CS6301.010: Machine Learning for Engineers and Scientists (Spring '19)

***Instructor**: Gautam Kunapuli*
Due**: In class, **February 25 (Monday)

Homework 2

The report component of this assignment is the **hard copy** of this homework, along with your answers to questions, and is **due at the start of class on Monday, February 25, 2019**.

The **electronic version** of this homework **must be uploaded on eLearning by 9:59am Central Standard Time, Monday, February 25, 2019**. All deadlines are hard and without exceptions unless permission was obtained from the instructor **in advance**.

You may work in groups to discuss the problems and work through solutions together. However, you must **write up your solutions on your own**, without copying another student's work or letting another student copy your work. In your solution for each problem, you must write down the names of your partner (if any); this will not affect your grade.

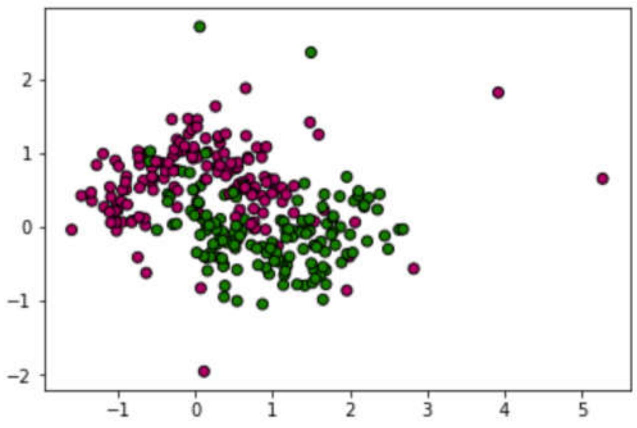
1. **Support Vector Machines with Synthetic Data**, 50 points.

For this problem, we will generate synthetic data for a nonlinear binary classification problem and partition it into training, validation and test sets. Our goal is to understand the behavior of SVMs with Radial-Basis Function (RBF) kernels with different values of C and γ.

In [10]:
```
#
# DO NOT EDIT THIS FUNCTION; IF YOU WANT TO PLAY AROUND WITH DATA GENERATION,
# MAKE A COPY OF THIS FUNCTION AND THEN EDIT
#
import numpy as np
from sklearn.datasets import make_moons
from sklearn.model_selection import train_test_split
import matplotlib.pyplot as plt
from matplotlib.colors import ListedColormap

def generate_data(n_samples, tst_frac=0.2, val_frac=0.2):
  # Generate a non-linear data set
  X, y = make_moons(n_samples=n_samples, noise=0.25, random_state=42)

  # Take a small subset of the data and make it VERY noisy; that is, generate ou
tliers
  m = 30
  np.random.seed(42)
  ind = np.random.permutation(n_samples)[:m]
  X[ind, :] += np.random.multivariate_normal([0, 0], np.eye(2), (m, ))
  y[ind] = 1 - y[ind]

  # Plot this data
  cmap = ListedColormap(['#b30065', '#178000'])
  plt.scatter(X[:, 0], X[:, 1], c=y, cmap=cmap, edgecolors='k')

  # First, we use train_test_split to partition (X, y) into training and test se
ts
  X_trn, X_tst, y_trn, y_tst = train_test_split(X, y, test_size=tst_frac,
                                                random_state=42)

  # Next, we use train_test_split to further partition (X_trn, y_trn) into train
ing and validation sets
  X_trn, X_val, y_trn, y_val = train_test_split(X_trn, y_trn, test_size=val_frac
,
                                                random_state=42)

  return (X_trn, y_trn), (X_val, y_val), (X_tst, y_tst)
```

