

# 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  $X_1$  and  $X_2$  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  $\sigma = 1$ .
- 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 classification rules, estimated with the test sets, as a function of  $n$ .

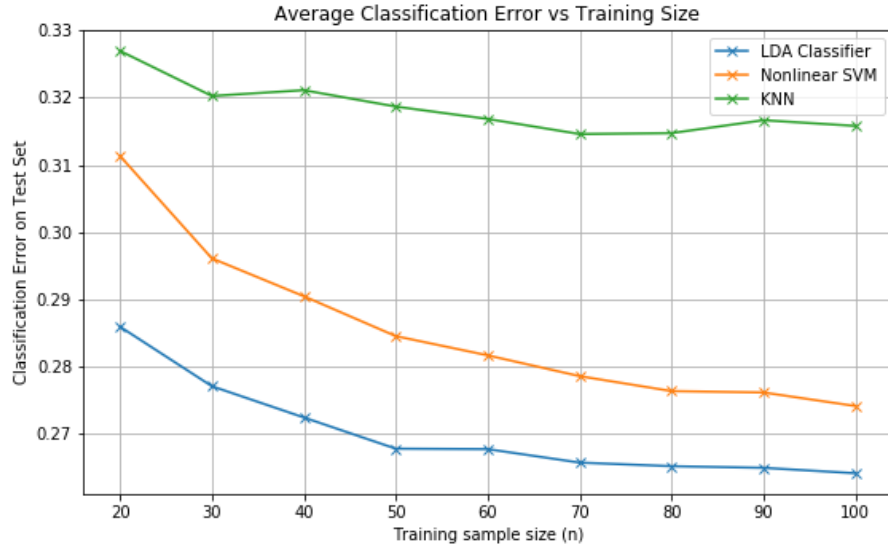


Figure 1: Average Classification Error on Test Set for different classifiers  $\sigma=1$

- Next we plot the average classification errors of the LDA, 3NN, and linear SVM classification rules, estimated with the test sets, as a function of  $n$  with  $\sigma=2$ .

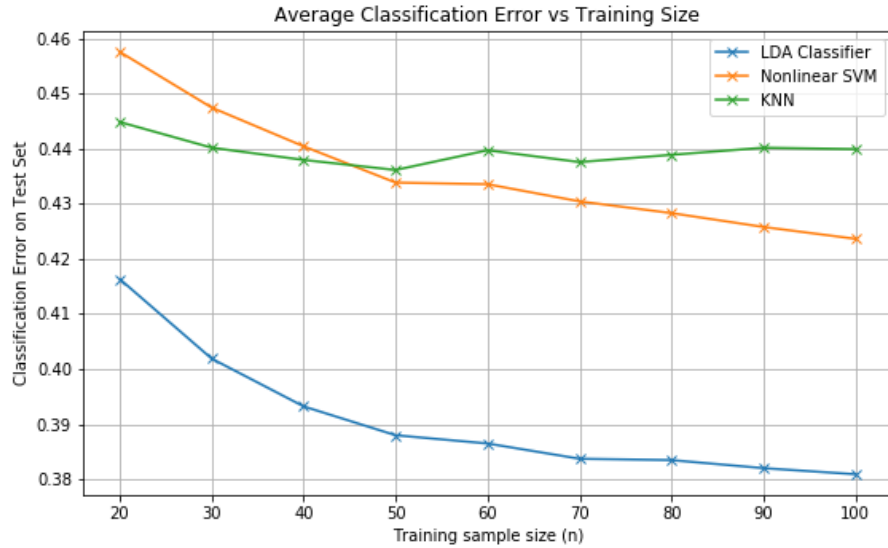


Figure 2: Average Classification Error on Test Set for different classifiers  $\sigma=2$

## 1.2 (b)

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

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

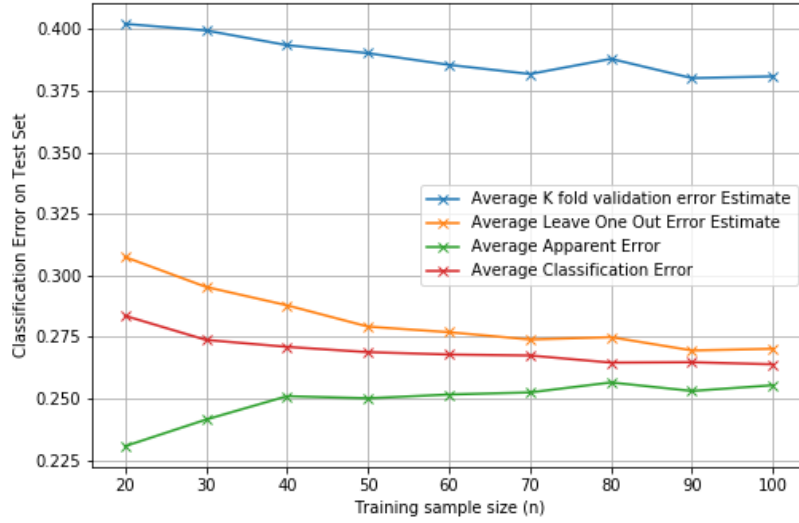


Figure 3: Average Error Estimates and Average Classification Error on Test Set for LDA  $\sigma=1$

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

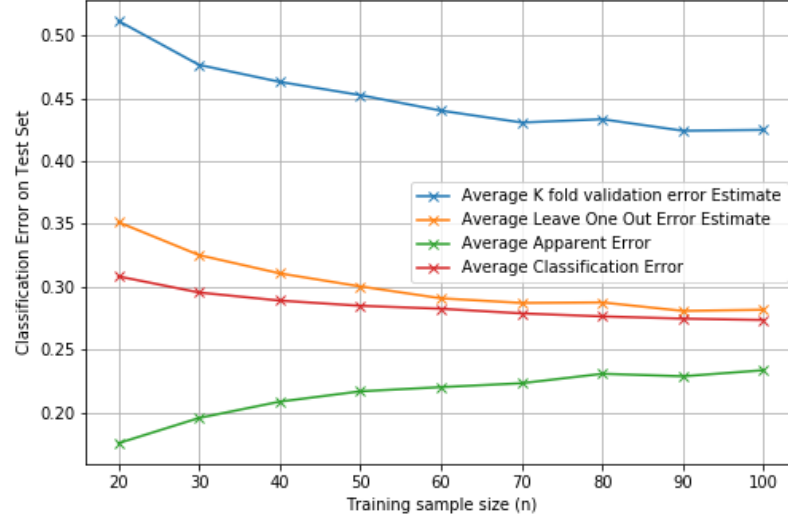


Figure 4: Average Error Estimates and Average Classification Error on Test Set for KNN  $\sigma=1$

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

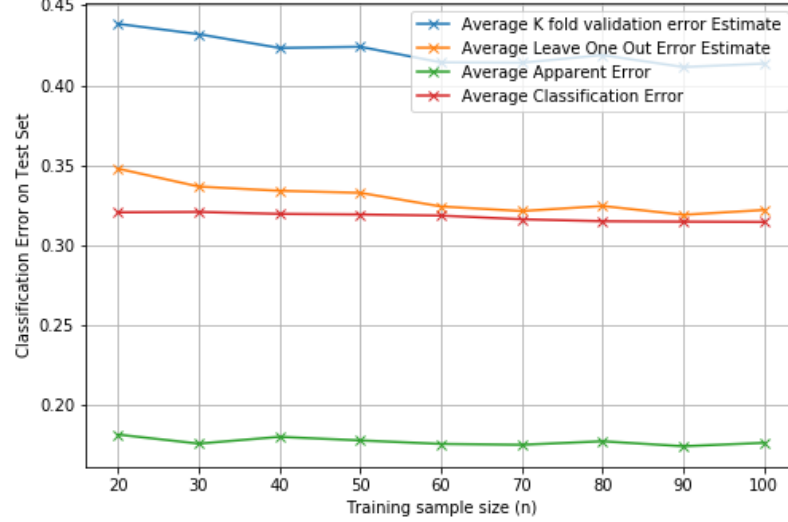


Figure 5: Average Error Estimates and Average Classification Error on Test Set for SVM  $\sigma=1$

\* the Y axis label is supposed to be just "Classification Error"

- Now we have  $\sigma=2$ . We can expect to see higher error rates due to a lower ease of separability.

