3615
             0.31091667 0.42218333]
 [0.36842857 0.31951429 0.42804286]
 [0.371225
             0.3233625 0.4258625 ]
 [0.37271111 0.32636667 0.42763333]
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                        0.4276
                                  ]]
score loo [[0.51465
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 [0.54993333 0.50176667 0.53506667]
 [0.573375
             0.52335
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 [0.5855
                        0.54992
             0.53636
 [0.58616667 0.5413
                        0.54758333]
 [0.59504286 0.55318571 0.55492857]
 [0.600725
             0.5561
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 [0.60526667 0.5625
                        0.55468889]
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            0.56197
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score avg [[0.66725
                       0.87095
                                  0.75975
                                            ]
 [0.65463333 0.84006667 0.76326667]
 [0.65005
             0.8131
                        0.76875
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             0.79598
                        0.7696
                                  ]
 [0.63685
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                                  ٦
 [0.63767143 0.7699
                        0.7709
                                  ]
 [0.6362
             0.75865
                        0.771625
 [0.63604444 0.75071111 0.77153333]
 [0.63198
             0.74166
                        0.77189
                                  ]]
score avg [[0.5850225 0.5435975 0.5558825]
 [0.5980475 0.550245 0.556865 ]
 [0.6064025 0.55752
                      0.559835 ]
 [0.610645 0.5624775 0.5620175]
 [0.6139225 0.566785 0.56079 ]
 [0.6144275 0.569565 0.5618625]
                      0.5619425]
 [0.6170375 0.57271
 [0.61893
            0.5761625 0.5644725]
 [0.61806
            0.5760975 0.5614225]]
```

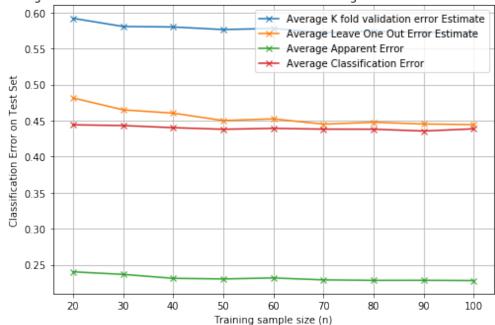




Average Classification Error and Error Estimates vs Training Size for SVM Classification Rule







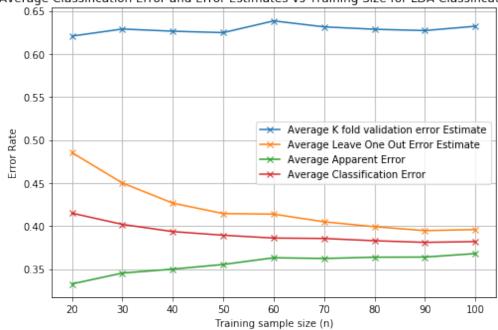
```
In [108]: #plot error curves for LDA
          fig, ax = plt.subplots(figsize=[8,5])
          plt.plot(nlist,1-score_avgkf[:,0],marker='x',label='Average K fold validation error
          plt.plot(nlist,1-score_avgloo[:,0],marker='x',label='Average Leave One Out Error Est
          plt.plot(nlist,1-score_avg[:,0],marker='x',label='Average Apparent Error')
          plt.plot(nlist,1-score_avgcl[:,0],marker='x',label='Average Classification Error')
          plt.title('Average Classification Error and Error Estimates vs Training Size for LDA
          plt.ylabel('Error Rate')
          plt.xlabel('Training sample size (n)')
          fig.tight_layout()
          ax.legend()
          plt.grid(True)
          plt.show
          fig.savefig('hw2_17b.png')
          #plot error curves for SVM
          fig, ax = plt.subplots(figsize=[8,5])
          plt.plot(nlist,1-score_avgkf[:,1],marker='x',label='Average K fold validation error
          plt.plot(nlist,1-score_avgloo[:,1],marker='x',label='Average Leave One Out Error Est
          plt.plot(nlist,1-score_avg[:,1],marker='x',label='Average Apparent Error')
          plt.plot(nlist,1-score_avgcl[:,1],marker='x',label='Average Classification Error')
          plt.title('Average Classification Error and Error Estimates vs Training Size for SVM
          plt.ylabel('Error Rate')
```

plt.xlabel('Training sample size (n)')

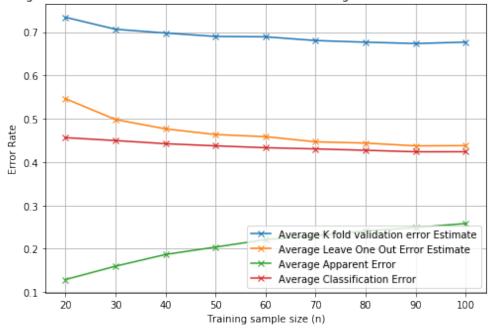
fig.tight_layout()