In [11]:
```
#
#  DO NOT EDIT THIS FUNCTION; IF YOU WANT TO PLAY AROUND WITH VISUALIZATION,
#  MAKE A COPY OF THIS FUNCTION AND THEN EDIT
#

def visualize(models, param, X, y):
  # Initialize plotting
  if len(models) % 3 == 0:
    nrows = len(models) // 3
  else:
    nrows = len(models) // 3 + 1

  fig, axes = plt.subplots(nrows=nrows, ncols=3, figsize=(15, 5.0 * nrows))
  cmap = ListedColormap(['#b30065', '#178000'])

  # Create a mesh
  xMin, xMax = X[:, 0].min() - 1, X[:, 0].max() + 1
  yMin, yMax = X[:, 1].min() - 1, X[:, 1].max() + 1
  xMesh, yMesh = np.meshgrid(np.arange(xMin, xMax, 0.01),
                             np.arange(yMin, yMax, 0.01))

  for i, (p, clf) in enumerate(models.items()):
    # if i > 0:
    #   break
    r, c = np.divmod(i, 3)
    ax = axes[r, c]

    # Plot contours
    zMesh = clf.decision_function(np.c_[xMesh.ravel(), yMesh.ravel()])
    zMesh = zMesh.reshape(xMesh.shape)
    ax.contourf(xMesh, yMesh, zMesh, cmap=plt.cm.PiYG, alpha=0.6)

    if (param == 'C' and p > 0.0) or (param == 'gamma'):
      ax.contour(xMesh, yMesh, zMesh, colors='k', levels=[-1, 0, 1],
                 alpha=0.5, linestyles=['--', '-', '--'])

    # Plot data
    ax.scatter(X[:, 0], X[:, 1], c=y, cmap=cmap, edgecolors='k')
    ax.set_title('{0} = {1}'.format(param, p))
```

In [12]:
```
# Generate the data
n_samples = 300    # Total size of data set
(X_trn, y_trn), (X_val, y_val), (X_tst, y_tst) = generate_data(n_samples)
```



a. (25 points) The effect of the regularization parameter, C

Complete the Python code snippet below that takes the generated synthetic 2-d data as input and learns non-linear SVMs. Use scikit-learn's SVC (https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html) function to learn SVM models with **radial-basis kernels** for fixed γ and various choices of $C \in \{10^{-3}, 10^{-2} \cdots, 1, \cdots 10^5\}$. The value of γ is fixed to $\gamma = \frac{1}{d \cdot \sigma_X}$, where d is the data dimension and σ_X is the standard deviation of the data set X. SVC can automatically use these setting for γ if you pass the argument gamma = 'scale' (see documentation for more details).

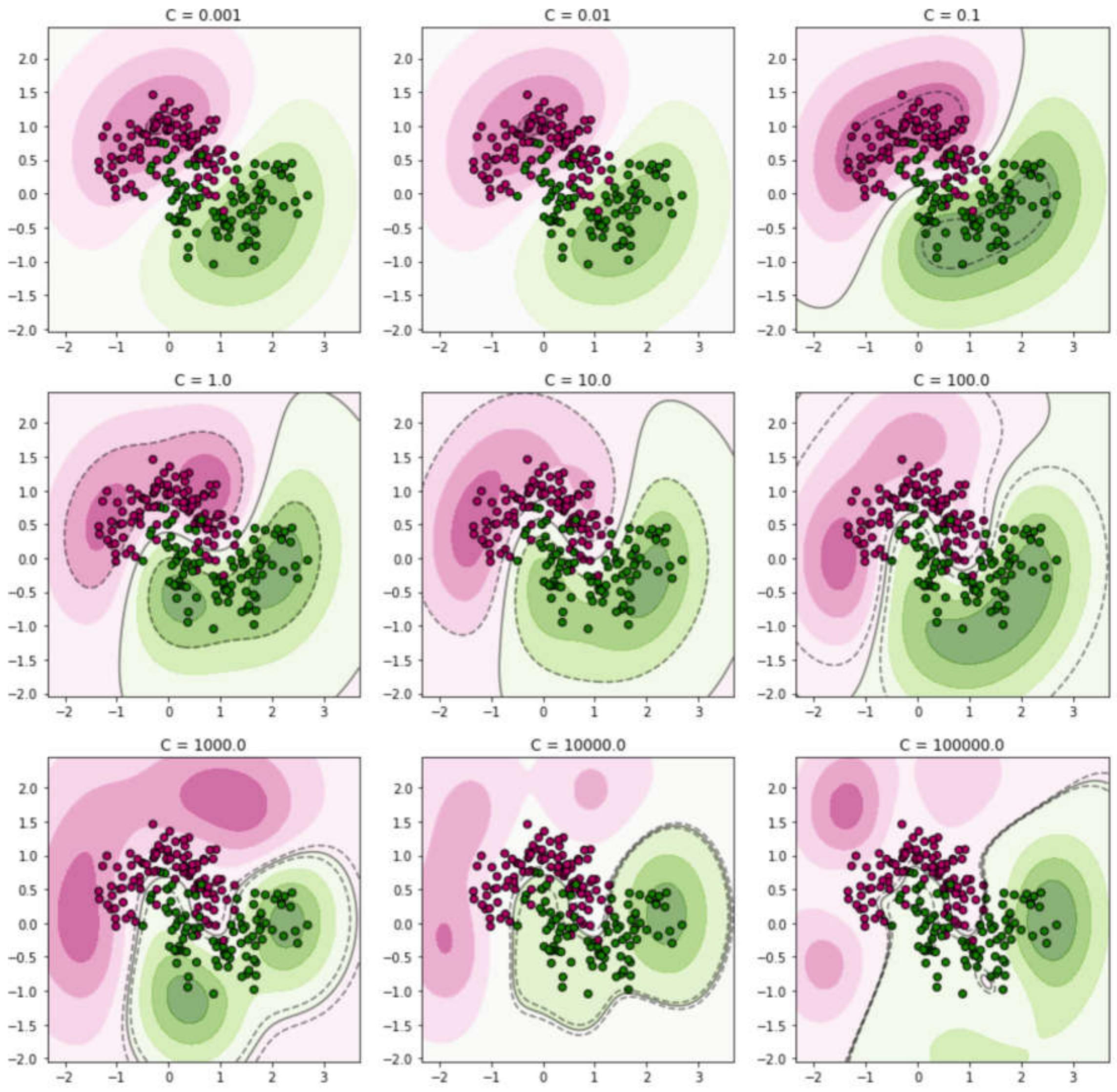
Plot: For each classifier, compute **both** the **training error** and the **validation error**. Plot them together, making sure to label the axes and each curve clearly.