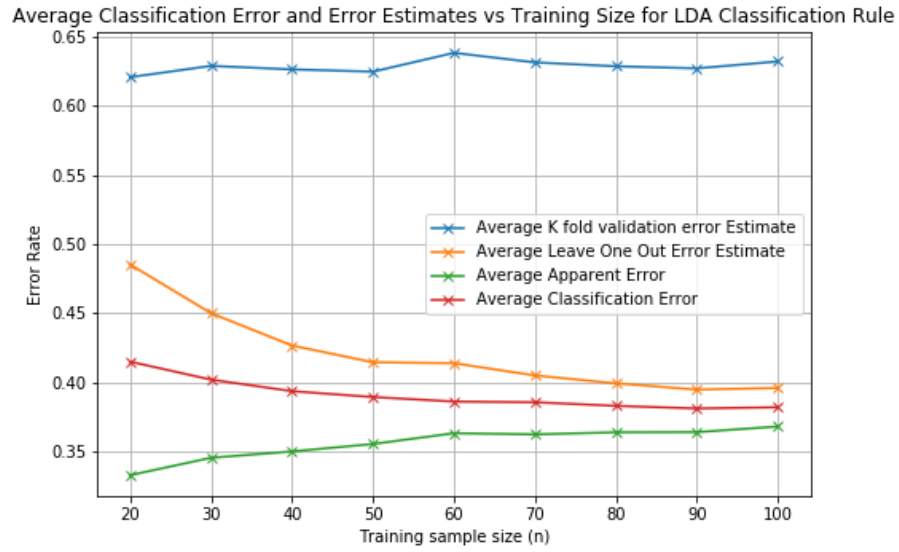


Figure 6: Average Error Estimates and Average Classification Error on Test Set for LDA  $\sigma=2$

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

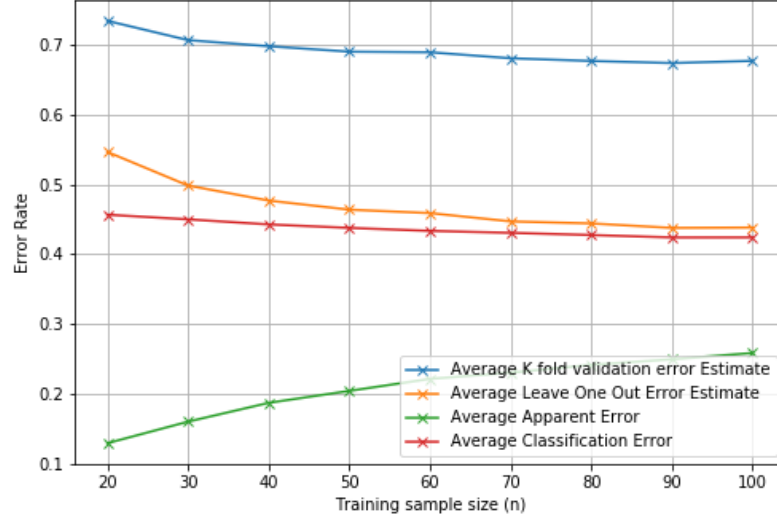


Figure 7: Average Error Estimates and Average Classification Error on Test Set for KNN  $\sigma=2$

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

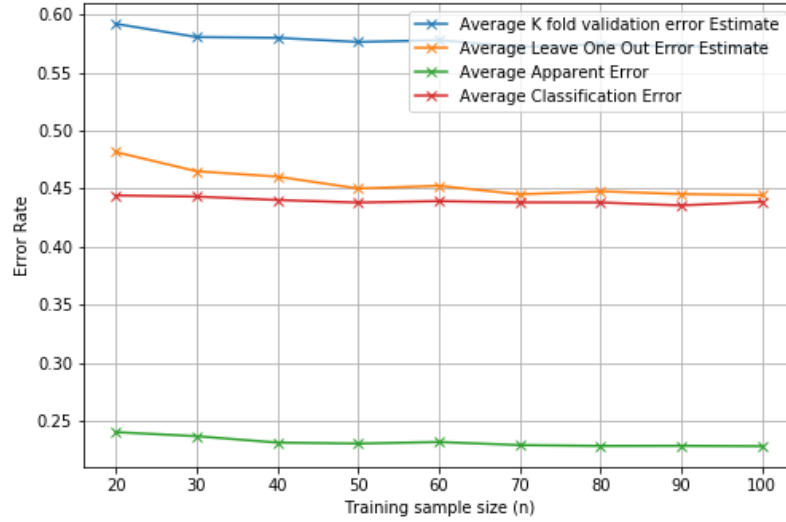


Figure 8: Average Error Estimates and Average Classification Error on Test Set for SVM  $\sigma=2$

\* 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.
- In some cases we have an increasing apparent error, which I am unable to explain. It is expected that as the training size  $n$  increases, the apparent error should decrease due to over fitting.
- 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.
- 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 classification 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.

## 2 Assignment2

- We consider LDA and 3NN as classification 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	Features	(Fe,)	(C, Fe)	(C, Ni, Fe)	(C, N, Fe, Mn)	(N, Ni, Fe, Si, Cr)
1	LDA_apparent Error	0.12	0.04	0.04	0.04	0
2	Features	(Mn,)	(C, Mn)	(C, N, Mn)	(C, N, Ni, Fe)	(C, N, Ni, Fe, Mn)
3	KNN_apparent Error	0.04	0.04	0.04	0.04	0.04
4	Features	(Ni,)	(N, Ni)	(C, Ni, Fe)	(C, N, Ni, Si)	(C, Fe, Mn, Si, Cr)
5	LDA_test Error	0.122449	0.0714286	0.0612245	0.0510204	0.0408163
6	Features	(Ni,)	(Ni, Fe)	(C, Ni, Fe)	(C, N, Ni, Fe)	(C, N, Ni, Fe, Mn)
7	KNN_test Error	0.0918367	0.0612245	0.0612245	0.0612245	0.0612245

Figure 9: Exhaustive Search with Feature Sets and Errors

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

	Categories	1st Feature	2nd Feature	3rd Feature	4th Feature	5th Feature
0	Features	Fe	C	Ni	Mn	N
1	LDA_apparent Error	0.12	0.04	0.04	0.04	0.04
2	Features	Mn	C	N	Si	Ni
3	KNN_apparent Error	0.04	0.04	0.04	0.04	0.08
4	Features	Ni	N	C	Si	Mn
5	LDA_test Error	0.122449	0.0714286	0.0714286	0.0510204	0.0918367
6	Features	Ni	Fe	C	N	Mn
7	KNN_test Error	0.0918367	0.0612245	0.0612245	0.0612245	0.0612245

Figure 10: Exhaustive 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:





Figure 11: Exhaustive Search with Feature Sets and Errors

### 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 gaussian 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
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)

#accuracy 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. ]]
[714.0849999999974, 688.6650000000003, 673.0324999999997]
scoreavg 0 0.714084999999974
[714.0849999999974, 688.6650000000003, 673.0324999999997]
scoreavg 1 0.6886650000000003
[714.0849999999974, 688.6650000000003, 673.0324999999997]
scoreavg 2 0.6730324999999997
[722.9525000000006, 703.9200000000001, 679.7474999999995]
scoreavg 0 0.7229525000000006
[722.9525000000006, 703.9200000000001, 679.7474999999995]
scoreavg 1 0.7039200000000001
[722.9525000000006, 703.9200000000001, 679.7474999999995]
scoreavg 2 0.6797474999999995
[727.6049999999984, 709.5599999999994, 678.8874999999991]
scoreavg 0 0.7276049999999984
[727.6049999999984, 709.5599999999994, 678.8874999999991]
scoreavg 1 0.7095599999999994
[727.6049999999984, 709.5599999999994, 678.8874999999991]
scoreavg 2 0.6788874999999991
[732.2525000000014, 715.4950000000007, 681.3250000000003]
scoreavg 0 0.7322525000000014
[732.2525000000014, 715.4950000000007, 681.3250000000003]
scoreavg 1 0.7154950000000007
[732.2525000000014, 715.4950000000007, 681.3250000000003]
scoreavg 2 0.6813250000000003
[732.3200000000002, 718.3600000000005, 683.1699999999997]
scoreavg 0 0.7323200000000002
[732.3200000000002, 718.3600000000005, 683.1699999999997]
scoreavg 1 0.7183600000000004
[732.3200000000002, 718.3600000000005, 683.1699999999997]
scoreavg 2 0.6831699999999997
[734.3250000000002, 721.4550000000013, 685.4149999999996]
scoreavg 0 0.7343250000000001
[734.3250000000002, 721.4550000000013, 685.4149999999996]
scoreavg 1 0.7214550000000013
[734.3250000000002, 721.4550000000013, 685.4149999999996]
scoreavg 2 0.6854149999999997
[734.8600000000004, 723.68, 685.2775]

```

