# hwk4-skeleton-code

### March 7, 2019

```
In [3]: import numpy as np
    import matplotlib.pyplot as plt
    import sklearn
    import scipy.spatial
    import functools
    from scipy.spatial.distance import cdist
    import warnings
    warnings.filterwarnings('ignore')

%matplotlib inline
```

### 6.2 Kernels and Kernel Machines

#### 6.2.1

Write functions to compute the RBF and polynomial kernels.

```
In [2]: ### Kernel function generators
        def linear_kernel(X1, X2):
            Computes the linear kernel between two sets of vectors.
            Args:
                 X1 - an n1xd matrix with vectors x1_1, \ldots, x1_n1 in the rows
                 X2 - an n2xd matrix with vectors x2_1, \ldots, x2_n2 in the rows
            Returns:
                 matrix of size n1xn2, with x1_i^T x2_j in position i, j
            return np.dot(X1,np.transpose(X2))
        def RBF_kernel(X1,X2,sigma):
             11 11 11
             Computes the RBF kernel between two sets of vectors
                 X1 - an n1xd matrix with vectors x1_1, \ldots, x1_n1 in the rows
                 X2 - an n2xd matrix with vectors x2_1, \ldots, x2_n2 in the rows
                 sigma - the bandwidth (i.e. standard deviation) for the RBF/Gaussian kernel
            Returns:
                 matrix of size n1xn2, with exp(-|/x1_i-x2_j|/^2/(2 \text{ sigma}^2)) in position i, j
```

```
return np.exp(-cdist(X1,X2,'sqeuclidean')/(2*sigma**2))

def polynomial_kernel(X1, X2, offset, degree):
    """

Computes the inhomogeneous polynomial kernel between two sets of vectors
Args:
    X1 - an n1xd matrix with vectors x1_1,...,x1_n1 in the rows
    X2 - an n2xd matrix with vectors x2_1,...,x2_n2 in the rows
    offset, degree - two parameters for the kernel
Returns:
    matrix of size n1xn2, with (offset + <x1_i,x2_j>)^degree in position i,j
"""

return (offset + X1@X2.T)**degree
```

# 6.2.2

Use the linear kernel function defined in the code to compute the kernel matrix on the set of points  $x_0 \in \mathcal{D}_X = \{-4, -1, 0, 2\}$ . Include both the code and the output.

## 6.2.3.a

```
In [4]: # PLot kernel machine functions
    plot_step = .01
    xpts = np.arange(-6.0, 6, plot_step).reshape(-1,1)
    prototypes = np.array([-4,-1,0,2]).reshape(-1,1)

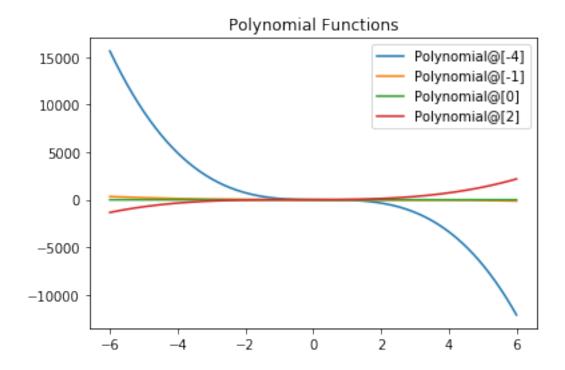
# Linear kernel
    y = linear_kernel(prototypes, xpts)
    for i in range(len(prototypes)):
        label = "Linear@"+str(prototypes[i,:])
        plt.plot(xpts, y[i,:], label=label)
    plt.legend(loc = 'best')
    plt.title('Linear Functions')
    plt.show()
```

# Linear Functions 20 10 0 -10Linear@[-4] Linear@[-1] Linear@[0] -20 Linear@[2] 2 -6 -4 -2 0 4 6

### 6.2.3.b

```
In [5]: # PLot kernel machine functions
    plot_step = .01
    xpts = np.arange(-6.0, 6, plot_step).reshape(-1,1)
    prototypes = np.array([-4,-1,0,2]).reshape(-1,1)

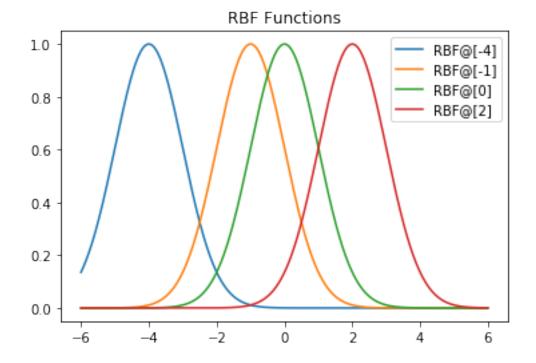
# Linear kernel
    y = polynomial_kernel(prototypes, xpts, 1,3)
    for i in range(len(prototypes)):
        label = "Polynomial@"+str(prototypes[i,:])
        plt.plot(xpts, y[i,:], label=label)
    plt.legend(loc = 'best')
    plt.title('Polynomial Functions')
    plt.show()
```