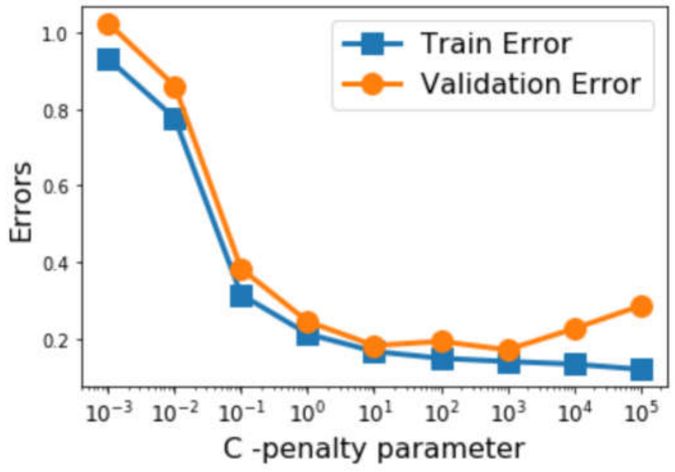
Discussion: How do the training error and the validation error change with C? Based on the visualization of the models and their resulting classifiers, how does changing C change the models? Explain in terms of minimizing the SVM's objective function $\frac{1}{2}\mathbf{w}'\mathbf{w} \, + \, C \, \Sigma_{i=1}^n \, \ell(\mathbf{w} \mid \mathbf{x}_i, y_i)$, where ℓ is the hinge loss for each training example $(\mathbf{x}_i, y_i)$.

Final Model Selection: Use the validation set to select the best the classifier corresponding to the best value, C_{best}. Report the accuracy on the **test set** for this selected best SVM model. *Note: You should report a single number, your final test set accuracy on the model corresponding to $C*{best}$_.