```

scoreavg 0 0.7348600000000004
[734.8600000000004, 723.68, 685.2775]
scoreavg 1 0.72368
[734.8600000000004, 723.68, 685.2775]
scoreavg 2 0.6852775
[735.1024999999997, 723.8874999999998, 683.3574999999998]
scoreavg 0 0.7351024999999998
[735.1024999999997, 723.8874999999998, 683.3574999999998]
scoreavg 1 0.7238874999999998
[735.1024999999997, 723.8874999999998, 683.3574999999998]
scoreavg 2 0.6833574999999998
[735.9074999999998, 725.9024999999997, 684.205]
scoreavg 0 0.7359074999999998
[735.9074999999998, 725.9024999999997, 684.205]
scoreavg 1 0.7259024999999997
[735.9074999999998, 725.9024999999997, 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')

```

```

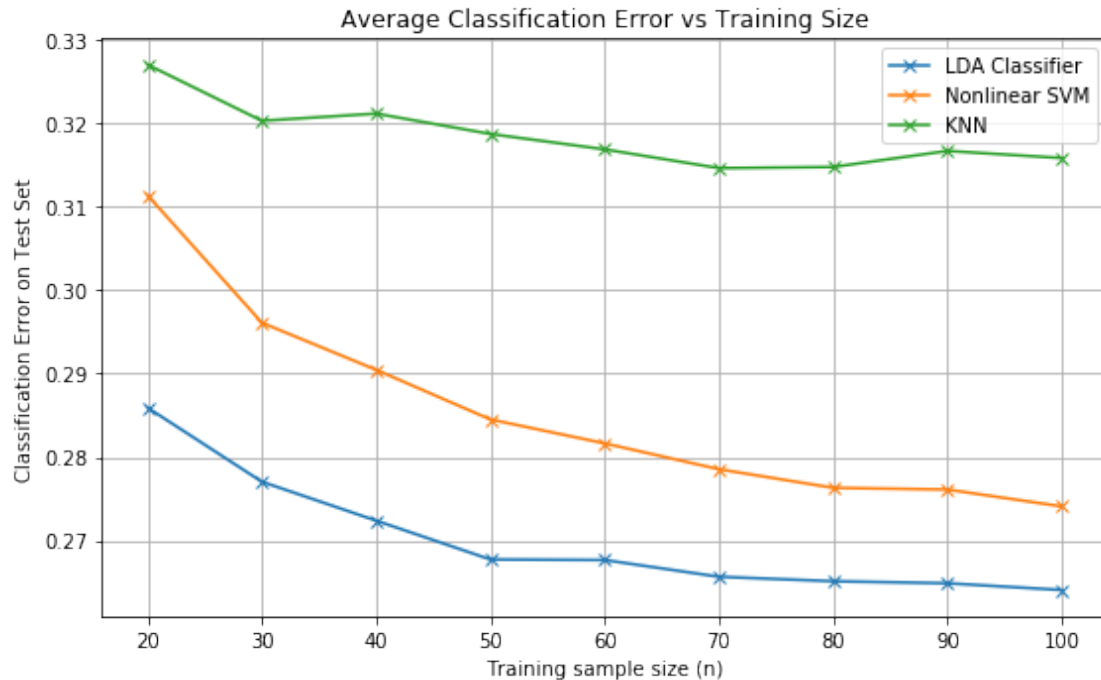
C:\Users\aksha\Anaconda3\lib\site-packages\ipykernel_launcher.py:6: MatplotlibDeprecationWarning:
  Future behavior will be consistent with the long-time default:
  plot commands add elements without first clearing the
  Axes and/or Figure.

```

```

C:\Users\aksha\Anaconda3\lib\site-packages\matplotlib\__init__.py:911: MatplotlibDeprecationWarning:
  mplDeprecation)
C:\Users\aksha\Anaconda3\lib\site-packages\matplotlib\rcsetup.py:156: MatplotlibDeprecationWarning:
  mplDeprecation)

```



```
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))

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 gaussian 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
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)

#accuracy 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 [[4.  0.8]
     [0.8 4.  ]]
[583.6624999999991, 542.4375000000008, 555.1675]
scoreavg 0 0.5836624999999991
[583.6624999999991, 542.4375000000008, 555.1675]
scoreavg 1 0.5424375000000008
[583.6624999999991, 542.4375000000008, 555.1675]
scoreavg 2 0.5551675
[598.1074999999998, 552.5524999999999, 559.8300000000002]
scoreavg 0 0.5981074999999998
[598.1074999999998, 552.5524999999999, 559.8300000000002]
scoreavg 1 0.5525524999999999
[598.1074999999998, 552.5524999999999, 559.8300000000002]
scoreavg 2 0.5598300000000002
[606.775, 559.5799999999997, 562.0499999999997]
scoreavg 0 0.606775
[606.775, 559.5799999999997, 562.0499999999997]
scoreavg 1 0.5595799999999997
[606.775, 559.5799999999997, 562.0499999999997]
scoreavg 2 0.5620499999999997
[612.0074999999998, 566.1625000000001, 563.8750000000005]
scoreavg 0 0.6120074999999998
[612.0074999999998, 566.1625000000001, 563.8750000000005]
scoreavg 1 0.5661625000000001
[612.0074999999998, 566.1625000000001, 563.8750000000005]
scoreavg 2 0.5638750000000005
[613.5049999999998, 566.4575, 560.2950000000003]
scoreavg 0 0.6135049999999998
[613.5049999999998, 566.4575, 560.2950000000003]
scoreavg 1 0.5664575
[613.5049999999998, 566.4575, 560.2950000000003]
scoreavg 2 0.5602950000000003
[616.275, 569.5699999999999, 562.4374999999993]
scoreavg 0 0.616275

```



```

[616.275, 569.5699999999999, 562.4374999999993]
scoreavg 1 0.5695699999999999
[616.275, 569.5699999999999, 562.4374999999993]
scoreavg 2 0.5624374999999994
[616.5199999999999, 571.7, 561.1224999999995]
scoreavg 0 0.6165199999999998
[616.5199999999999, 571.7, 561.1224999999995]
scoreavg 1 0.5717000000000001
[616.5199999999999, 571.7, 561.1224999999995]
scoreavg 2 0.5611224999999995
[617.9774999999993, 574.2150000000001, 559.8374999999993]
scoreavg 0 0.6179774999999993
[617.9774999999993, 574.2150000000001, 559.8374999999993]
scoreavg 1 0.5742150000000001
[617.9774999999993, 574.2150000000001, 559.8374999999993]
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')

```