```
ax.legend()
plt.grid(True)
plt.show
fig.savefig('hw2_18b.png')
#plot error curves for KNN
fig, ax = plt.subplots(figsize=[8,5])
plt.plot(nlist,1-score_avgkf[:,2],marker='x',label='Average K fold validation error )
plt.plot(nlist,1-score_avgloo[:,2],marker='x',label='Average Leave One Out Error Est
plt.plot(nlist,1-score_avg[:,2],marker='x',label='Average Apparent Error')
plt.plot(nlist,1-score_avgcl[:,2],marker='x',label='Average Classification Error')
plt.title('Average Classification Error and Error Estimates vs Training Size for KNN
plt.ylabel('Error Rate')
plt.xlabel('Training sample size (n)')
fig.tight_layout()
ax.legend()
plt.grid(True)
plt.show
fig.savefig('hw2_19b.png')
```

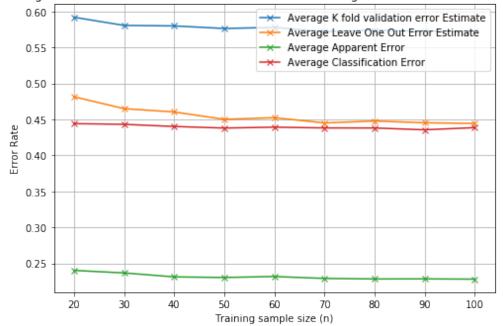




Average Classification Error and Error Estimates vs Training Size for SVM Classification Rule





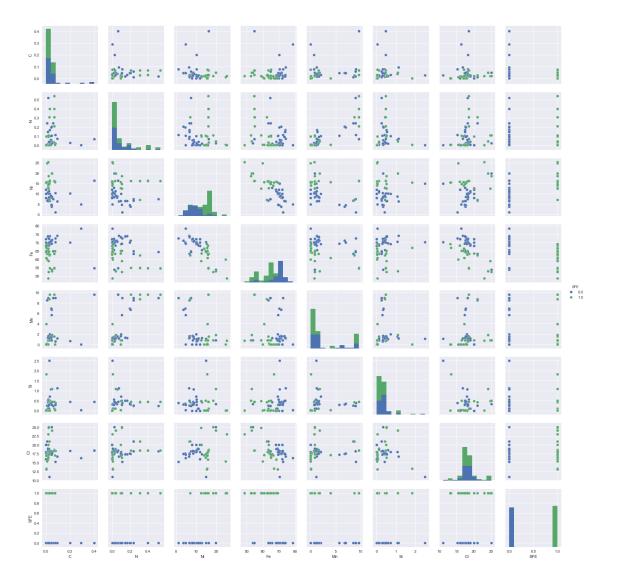


HW2_2trial2

November 1, 2018