In [20]:
```
# Learn support vector classifiers with a radial-basis function kernel with
# fixed gamma = 1 / (n_features * X.std()) and different values of C
C_range = np.arange(-3.0, 6.0, 1.0)
C_values = np.power(10.0, C_range)
C_models = dict()
C_trnErr = dict()
C_valErr = dict()
C_tstErr = dict()
#import sklearn
import numpy as np
import matplotlib.pyplot as plt
from sklearn.svm import SVC
from sklearn import svm
from sklearn.metrics import hinge_loss
for C in C_values:
  C_models[C]=SVC(C,gamma='scale')
  C_models[C].fit(X_trn,y_trn)
  #w=models[C].get_params()
  C_trnErr[C]=hinge_loss(y_trn,C_models[C].decision_function(X_trn))
  C_valErr[C]=hinge_loss(y_val,C_models[C].decision_function(X_val))

  #hinge_trn = (np.ones(len(y_trn)) - np.multiply(y_trn,models[C].decision_funct
ion(X_trn)))
  #te = [max(0,h) for h in hinge_trn]
  #trnErr[C] = sum(te)
  #hinge_val = (np.ones(len(y_val)) - np.multiply(y_val,models[C].decision_funct
ion(X_val)))
  #ve = [max(0,h) for h in hinge_val]
  #valErr[C] = sum(ve)

#print(C_trnErr)
#print(C_valErr)

visualize(C_models, 'C', X_trn, y_trn)
plt.figure()
plt.semilogx(C_trnErr.keys(), C_trnErr.values(), marker='s', linewidth=3, marker
size=12)
plt.semilogx(C_valErr.keys(), C_valErr.values(), marker='o', linewidth=3, marker
size=12)
plt.xlabel('C -penalty parameter', fontsize=16)
plt.ylabel('Errors', fontsize=16)
plt.xticks(list(C_valErr.keys()), fontsize=12)
plt.legend([ 'Train Error','Validation Error'], fontsize=16)

# Insert your code here to perform model selection
C_minvalerr = min(C_valErr.values())
for C in C_values:
    if C_valErr[C]== C_minvalerr:
        C_best = C
print('Based on least validation error, the best value of C would be',C_best,' w
ith error',C_minvalerr,'and the corresponding model has accuracy',100*C_models[C
].score(X_tst,y_tst),'%')
```

```
Based on least validation error, the best value of C would be 1000.0  with err
or 0.1720885325527015 and the corresponding model has accuracy 65.0 %
```





b. (25 points) The effect of the RBF kernel parameter, γ

Complete the Python code snippet below that takes the generated synthetic 2-d data as input and learns various non-linear SVMs. Use scikit-learn's SVC (https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html) function to learn SVM models with **radial-basis kernels** for fixed C and various choices of $\gamma \in \{10^{-2}, 10^{-1}\, 1, 10,\ 10^2\ 10^3\}$. The value of C is fixed to $C = 10$.

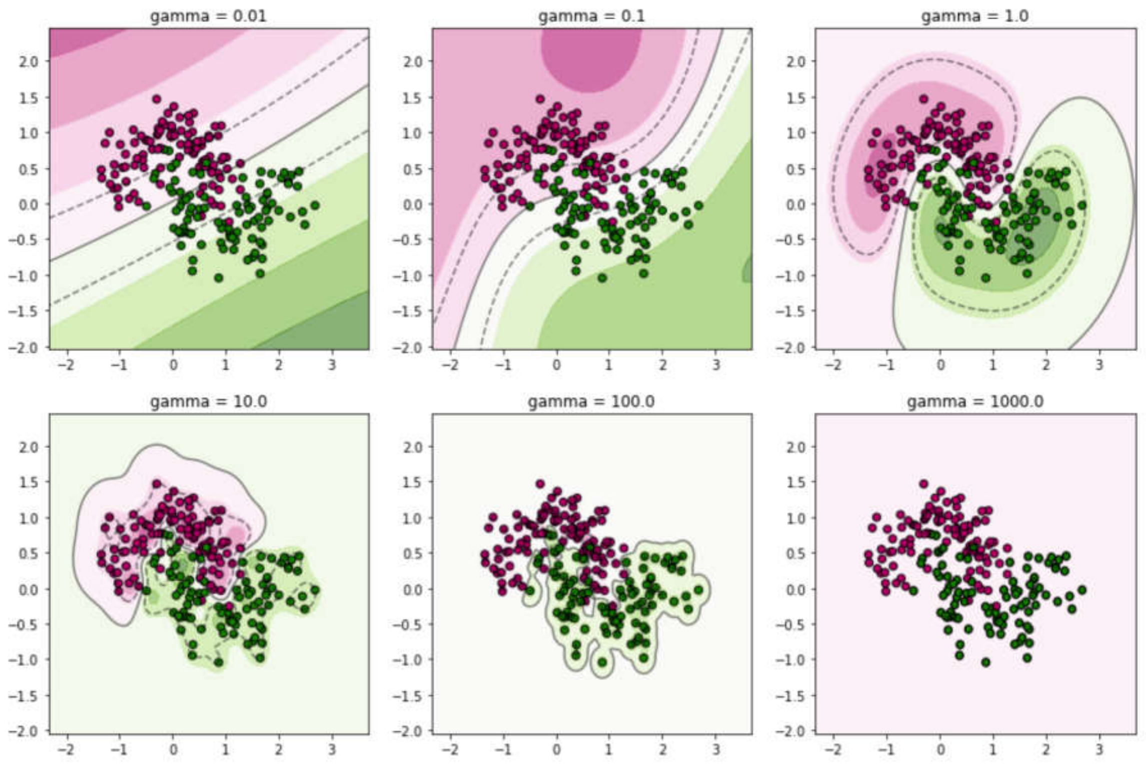
Plot: For each classifier, compute **both** the **training error** and the **validation error**. Plot them together, making sure to label the axes and each curve clearly.