```

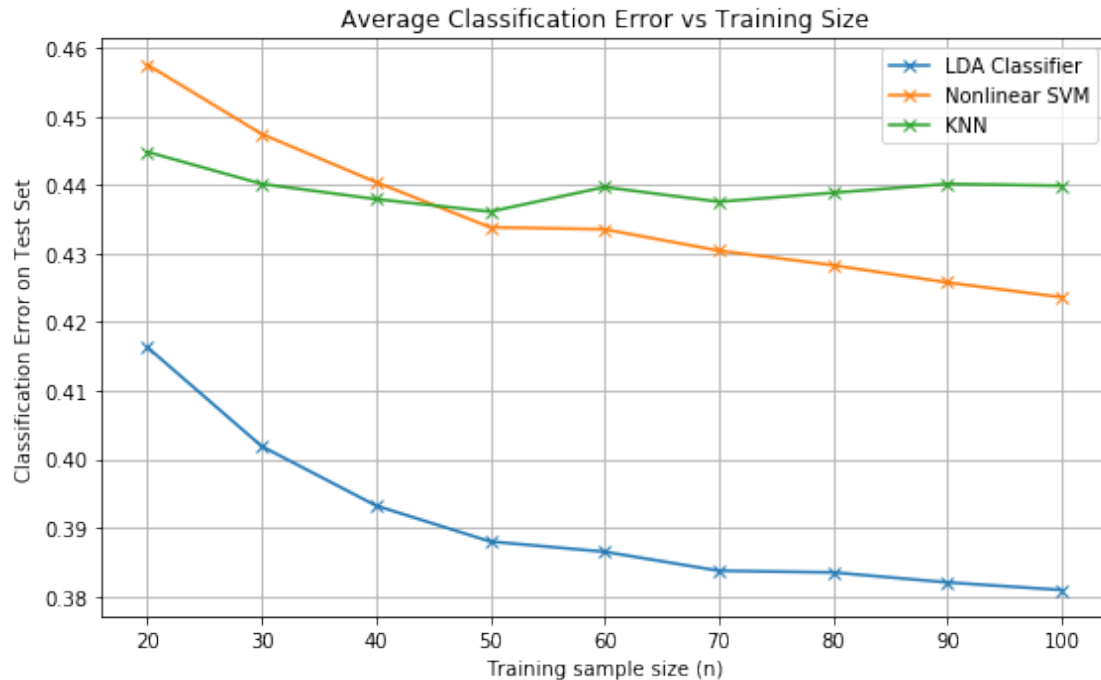
C:\Users\aksha\Anaconda3\lib\site-packages\ipykernel_launcher.py:6: MatplotlibDeprecationWarning:
  Future behavior will be consistent with the long-time default:
  plot commands add elements without first clearing the
  Axes and/or Figure.

```

```

C:\Users\aksha\Anaconda3\lib\site-packages\matplotlib\__init__.py:911: MatplotlibDeprecationWarning:
  mplDeprecation)
C:\Users\aksha\Anaconda3\lib\site-packages\matplotlib\rcsetup.py:156: MatplotlibDeprecationWarning:
  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_c1=[0,0,0]
#import pdb; pdb.set_trace()
for rep_i in range(0,1000):

    #import pdb; pdb.set_trace()
    #create sample two gaussian 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)

#accuracy 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)

#accuracy 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)

#accuracy 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)

#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)

#accuracy 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 avgcl',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)')

```

```

fig.tight_layout()
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 Estimate')
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 Estimate')
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]
      [0.2 1. ]]
count of n 1
score kf [[0.59785 0.48825 0.56155]
          [0.      0.      0.      ]
          [0.      0.      0.      ]
          [0.      0.      0.      ]
          [0.      0.      0.      ]
          [0.      0.      0.      ]
          [0.      0.      0.      ]
          [0.      0.      0.      ]

```

```

score loo [[0.6925 0.6485 0.6521]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score avg [[0.76935 0.8246 0.8184 ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score avg [[0.716375 0.6917125 0.6794275]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
count of n 2
score kf [[0.59785 0.48825 0.56155 ]
[0.60053333 0.5233 0.568 ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score loo [[0.6925 0.6485 0.6521 ]
[0.70466667 0.67476667 0.6633 ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score avg [[0.76935 0.8246 0.8184 ]
[0.75853333 0.8045 0.82406667]

```



```

[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score avg [[0.716375  0.6917125 0.6794275]
[0.72618  0.7045625 0.6791725]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
count of n 3
score kf [[0.59785  0.48825  0.56155  ]
[0.60053333 0.5233  0.568  ]
[0.6065  0.536825  0.576625 ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score loo [[0.6925  0.6485  0.6521  ]
[0.70466667 0.67476667 0.6633  ]
[0.712125  0.689325  0.66595  ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score avg [[0.76935  0.8246  0.8184  ]
[0.75853333 0.8045  0.82406667]
[0.749025  0.7915  0.819825  ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      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.      0.      0.      ]

```

```

[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
count of n 4
score kf [[0.59785    0.48825    0.56155    ]
[0.60053333 0.5233     0.568      ]
[0.6065     0.536825  0.576625  ]
[0.60976    0.5474    0.57588    ]
[0.         0.         0.         ]
[0.         0.         0.         ]
[0.         0.         0.         ]
[0.         0.         0.         ]
[0.         0.         0.         ]]
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    ]
[0.         0.         0.         ]
[0.         0.         0.         ]
[0.         0.         0.         ]
[0.         0.         0.         ]
[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.         0.         0.         ]
[0.         0.         0.         ]
[0.         0.         0.         ]
[0.         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.         0.         0.         ]
[0.         0.         0.         ]
[0.         0.         0.         ]
[0.         0.         0.         ]
[0.         0.         0.         ]]
count of n 5
score kf [[0.59785    0.48825    0.56155    ]
[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.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
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    ]
[0.72305    0.7092     0.67575    ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[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.      0.      0.      ]
[0.      0.      0.      ]
[0.      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.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
count of n 6
score kf [[0.59785     0.48825     0.56155     ]
[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      0.6485      0.6521      ]
[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    0.8246    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.      0.      0.      ]
[0.      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]
[0.7325075   0.721205   0.6837525]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
count of n 7
score kf [[0.59785    0.48825    0.56155    ]
[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.      0.      0.      ]
[0.      0.      0.      ]]
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    ]
[0.72305     0.7092     0.67575    ]
[0.72601429 0.71288571 0.67862857]
[0.7250625   0.712475   0.67545    ]
[0.      0.      0.      ]
[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.      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]
[0.7325075  0.721205   0.6837525]
[0.7354     0.72361    0.6849825]
[0.         0.         0.         ]
[0.         0.         0.         ]]
count of n 8
score kf [[0.59785    0.48825    0.56155    ]
[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.         0.         0.         ]]
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     ]
[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     ]
[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     0.72361    0.6849825]
[0.7352425  0.725385   0.685275  ]
[0.         0.         0.         ]]
count of n 9
score kf [[0.59785    0.48825    0.56155    ]