```
In [2]: import numpy as np
        import pandas as pd
        import matplotlib.pyplot as plt
        import seaborn as sns
        f=open('SFE_Test_Data.txt','r')
        SFE_testf=f.read()
        f.close
        f=open('SFE_Train_Data.txt','r')
        SFE_trainf=f.read()
        f.close
Out[2]: <function TextIOWrapper.close()>
In [3]: def list_concat(word):
            out=''
            for i in word:
                out+=i
            return(out)
In [4]: temp=[]
        SFE_train=[]
        for t in SFE_trainf:
            if(t!='\n' and t!='\t'):
                temp.append(t)
            else:
                SFE_train.append(temp)
                temp=[]
        temp=[]
        SFE_test=[]
        for t in SFE_testf:
            if (t!='\n') and t!='\t'):
                temp.append(t)
            else:
                SFE_test.append(temp)
                temp=[]
In [5]: SFE_train1=[]
        for i in SFE_train:
```

```
SFE_train1.append(list_concat(i))
        SFE_test1=[]
        for i in SFE_test:
            SFE_test1.append(list_concat(i))
In [6]: cols=SFE_train1[0:8]
        train=SFE_train1[8:len(SFE_train1)]
        cols=SFE_test1[0:8]
        test=SFE_test1[8:len(SFE_test1)]
In [7]: train3=[]
        for i in train:
            if (i=='High'):
                train3.append(float(1))
            elif (i=='Low'):
                train3.append(float(0))
            else:
                train3.append(float(i))
        test3=[]
        for i in test:
            if (i=='High'):
                test3.append(float(1))
            elif (i=='Low'):
                test3.append(float(0))
            else:
                test3.append(float(i))
In [8]: train1=np.array(train3)
        test1=np.array(test3)
In [9]: train4=np.reshape(train1,(25,8))
        test4=np.reshape(test1,(int(len(test1)/8),8))
In [10]: len(test1)/8
Out[10]: 98.0
In [11]: traindf=pd.DataFrame(data=train4,columns=cols)
         testdf=pd.DataFrame(data=test4,columns=cols)
In [12]: testdf
         #scatterplot
         sns.set()
         sns.pairplot(testdf, size = 2.5,hue='SFE')
         plt.show();
```



```
In [13]: import numpy as np
        import matplotlib.pyplot as plt
        from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
        from sklearn.neighbors import KNeighborsClassifier
        from itertools import combinations

#Exhaustive search
        #Obtain combinations of size r
        train_cols=traindf.columns[0:7]
        test_cols=testdf.columns[0:7]

all_combs=[]
        all_combs_feat=[]
        for ncomb in range(1,6):
```

```
col_comb = list(combinations(train_cols, ncomb))
             count=0
             score_combs=np.zeros([len(col_comb),4])
             sel_feat=[]
             print('N features', ncomb)
             #import pdb; pdb.set trace()
             for col_i in col_comb :
                 X_train=traindf.loc[:,col_i]
                 Y_train=traindf.loc[:,'SFE']
                 X_test=testdf.loc[:,col_i]
                 Y_test=testdf.loc[:,'SFE']
                 #model1
                 model1 = LinearDiscriminantAnalysis()
                 model1.fit(X_train, Y_train)
                 LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None,
                 solver='svd', store covariance=False, tol=0.0001)
                 #model2
                 model2 = KNeighborsClassifier(n_neighbors=3)
                 model2.fit(X_train, Y_train)
                 KNeighborsClassifier(...)
                 #acccuracy for this iteration
                 score_combs[count,0]=model1.score(X_train,Y_train)
                 score_combs[count,1]=model2.score(X_train,Y_train)
                 score_combs[count,2]=model1.score(X_test,Y_test)
                 score_combs[count,3]=model2.score(X_test,Y_test)
                 #print('Count score',score_combs)
                 count+=1
                 sel_feat.append(col_i)
             all combs feat.append(sel feat)
             all_combs.append(score_combs)
N features 1
N features 2
N features 3
N features 4
N features 5
In [14]: x=all_combs[0][:,0]
In [15]: all_combs_feat[0]
Out[15]: [('C',), ('N',), ('Ni',), ('Fe',), ('Mn',), ('Si',), ('Cr',)]
```

#combinations of features