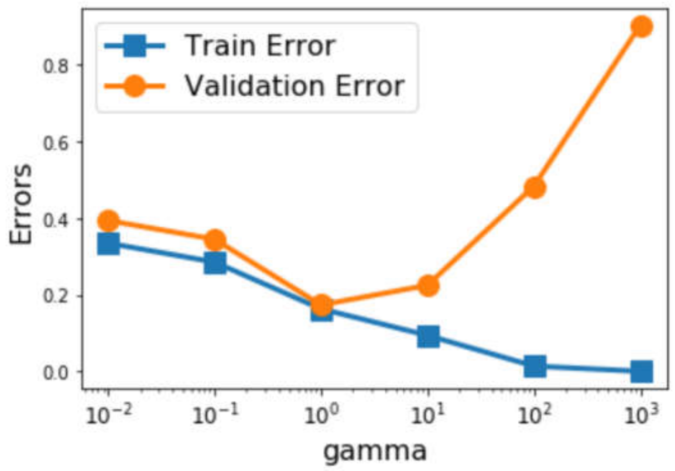
Discussion: How do the training error and the validation error change with γ? Based on the visualization of the models and their resulting classifiers, how does changing γ change the models? Explain in terms of the functional form of the RBF kernel, $\kappa(\mathbf{x},\, \mathbf{z}) \,=\, \exp(-\gamma \cdot \|\mathbf{x} - \mathbf{z}\|^2)$

Final Model Selection: Use the validation set to select the best the classifier corresponding to the best value, γ_{best}. Report the accuracy on the **test set** for this selected best SVM model. *Note: You should report a single number, your final test set accuracy on the model corresponding to $\gamma*{best}$_.

In [21]:
```
# Learn support vector classifiers with a radial-basis function kernel with
# fixed C = 10.0 and different values of gamma
gamma_range = np.arange(-2.0, 4.0, 1.0)
gamma_values = np.power(10.0, gamma_range)

G_models = dict()
G_trnErr = dict()
G_valErr = dict()
import numpy as np
import matplotlib.pyplot as plt
from sklearn.svm import SVC

for G in gamma_values:
    G_models[G]=SVC(C=10,gamma=G)
    G_models[G].fit(X_trn,y_trn)
    G_trnErr[G]=hinge_loss(y_trn,G_models[G].decision_function(X_trn))
    G_valErr[G]=hinge_loss(y_val,G_models[G].decision_function(X_val))

    #w=models[G].get_params()
    #hinge_trn = (np.ones(len(y_trn)) - np.multiply(y_trn,models[G].decision_fun
ction(X_trn)))
    #te = [max(0,h) for h in hinge_trn]
    #trnErr[G] = sum(te)
    #hinge_val = (np.ones(len(y_val)) - np.multiply(y_val,models[G].decision_fun
ction(X_val)))
    #ve = [max(0,h) for h in hinge_val]
    #valErr[G] = sum(ve)

visualize(G_models, 'gamma', X_trn, y_trn)
#print(trnErr)
#print(valErr)

plt.figure()
plt.semilogx(G_trnErr.keys(), G_trnErr.values(), marker='s', linewidth=3, marker
size=12)
plt.semilogx(G_valErr.keys(), G_valErr.values(), marker='o', linewidth=3, marker
size=12)
plt.xlabel('gamma', fontsize=16)
plt.ylabel('Errors', fontsize=16)
plt.xticks(list(G_valErr.keys()), fontsize=12)
plt.legend([ 'Train Error','Validation Error'], fontsize=16)

# Insert your code here to perform model selection
G_minvalerr = min(G_valErr.values())
for G in gamma_values:
    if G_valErr[G]== G_minvalerr:
        gamma_best = G
print('Based on least validation error, the best value of gamma would be',gamma_
best,' with error',G_minvalerr,'and the corresponding model has accuracy',100*C_
models[G].score(X_tst,y_tst),'%')
```

```
Based on least validation error, the best value of gamma would be 1.0  with er
ror 0.17312453018008142 and the corresponding model has accuracy 66.6666666666
6666 %
```





2. **Breast Cancer Diagnosis with Support Vector Machines**, 25 points.