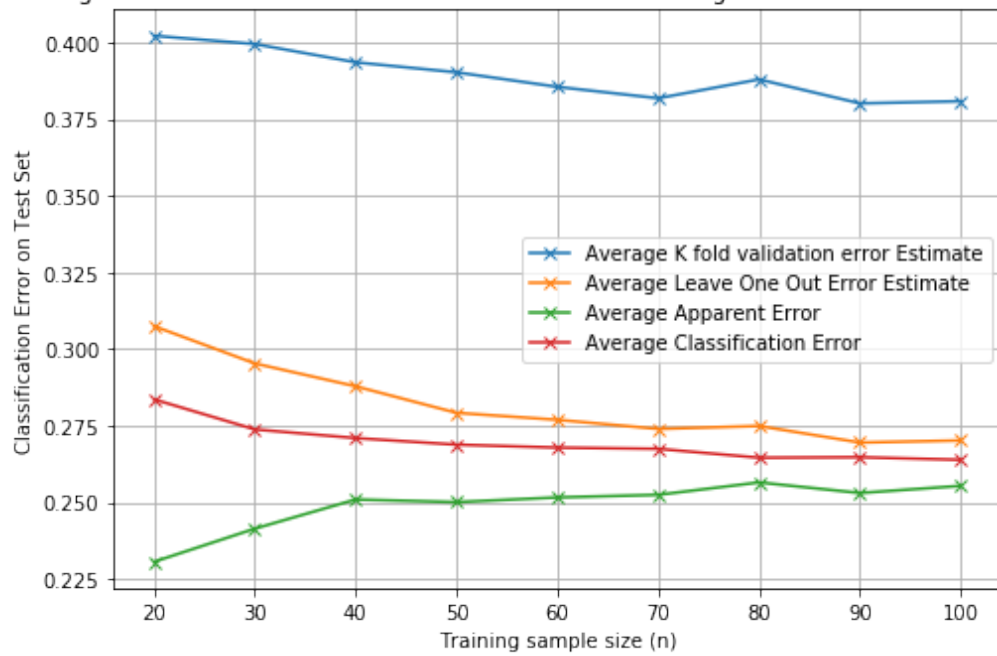
```

```

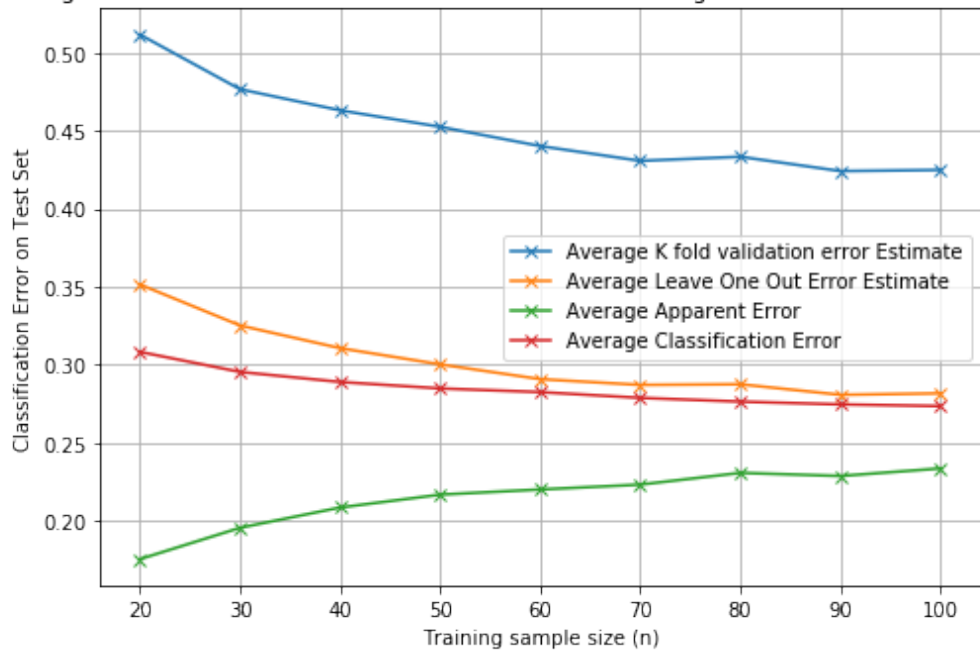
[0.60053333 0.5233      0.568      ]
[0.6065      0.536825   0.576625   ]
[0.60976     0.5474     0.57588     ]
[0.6145      0.55973333 0.58565     ]
[0.61821429 0.56921429 0.58587143]
[0.6120625   0.5665875   0.5811      ]
[0.61988889 0.57577778 0.58855556]
[0.61918     0.57506     0.58643     ]]
score 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     ]
[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     ]]
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      ]
[0.74458     0.76644     0.82358     ]]
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      0.72361     0.6849825]
[0.7352425   0.725385    0.685275   ]
[0.7360875   0.7264575   0.6854525]]

```

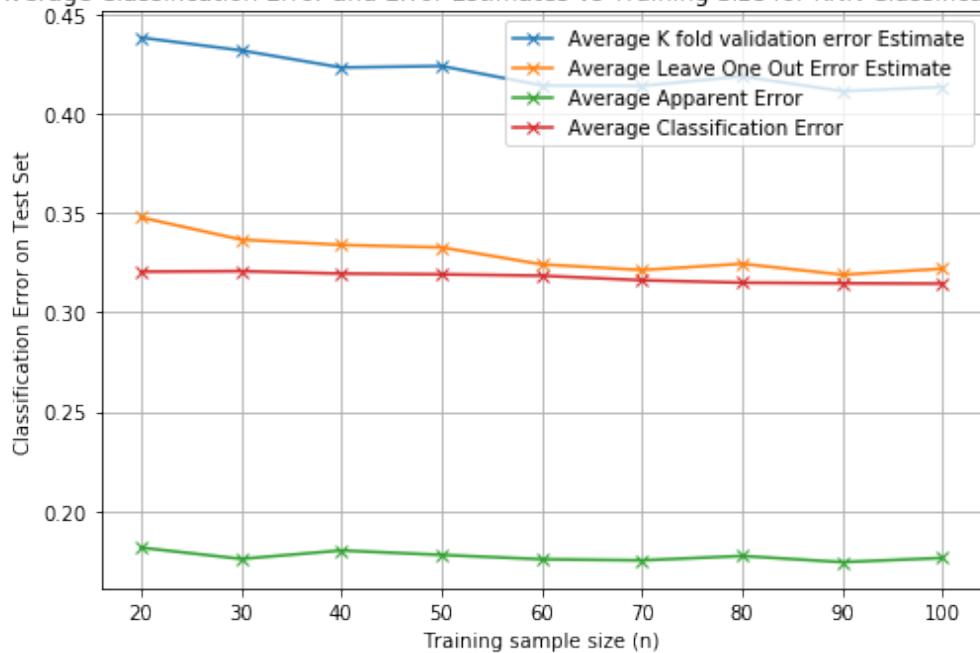
Average Classification Error and Error Estimates vs Training Size for LDA Classification Rule



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



Average Classification Error and Error Estimates vs Training Size for KNN 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_c1=[0,0,0]
#import pdb; pdb.set_trace()
for rep_i in range(0,1000):

    #import pdb; pdb.set_trace()
    #create sample two gaussian 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)

#accuracy 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)

#accuracy 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)

#accuracy 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)

#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)

#accuracy 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 avgcl',score_avgcl)

```

```

cov [[4.  0.8]
     [0.8 4. ]]
count of n 1
score kf [[0.37915 0.2659  0.4081 ]
          [0.      0.      0.      ]
          [0.      0.      0.      ]
          [0.      0.      0.      ]
          [0.      0.      0.      ]

```

```

[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score loo [[0.51465 0.45365 0.51855]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score avg [[0.66725 0.87095 0.75975]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score avg [[0.5850225 0.5435975 0.5558825]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[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.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score loo [[0.51465      0.45365      0.51855      ]
[0.54993333 0.50176667 0.53506667]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]

```

```

[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.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score avg [[0.5850225 0.5435975 0.5558825]
[0.5980475 0.550245  0.556865  ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
count of n 3
score kf [[0.37915  0.2659  0.4081  ]
[0.37093333 0.2935  0.41946667]
[0.373475  0.302225  0.42015  ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score loo [[0.51465  0.45365  0.51855  ]
[0.54993333 0.50176667 0.53506667]
[0.573375  0.52335  0.539675  ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score avg [[0.66725  0.87095  0.75975  ]
[0.65463333 0.84006667 0.76326667]
[0.65005  0.8131  0.76875  ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]
[0.      0.      0.      ]]
score avg [[0.5850225 0.5435975 0.5558825]

```

```

[0.5980475 0.550245 0.556865 ]
[0.6064025 0.55752 0.559835 ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]]
count of n 4
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. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]]
score loo [[0.51465 0.45365 0.51855 ]
[0.54993333 0.50176667 0.53506667]
[0.573375 0.52335 0.539675 ]
[0.5855 0.53636 0.54992 ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]]
score avg [[0.66725 0.87095 0.75975 ]
[0.65463333 0.84006667 0.76326667]
[0.65005 0.8131 0.76875 ]
[0.64464 0.79598 0.7696 ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]]
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. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]
[0. 0. 0. ]]
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]
[0.        0.        0.        ]
[0.        0.        0.        ]
[0.        0.        0.        ]
[0.        0.        0.        ]]
score loo [[0.51465   0.45365   0.51855   ]
[0.54993333 0.50176667 0.53506667]
[0.573375   0.52335   0.539675   ]
[0.5855     0.53636   0.54992   ]
[0.58616667 0.5413    0.54758333]
[0.        0.        0.        ]
[0.        0.        0.        ]
[0.        0.        0.        ]
[0.        0.        0.        ]]
score avg [[0.66725   0.87095   0.75975   ]
[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.        0.        0.        ]
[0.        0.        0.        ]
[0.        0.        0.        ]
[0.        0.        0.        ]]
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.        0.        0.        ]
[0.        0.        0.        ]
[0.        0.        0.        ]
[0.        0.        0.        ]]
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.        0.        0.        ]
[0.        0.        0.        ]
[0.        0.        0.        ]]
score loo [[0.51465   0.45365   0.51855   ]
[0.54993333 0.50176667 0.53506667]
[0.573375   0.52335   0.539675   ]
[0.5855     0.53636   0.54992   ]