```
In [16]: from operator import itemgetter
         maxscore=[]
         maxscore_feat=[]
         maxscore.append(max(enumerate(x), key=itemgetter(1))[1])
         maxscore_feat.append(all_combs_feat[0][max(enumerate(x), key=itemgetter(1))[0]])
In [17]: type(maxscore_feat)
Out[17]: list
In [18]: score_max=[]
         feat_set=[]
         #number of features to be considered
         for nfeat in range (0,5):
             maxscore=[]
             best_feat=[]
             #different models and err types
             for i in range (0,4):
                 x=all_combs[nfeat][:,i]
                 maxscore.append(max(enumerate(x), key=itemgetter(1))[1])
                 best_feat.append(all_combs_feat[nfeat][max(enumerate(x), key=itemgetter(1))[0]
             score_max.append(maxscore)
             feat_set.append(best_feat)
In [36]: feat_set[0]
Out[36]: [('Fe',), ('Mn',), ('Ni',), ('Ni',)]
In [19]: test_errlda=[]
         test_errknn=[]
         for nfeat in range(0,5):
             #two models
             err1=[]
             err2=[]
             for i in range (0,2):
                 col_i=feat_set[nfeat][i]
                 X_train=traindf.loc[:,col_i]
                 Y_train=traindf.loc[:,'SFE']
                 X_test=testdf.loc[:,col_i]
                 Y_test=testdf.loc[:,'SFE']
                 #model1
                 model1 = LinearDiscriminantAnalysis()
                 model1.fit(X_train, Y_train)
                 LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None,
                 solver='svd', store_covariance=False, tol=0.0001)
```

```
#model2
                 model2 = KNeighborsClassifier(n_neighbors=3)
                 model2.fit(X_train, Y_train)
                 KNeighborsClassifier(...)
                 #acccuracy for this iteration
                 #import pdb; pdb.set trace()
                 if (i==0):
                     err1.append(1-model1.score(X_test,Y_test))
                 else:
                     err2.append(1-model2.score(X_test,Y_test))
             test_errlda.append(err1)
             test_errknn.append(err2)
In [20]: test_errlda[0]
Out[20]: [0.1428571428571429]
In [21]: varlda_app=[]
         varknn_app=[]
         errlda_app=[]
         errlda_test=[]
         errknn_app=[]
         errknn_test=[]
         for i in range(0,5):
             varlda_app.append(feat_set[i][0])
             varknn_app.append(feat_set[i][2])
             errlda_app.append(1-score_max[i][0])
             errlda_test.append(test_errlda[i])
             errknn app.append(1-score max[i][2])
             errknn_test.append(test_errknn[i])
In [51]: errlda_app[0]
Out[51]: 0.12
In [22]: dat=[]
         for i in range (0,6):
             dat.append([])
         dat[0].append('LDA Based Features')
         dat[1].append('LDA best apparent Error')
         dat[2].append('LDA test Error')
         dat[3].append('KNN Based Features')
         dat[4].append('KNN apparent Error')
         dat[5].append('KNN_test Error')
         for i in range(0,5):
```