For this problem, we will use the Wisconsin Breast Cancer (https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic)) data set, which has already been pre-processed and partitioned into training, validation and test sets. Numpy's loadtxt (https://docs.scipy.org/doc/numpy-1.13.0/reference/generated/numpy.loadtxt.html) command can be used to load CSV files.

In [22]:
```
y_wbcd_trn=np.loadtxt(r"wdbc_trn.csv",delimiter=',')[:,0]
X_wbcd_trn=np.loadtxt(r"wdbc_trn.csv",delimiter=',')[:,1:]
y_wbcd_val=np.loadtxt(r"wdbc_val.csv",delimiter=',')[:,0]
X_wbcd_val=np.loadtxt(r"wdbc_val.csv",delimiter=',')[:,1:]
y_wbcd_tst=np.loadtxt(r"wdbc_tst.csv",delimiter=',')[:,0]
X_wbcd_tst=np.loadtxt(r"wdbc_tst.csv",delimiter=',')[:,1:]
```

Use scikit-learn's SVC (https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html) function to learn SVM models with **radial-basis kernels** for **each combination** of $C \in \{10^{-2}, 10^{-1}, 1, 10^{1}, \cdots 10^{4}\}$ and $\gamma \in \{10^{-3}, 10^{-2}\ 10^{-1}, 1,\ 10,\ 10^{2}\}$. Print the tables corresponding to the training and validation errors.

Final Model Selection: Use the validation set to select the best the classifier corresponding to the best parameter values, C_{best} and γ_{best}. Report the accuracy on the **test set** for this selected best SVM model. *Note: You should report a single number, your final test set accuracy on the model corresponding to $C*{best}$and$\gamma*{best}$$.

In [23]:
```
gamma_range = np.arange(-3.0, 3.0, 1.0)
gamma_values = np.power(10.0, gamma_range)
C_range = np.arange(-2.0, 5.0, 1.0)
C_values = np.power(10.0, C_range)

BC_models = dict()
BC_trnErr = dict()
BC_valErr = dict()
BC_minvalerr = dict()
import numpy as np
import matplotlib.pyplot as plt

from sklearn.svm import SVC

for G in gamma_values:
    for C in C_values:
        BC_models[(G,C)]=SVC(C=C,gamma=G)
        BC_models[(G,C)].fit(X_wbcd_trn,y_wbcd_trn)
        BC_trnErr[(G,C)]=hinge_loss(y_wbcd_trn,BC_models[(G,C)].decision_functio
n(X_wbcd_trn))
        BC_valErr[(G,C)]=hinge_loss(y_wbcd_val,BC_models[(G,C)].decision_functio
n(X_wbcd_val))

BC_minvalerr = min(BC_valErr.values())
for G in gamma_values:
    for C in C_values:
        print('\n','gamma-C =',(G,C),'\n','training error',BC_trnErr[(G,C)],'\n'
,'validation error',BC_valErr[(G,C)],'\n','accuracy',BC_models[(G,C)].score(X_wb
cd_tst,y_wbcd_tst),'\n')

# Insert your code here to perform model selection

for G in gamma_values:
    for C in C_values:
        if BC_valErr[(G,C)] == BC_minvalerr:
            best_pair = (G,C)
print('Based on least validation error the best gamma-C pair is ',best_pair,'wit
h validation error',BC_minvalerr,'and the corresponding accuracy is',100*BC_mode
ls[best_pair].score(X_wbcd_tst,y_wbcd_tst),'%')
```

```
gamma-C = (0.001, 0.01)
training error 0.7208184768103563
validation error 0.7256813479326054
accuracy 0.6260869565217392


gamma-C = (0.001, 0.1)
training error 0.5179192813778993
validation error 0.5263786967173579
accuracy 0.7217391304347827


gamma-C = (0.001, 1.0)
training error 0.19672329762276422
validation error 0.2319876477038771
accuracy 0.9391304347826087


gamma-C = (0.001, 10.0)
training error 0.09701456859151125
validation error 0.13388256372479423
accuracy 0.9565217391304348


gamma-C = (0.001, 100.0)
training error 0.039733445101810476
validation error 0.08999117182651394
accuracy 0.9826086956521739


gamma-C = (0.001, 1000.0)
training error 0.017331117265180534
validation error 0.09480186699532406
accuracy 0.9565217391304348


gamma-C = (0.001, 10000.0)
training error 8.947564670306962e-06
validation error 0.11207298877748234
accuracy 0.9391304347826087


gamma-C = (0.01, 0.01)
training error 0.6193448509258744
validation error 0.6289289720713183
accuracy 0.6260869565217392


gamma-C = (0.01, 0.1)
training error 0.22399080644054883
validation error 0.25933367549441083
accuracy 0.9565217391304348


gamma-C = (0.01, 1.0)
training error 0.09541062284939203
validation error 0.13633800940688717
accuracy 0.9652173913043478


gamma-C = (0.01, 10.0)
training error 0.0334452063038933
validation error 0.09246126318517811
accuracy 0.9826086956521739


gamma-C = (0.01, 100.0)
training error 0.009753332952597648
validation error 0.08178962641844872
```