```



```

[0.58616667 0.5413      0.54758333]
[0.59504286 0.55318571 0.55492857]
[0.          0.          0.          ]
[0.          0.          0.          ]
[0.          0.          0.          ]]
score avg [[0.66725      0.87095      0.75975      ]
[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      ]
[0.          0.          0.          ]
[0.          0.          0.          ]
[0.          0.          0.          ]]
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.          0.          0.          ]
[0.          0.          0.          ]
[0.          0.          0.          ]]
count of n 7
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]
[0.371225 0.3233625 0.4258625 ]
[0.          0.          0.          ]
[0.          0.          0.          ]]
score loo [[0.51465      0.45365      0.51855      ]
[0.54993333 0.50176667 0.53506667]
[0.573375 0.52335 0.539675 ]
[0.5855 0.53636 0.54992 ]
[0.58616667 0.5413      0.54758333]
[0.59504286 0.55318571 0.55492857]
[0.600725 0.5561      0.5523125 ]
[0.          0.          0.          ]
[0.          0.          0.          ]]
score avg [[0.66725      0.87095      0.75975      ]
[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      ]

```

```

[0.6362      0.75865      0.771625   ]
[0.          0.          0.          ]
[0.          0.          0.          ]]
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]
[0.          0.          0.          ]
[0.          0.          0.          ]]
count of n 8
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]
[0.371225 0.3233625 0.4258625 ]
[0.37271111 0.32636667 0.42763333]
[0.          0.          0.          ]]
score loo [[0.51465      0.45365      0.51855      ]
[0.54993333 0.50176667 0.53506667]
[0.573375 0.52335 0.539675 ]
[0.5855 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.          0.          0.          ]]
score avg [[0.66725      0.87095      0.75975      ]
[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 ]
[0.6362 0.75865 0.771625 ]
[0.63604444 0.75071111 0.77153333]
[0.          0.          0.          ]]
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]
[0.61893 0.5761625 0.5644725]

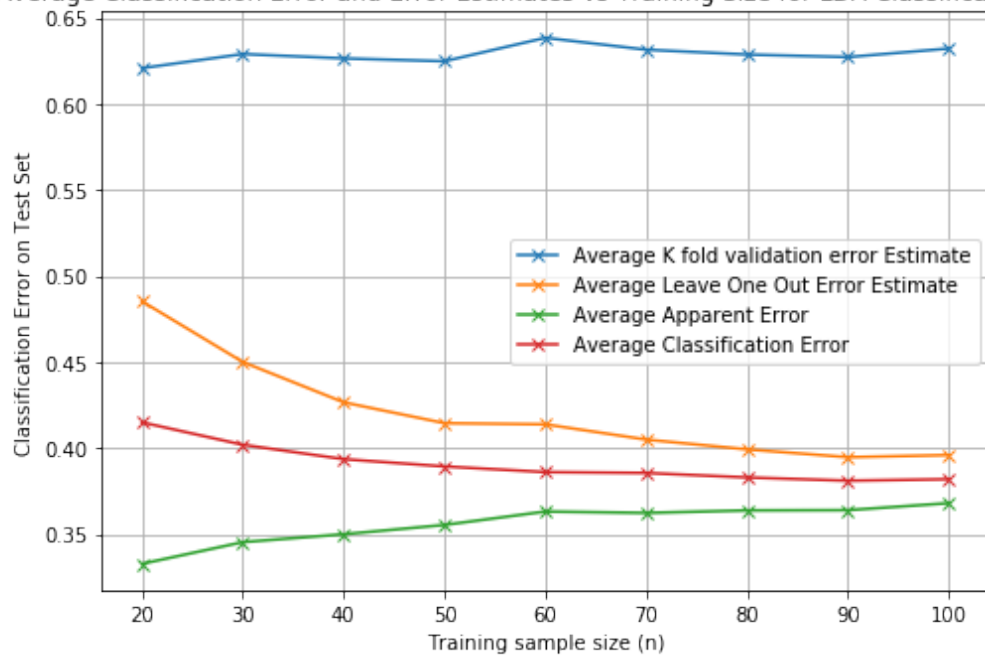
```

```

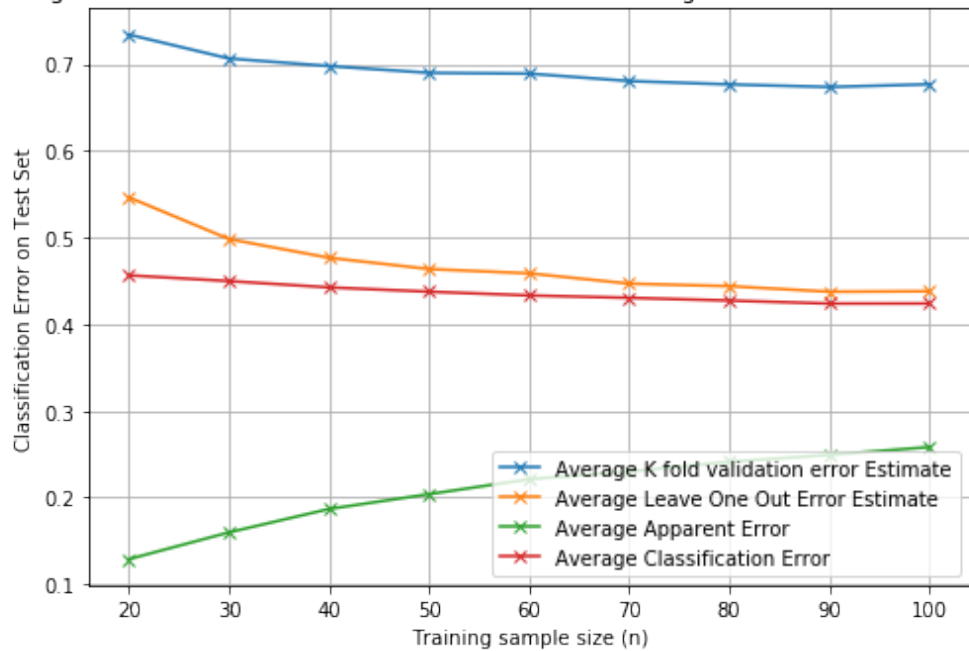
[0.      0.      0.      ]]
count of n 9
score kf [[0.37915    0.2659    0.4081    ]
[0.37093333 0.2935    0.41946667]
[0.373475   0.302225   0.42015    ]
[0.37512    0.31006    0.42372    ]
[0.3615     0.31091667 0.42218333]
[0.36842857 0.31951429 0.42804286]
[0.371225   0.3233625   0.4258625   ]
[0.37271111 0.32636667 0.42763333]
[0.36773    0.32323    0.4276    ]]
score loo [[0.51465    0.45365    0.51855    ]
[0.54993333 0.50176667 0.53506667]
[0.573375   0.52335    0.539675   ]
[0.5855     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]
[0.60404    0.56197    0.5556    ]]
score avg [[0.66725    0.87095    0.75975    ]
[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    ]
[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]
[0.6170375 0.57271 0.5619425]
[0.61893 0.5761625 0.5644725]
[0.61806 0.5760975 0.5614225]]