```
dat[0].append(varlda_app[i])
             dat[1].append(errlda_app[i])
             dat[2].append(errlda_test[i])
             dat[3].append(varknn_app[i])
             dat[4].append(errknn_app[i])
             dat[5].append(errknn_test[i])
In [23]: feat_set[0][0]
Out[23]: ('Fe',)
In [24]: labs=['Categories','1 Feature','2 Features','3 Features','4 Features','5 Features']
         df1=pd.DataFrame(data=dat,columns=labs)
         df1
Out [24]:
                                                  1 Feature
                                                                         2 Features
                          Categories
                                                                            (C, Fe)
                 LDA Based Features
                                                      (Fe,)
         1
            LDA best apparent Error
                                                       0.12
                                                                               0.04
         2
                      LDA test Error
                                      [0.1428571428571429]
                                                              [0.12244897959183676]
         3
                 KNN Based Features
                                                      (Ni,)
                                                                            (N, Ni)
         4
                 KNN apparent Error
                                                   0.122449
                                                                          0.0714286
         5
                     KNN_test Error
                                      [0.2551020408163265]
                                                              [0.23469387755102045]
                         3 Features
                                                                           5 Features
                                                  4 Features
         0
                        (C, Ni, Fe)
                                              (C, N, Fe, Mn)
                                                                  (N, Ni, Fe, Si, Cr)
         1
                               0.04
                                                        0.04
                                      [0.11224489795918369]
         2
            [0.061224489795918324]
                                                                [0.16326530612244894]
         3
                        (C, Ni, Fe)
                                              (C, N, Ni, Si)
                                                                  (C, Fe, Mn, Si, Cr)
         4
                          0.0612245
                                                   0.0510204
                                                                            0.0408163
                                      [0.061224489795918324]
             [0.23469387755102045]
                                                               [0.061224489795918324]
In [25]: #Sequential forward search
         train_cols=traindf.columns[0:7]
         test_cols=testdf.columns[0:7]
         #initialize variables for storing features and scores
         all_combs=[]
         all_combs_feat=[]
         chosen_feat=[]
         score_max=[]
         for i in range (0,4):
             chosen_feat.append([])
             score_max.append([])
         feat_set=[]
         #keep adding one feature at a time
         for nfeat in range(1,6):
             #combinations of features
```

```
#keep track of remaining columns separately for each path
rem_cols=[]
for j in range (0,4):
    rem_cols.append([])
for i in range (0,4):
    for t in train_cols:
        if (t not in chosen_feat[i]):
            rem_cols[i].append(t)
score_combs=np.zeros([len(rem_cols[0]),4])
sel_feat=[]
for i in range (0,4):
    sel_feat.append([])
#for each of the four paths
for path in range (0,4):
    count=0
    for col_i in rem_cols[path]:
        X_train=traindf.loc[:,chosen_feat[path]+list([col_i])]
        Y_train=traindf.loc[:,'SFE']
        X_test=testdf.loc[:,chosen_feat[path]+list([col_i])]
        Y test=testdf.loc[:,'SFE']
        #import pdb; pdb.set_trace()
        #model1
        model1 = LinearDiscriminantAnalysis()
        model1.fit(X_train, Y_train)
        LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None
        solver='svd', store_covariance=False, tol=0.0001)
        #model2
        model2 = KNeighborsClassifier(n_neighbors=3)
        model2.fit(X_train, Y_train)
        KNeighborsClassifier(...)
        #acccuracy for this iteration
        if (path==0):
            score_combs[count,0]=model1.score(X_train,Y_train)
        elif(path==1):
            score_combs[count,1]=model2.score(X_train,Y_train)
        elif(path==2):
            score_combs[count,2]=model1.score(X_test,Y_test)
        else:
            score_combs[count,3]=model2.score(X_test,Y_test)
        count+=1
        sel_feat[path].append(col_i)
    #print('Chosen Features ',path,chosen_feat,'\n',score_combs)
all_combs.append(score_combs)
for i in range (0,4):
```

```
x=all_combs[nfeat-1][:,i]
                 maxscore=(max(enumerate(x), key=itemgetter(1))[1])
                 best_feat=(sel_feat[i][max(enumerate(x), key=itemgetter(1))[0]])
                 score_max[i].append(maxscore)
                 chosen_feat[i].append(best_feat)
             #all_combs_feat[i].append(chosen_feat)
             #import pdb; pdb.set trace()
In [33]: score_max[2]
Out [33]: [0.8775510204081632,
          0.9285714285714286,
          0.9285714285714286,
          0.9489795918367347,
          0.9081632653061225]
In [27]: chosen_feat
Out[27]: [['Fe', 'C', 'Ni', 'Mn', 'N'],
          ['Mn', 'C', 'N', 'Si', 'Ni'],
          ['Ni', 'N', 'C', 'Si', 'Mn'],
          ['Ni', 'Fe', 'C', 'N', 'Mn']]
In [220]: a=['p']
          b=['tt']
          c=list(b)
          a+c
Out[220]: ['p', 'tt']
In [62]: chosen_feat[0][0:1]
Out[62]: ['Fe']
In [26]: test_errlda=[]
         test_errknn=[]
         for nfeat in range(0,5):
             #two models
             err1=[]
             err2=[]
             for i in range(0,2):
                 col_i=chosen_feat[i][0:nfeat+1]
                 X_train=traindf.loc[:,col_i]
                 Y_train=traindf.loc[:,'SFE']
                 X_test=testdf.loc[:,col_i]
                 Y_test=testdf.loc[:,'SFE']
```