3. **Breast Cancer Diagnosis with k-Nearest Neighbors**, 25 points.

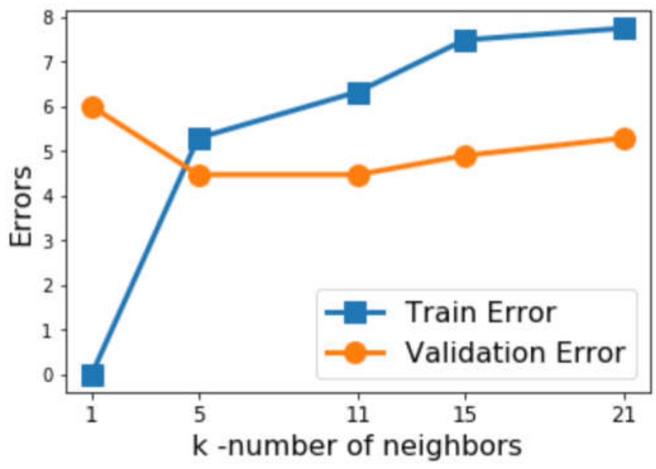
Use scikit-learn's k-nearest neighbor (https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html) classifier to learn models for Breast Cancer Diagnosis with $k \in \{1,\, 5,\, 11,\, 15,\, 21\}$, with the kd-tree algorithm.

Plot: For each classifier, compute **both** the **training error** and the **validation error**. Plot them together, making sure to label the axes and each curve clearly.

Final Model Selection: Use the validation set to select the best the classifier corresponding to the best parameter value, k_{best}. Report the accuracy on the **test set** for this selected best kNN model. *Note: You should report a single number, your final test set accuracy on the model corresponding to $k*{best}$_.

```
In [25]: knn_models=dict()
         knn_trnErr = dict()
         knn_valErr = dict()
         from scipy.spatial import distance
         import matplotlib.pyplot as plt
         from sklearn.neighbors import KNeighborsClassifier
         for k in (1,5,11,15,21):
             knn_models[k] = KNeighborsClassifier(n_neighbors=k,algorithm='kd_tree')
             knn_models[k].fit(X_wbcd_trn,y_wbcd_trn)
             knn_trnErr[k] = distance.euclidean(y_wbcd_trn,knn_models[k].predict(X_wbcd_t
         rn))
             knn_valErr[k] = distance.euclidean(y_wbcd_val,knn_models[k].predict(X_wbcd_v
         al))
         plt.figure()
         plt.plot(knn_trnErr.keys(), knn_trnErr.values(), marker='s', linewidth=3, marker
         size=12)
         plt.plot(knn_valErr.keys(), knn_valErr.values(), marker='o', linewidth=3, marker
         size=12)
         plt.xlabel('k -number of neighbors', fontsize=16)
         plt.ylabel('Errors', fontsize=16)
         plt.xticks(list(knn_valErr.keys()), fontsize=12)
         plt.legend([ 'Train Error','Validation Error'], fontsize=16)

         knn_minvalerr = min(knn_valErr.values())
         for k in (1,5,11,15,21):
             if knn_valErr[k]== knn_minvalerr:
                 k_best = k
         print('accuracy corresponding to the best value of k = (',k_best,'), is ',100*kn
         n_models[k].score(X_wbcd_tst,y_wbcd_tst),'%')
```

```
accuracy corresponding to the best value of k = ( 11 ), is  96.52173913043478
%
```



Discussion: Which of these two approaches, SVMs or kNN, would you prefer for this classification task? Explain.