```

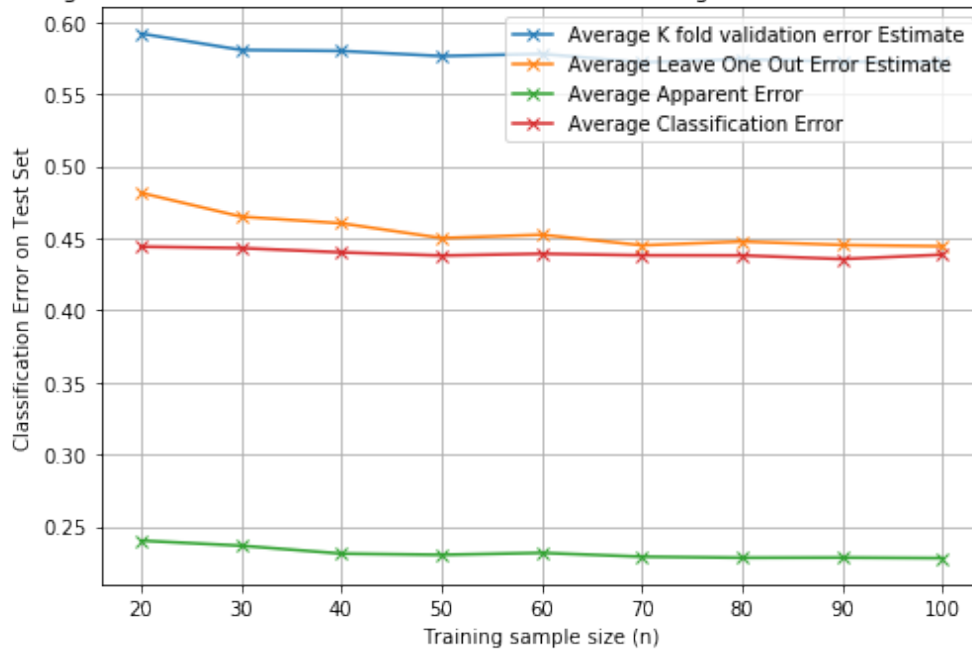
Average Classification Error and Error Estimates vs Training Size for LDA Classification Rule



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



Average Classification Error and Error Estimates vs Training Size for KNN 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 Estimate')
plt.plot(nlist,1-score_avgloo[:,0],marker='x',label='Average Leave One Out Error Estimate')
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 Estimate')
plt.plot(nlist,1-score_avgloo[:,1],marker='x',label='Average Leave One Out Error Estimate')
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()
```

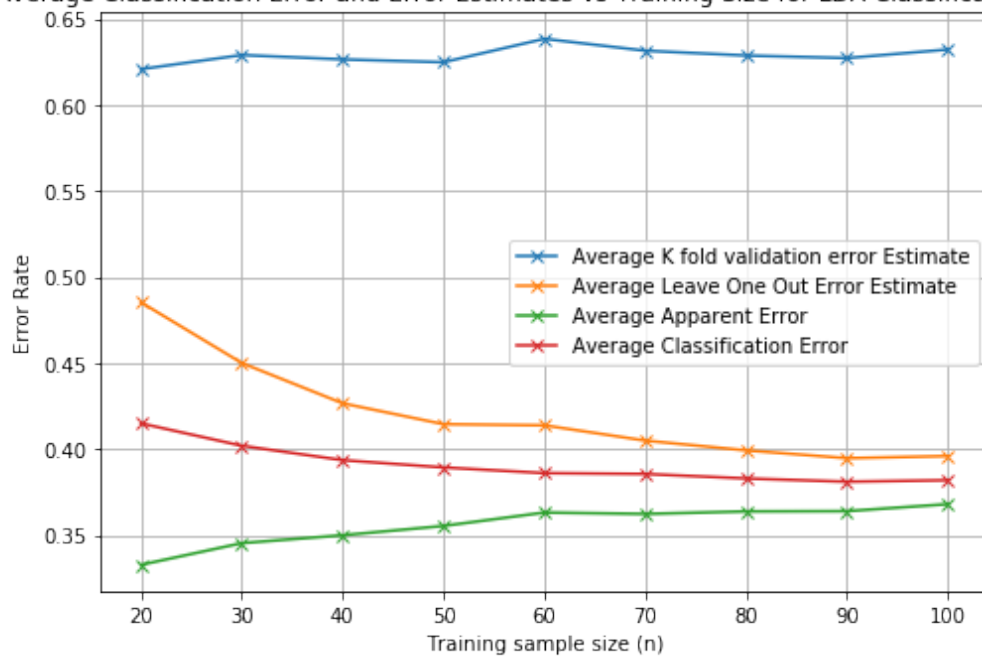
```

ax.legend()
plt.grid(True)
plt.show
fig.savefig('hw2_18b.png')

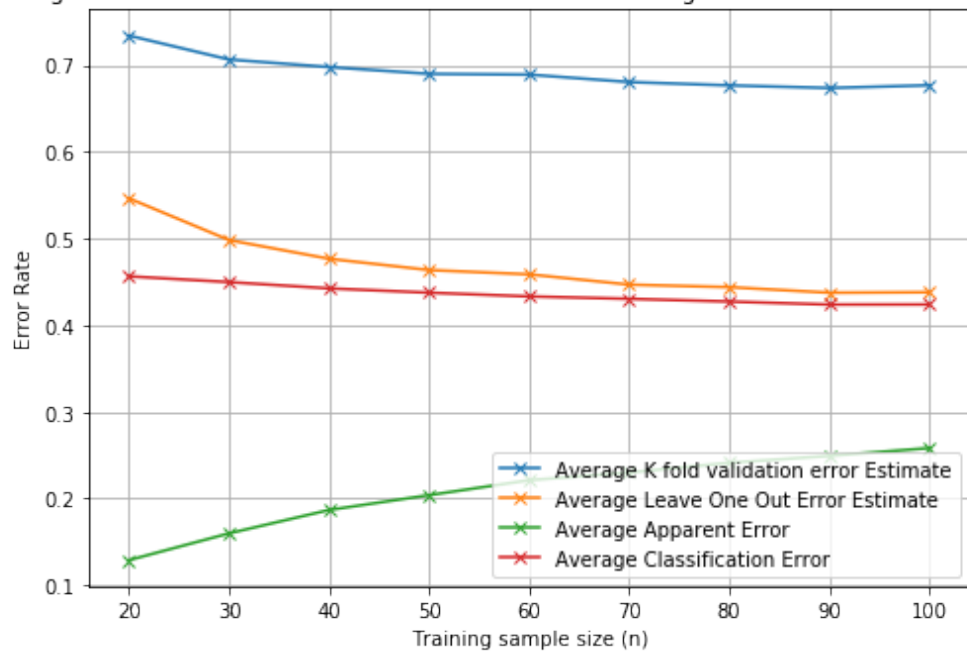
#plot error curves for KNN
fig, ax = plt.subplots(figsize=[8,5])
plt.plot(nlist,1-score_avgkf[:,2],marker='x',label='Average K fold validation error Estimate')
plt.plot(nlist,1-score_avgloo[:,2],marker='x',label='Average Leave One Out Error Estimate')
plt.plot(nlist,1-score_avg[:,2],marker='x',label='Average 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')

```

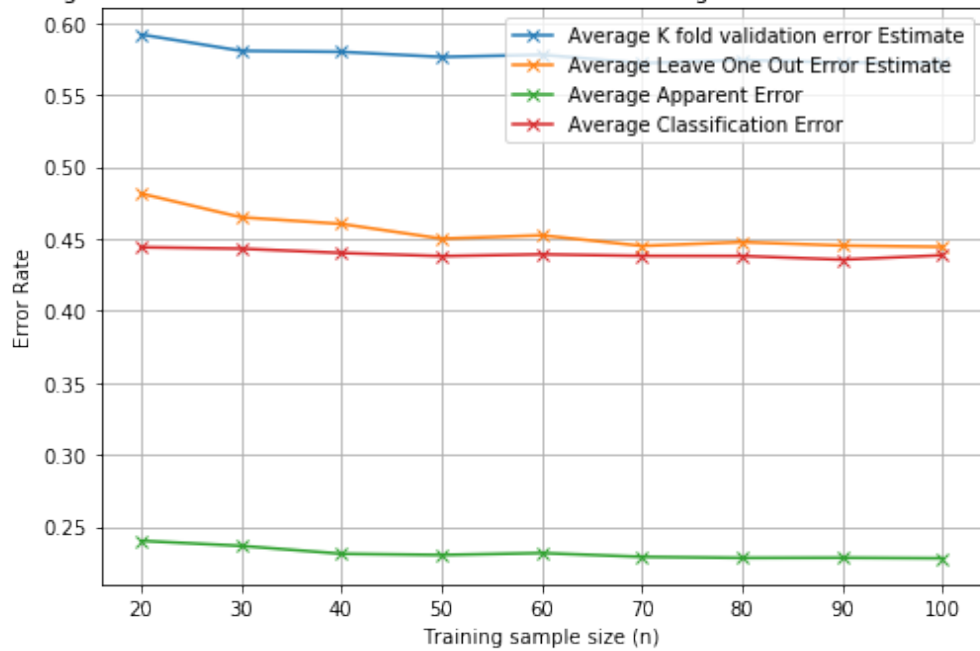
Average Classification Error and Error Estimates vs Training Size for LDA Classification Rule



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



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



# HW2\_2copy

October 30, 2018