```
#model1
                 model1 = LinearDiscriminantAnalysis()
                 model1.fit(X_train, Y_train)
                 LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None,
                 solver='svd', store_covariance=False, tol=0.0001)
                 #model2
                 model2 = KNeighborsClassifier(n_neighbors=3)
                 model2.fit(X_train, Y_train)
                 KNeighborsClassifier(...)
                 #acccuracy for this iteration
                 #import pdb; pdb.set_trace()
                 if (i==0):
                     err1.append(1-model1.score(X_test,Y_test))
                     err2.append(1-model2.score(X_test,Y_test))
             test_errlda.append(err1)
             test_errknn.append(err2)
In [34]: varlda_app=[]
         varknn app=[]
         errlda_app=[]
         errlda test=[]
         errknn_app=[]
         errknn_test=[]
         for i in range (0,5):
             varlda_app.append(chosen_feat[0][0:i+1])
             varknn_app.append(chosen_feat[1][0:i+1])
             errlda_app.append(1-score_max[0][i])
             errlda_test.append(test_errlda[i])
             errknn_app.append(1-score_max[1][i])
             errknn_test.append(test_errknn[i])
In [35]: dat=[]
         for i in range (0,6):
             dat.append([])
         dat[0].append('LDA Based Features')
         dat[1].append('LDA best apparent Error')
         dat[2].append('LDA test Error')
         dat[3].append('KNN Based Features')
         dat[4].append('KNN best apparent Error')
         dat[5].append('KNN_test Error')
         for i in range (0,5):
             dat[0].append(varlda_app[i])
```

```
dat[1].append(errlda_app[i])
             dat[2].append(errlda_test[i])
             dat[3].append(varknn_app[i])
             dat[4].append(errknn_app[i])
             dat[5].append(errknn_test[i])
In [36]: labs=['Categories','1 Feature','2 Features','3 Features','4 Features','5 Features']
         df1=pd.DataFrame(data=dat,columns=labs)
         df1
Out [36]:
                          Categories
                                                  1 Feature
                                                                         2 Features
                 LDA Based Features
                                                        [Fe]
                                                                             [Fe, C]
            LDA best apparent Error
                                                       0.12
                                                                                0.04
                      LDA test Error
                                       [0.1428571428571429]
         2
                                                              [0.12244897959183676]
                 KNN Based Features
         3
                                                        [Mn]
                                                                             [Mn, C]
            KNN best apparent Error
                                                       0.04
                                                                               0.04
         5
                      KNN_test Error
                                       [0.2551020408163265]
                                                              [0.23469387755102045]
                         3 Features
                                                  4 Features
                                                                          5 Features
         0
                        [Fe, C, Ni]
                                             [Fe, C, Ni, Mn]
                                                                  [Fe, C, Ni, Mn, N]
                               0.04
                                                        0.04
                                                                                 0.04
         1
         2
            [0.061224489795918324]
                                      [0.061224489795918324]
                                                               [0.09183673469387754]
         3
                         [Mn, C, N]
                                              [Mn, C, N, Si]
                                                                  [Mn, C, N, Si, Ni]
                               0.04
                                                        0.04
                                                                                 0.08
         4
         5
              [0.23469387755102045]
                                       [0.22448979591836737]
                                                               [0.09183673469387754]
In [307]: score_max[0]
Out[307]: [0.88, 0.96, 0.96, 0.96, 0.96]
```