```
In [241]: 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[241]: <function TextIOWrapper.close()>
```

```
In [54]: def list_concat(word):
out=''
for i in word:
out+=i
return(out)
```

```
In [55]: 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 [56]: 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 [57]: 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 [58]: 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 [59]: train1=np.array(train3)
        test1=np.array(test3)

In [60]: train4=np.reshape(train1,(25,8))
        test4=np.reshape(test1,(int(len(test1)/8),8))

In [61]: len(test1)/8

Out[61]: 98.0

In [62]: traindf=pd.DataFrame(data=train4,columns=cols)
        testdf=pd.DataFrame(data=test4,columns=cols)

In [244]: testdf
         #scatterplot
        sns.set()
        sns.pairplot(testdf, size = 2.5,hue='SFE')
        plt.show();

```



```
In [312]: 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):
```

```

#combinations of features
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(...)

    #accuracy 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 [83]: x=all_combs[0][:,0]
```

```
[0.72 0.52 0.84 0.88 0.6  0.68 0.6 ]
```

```
In [95]: all_combs_feat[0]
```

```
Out[95]: ('C',)
```

```
In [97]: 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 [105]: type(maxscore_feat)
```

```
Out[105]: list
```

```
In [118]: 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 [157]: varlda_app=[]
varlda_test=[]
varknn_app=[]
varknn_test=[]
errlda_app=[]
errlda_test=[]
errknn_app=[]
errknn_test=[]
for i in range(0,5):
    varlda_app.append(feat_set[i][0])
    varlda_test.append(feat_set[i][1])
    varknn_app.append(feat_set[i][2])
    varknn_test.append(feat_set[i][3])
    errlda_app.append(1-score_max[i][0])
    errlda_test.append(1-score_max[i][1])
    errknn_app.append(1-score_max[i][2])
    errknn_test.append(1-score_max[i][3])
```

```
In [201]: dat=[]
for i in range(0,8):
    dat.append([])
```

```

dat[0].append('Features')
dat[1].append('LDA_apparent Error')
dat[2].append('Features')
dat[3].append('KNN_apparent Error')
dat[4].append('Features')
dat[5].append('LDA_test Error')
dat[6].append('Features')
dat[7].append('KNN_test Error')

for i in range(0,5):
    dat[0].append(feats[i][0])
    dat[2].append(feats[i][1])
    dat[4].append(feats[i][2])
    dat[6].append(feats[i][3])
    dat[1].append(1-score_max[i][0])
    dat[3].append(1-score_max[i][1])
    dat[5].append(1-score_max[i][2])
    dat[7].append(1-score_max[i][3])

```

```

In [204]: labs=['Categories','1 Feature','2 Features','3 Features','4 Features','5 Features']
df1=pd.DataFrame(data=dat,columns=labs)
df1

```

```

Out[204]:

```

	Categories	1 Feature	2 Features	3 Features	4 Features \
0	Features	(Fe,)	(C, Fe)	(C, Ni, Fe)	(C, N, Fe, Mn)
1	LDA_apparent Error	0.12	0.04	0.04	0.04
2	Features	(Mn,)	(C, Mn)	(C, N, Mn)	(C, N, Ni, Fe)
3	KNN_apparent Error	0.04	0.04	0.04	0.04
4	Features	(Ni,)	(N, Ni)	(C, Ni, Fe)	(C, N, Ni, Si)
5	LDA_test Error	0.122449	0.0714286	0.0612245	0.0510204
6	Features	(Ni,)	(Ni, Fe)	(C, Ni, Fe)	(C, N, Ni, Fe)
7	KNN_test Error	0.0918367	0.0612245	0.0612245	0.0612245

	5 Features
0	(N, Ni, Fe, Si, Cr)
1	0
2	(C, N, Ni, Fe, Mn)
3	0.04
4	(C, Fe, Mn, Si, Cr)
5	0.0408163
6	(C, N, Ni, Fe, Mn)
7	0.0612245

```

In [311]: #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(...)

```

```

#accuracy 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 [300]: score\_max

```

Out[300]: [[0.88, 0.96, 0.96, 0.96, 0.96],
 [0.96, 0.96, 0.96, 0.96, 0.92],
 [0.8775510204081632,
 0.9285714285714286,
 0.9285714285714286,
 0.9489795918367347,
 0.9081632653061225],
 [0.9081632653061225,
 0.9387755102040817,
 0.9387755102040817,
 0.9387755102040817,
 0.9387755102040817]]

```

In [290]: all\_combs\_feat

```

Out[290]: [['Fe', 'C', 'Ni', 'Mn', 'N'],
 ['Mn', 'C', 'N', 'Si', 'Ni'],
 ['Ni', 'N', 'C', 'Si', 'Mn'],
 ['Ni', 'Fe', 'C', 'N', 'Mn']],
 [['Fe', 'C', 'Ni', 'Mn', 'N'],
 ['Mn', 'C', 'N', 'Si', 'Ni'],
 ['Ni', 'N', 'C', 'Si', 'Mn'],
 ['Ni', 'Fe', 'C', 'N', 'Mn']],
 [['Fe', 'C', 'Ni', 'Mn', 'N'],
 ['Mn', 'C', 'N', 'Si', 'Ni'],

```

```

['Ni', 'N', 'C', 'Si', 'Mn'],
['Ni', 'Fe', 'C', 'N', 'Mn']],
[['Fe', 'C', 'Ni', 'Mn', 'N'],
 ['Mn', 'C', 'N', 'Si', 'Ni'],
 ['Ni', 'N', 'C', 'Si', 'Mn'],
 ['Ni', 'Fe', 'C', 'N', 'Mn']],
[['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 [308]: dat=[]
          for i in range(0,8):
              dat.append([])

          dat[0].append('Features')
          dat[1].append('LDA_apparent Error')
          dat[2].append('Features')
          dat[3].append('KNN_apparent Error')
          dat[4].append('Features')
          dat[5].append('LDA_test Error')
          dat[6].append('Features')
          dat[7].append('KNN_test Error')

```

```

          for i in range(0,5):
              dat[0].append(chosen_feat[0][i])
              dat[2].append(chosen_feat[1][i])
              dat[4].append(chosen_feat[2][i])
              dat[6].append(chosen_feat[3][i])
              dat[1].append(1-score_max[0][i])
              dat[3].append(1-score_max[1][i])
              dat[5].append(1-score_max[2][i])
              dat[7].append(1-score_max[3][i])

```

```

In [310]: labs=['Categories', '1st Feature', '2nd Feature', '3rd Feature', '4th Feature', '5th Feature']
          df1=pd.DataFrame(data=dat, columns=labs)
          df1

```

```

Out[310]:
      Categories 1st Feature 2nd Feature 3rd Feature 4th Feature \
0      Features          Fe          C          Ni          Mn
1  LDA_apparent Error      0.12        0.04        0.04        0.04
2      Features          Mn          C          N          Si

```



3	KNN_apparent Error	0.04	0.04	0.04	0.04
4	Features	Ni	N	C	Si
5	LDA_test Error	0.122449	0.0714286	0.0714286	0.0510204
6	Features	Ni	Fe	C	N
7	KNN_test Error	0.0918367	0.0612245	0.0612245	0.0612245

	5th Feature
0	N
1	0.04
2	Ni
3	0.08
4	Mn
5	0.0918367
6	Mn
7	0.0612245

In [307]: score\_max[0]

Out[307]: [0.88, 0.96, 0.96, 0.96, 0.96]