## 6.2.3.c

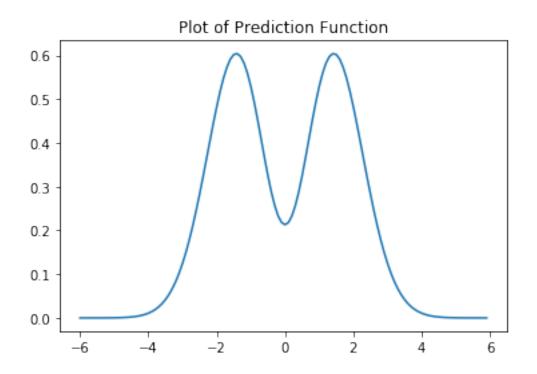
```
In [6]: # PLot kernel machine functions
    plot_step = .01
    xpts = np.arange(-6.0, 6, plot_step).reshape(-1,1)
    prototypes = np.array([-4,-1,0,2]).reshape(-1,1)

# Linear kernel
    y = RBF_kernel(prototypes, xpts, 1)
    for i in range(len(prototypes)):
        label = "RBF0"+str(prototypes[i,:])
        plt.plot(xpts, y[i,:], label=label)
    plt.legend(loc = 'best')
    plt.title('RBF Functions')
    plt.show()
```



#### 6.2.3.d

```
In [7]: class Kernel_Machine(object):
            def __init__(self, kernel, prototype_points, weights):
                Args:
                    kernel(X1, X2) - a function return the cross-kernel matrix between rows of X1
                    prototype_points - an Rxd matrix with rows mu_1,...,mu_R
                    weights - a vector of length R with entries w_1,...,w_R
                self.kernel = kernel
                self.prototype_points = prototype_points
                self.weights = weights
            def predict(self, X):
                Evaluates the kernel machine on the points given by the rows of X
                Args:
                    X - an nxd matrix with inputs x_1, \ldots, x_n in the rows
                Returns:
                    Vector of kernel machine evaluations on the n points in X. Specifically, jt
                        Sum_{i=1}^n w_i k(x_j, mu_i)
                11 11 11
                return self.kernel(X, self.prototype_points)@self.weights
In [8]: from functools import partial
        kernel = partial(RBF_kernel, sigma=1)
        x = np.array([[-1],[0],[1]])
        w = np.array([1,-1,1])
        model = Kernel_Machine(kernel=kernel, prototype_points=x, weights=w)
        x_pred = np.arange(-6.0, 6, 0.1).reshape(-1,1)
        y_pred = model.predict(x_pred)
        plt.plot(x_pred, y_pred)
        plt.title("Plot of Prediction Function")
        plt.show()
```

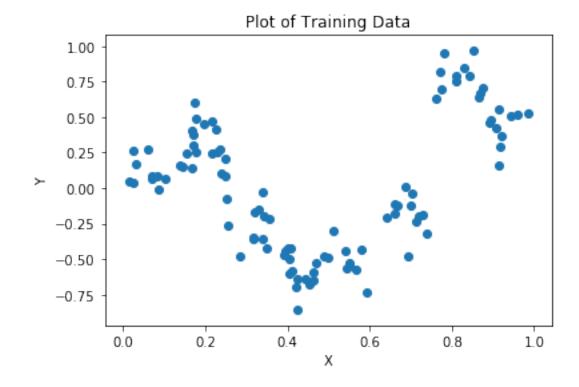


# 6.3 Kernel Ridge Regression

Load train & test data; Convert to column vectors so it generalizes well to data in higher dimensions.

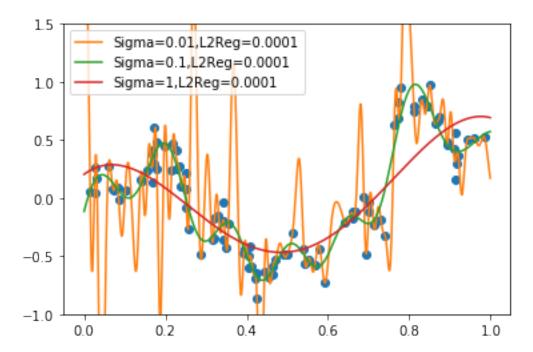
## 6.3.1

Plot the training data



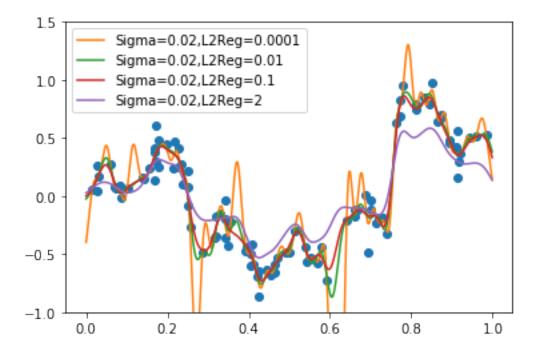
Complete the function train\_kernel\_ridge\_regression

Use the code provided to plot your fits to the training data for the RBF kernel with a fixed regularization parameter of 0.0001 for 3 different values of sigma: 0.01, 0.1, and 1.0. What values of sigma do you think would be more likely to over fit, and which less?



Lower values of  $\sigma$  are more prone to overfitting. With lower values of  $\sigma$ , the final prediction function is highly dependednt on local values of the training data.

Use the code provided to plot your fits to the training data for the RBF kernel with a fixed sigma of 0.02 and 4 different values of the regularization parameter  $\lambda$ : 0.0001, 0.01, 0.1, and 2.0. What happens to the prediction function as  $\lambda \to \infty$ ?



As  $\lambda \to \infty$ , the weights become smaller, eventually reaching 0. At this point the prediction function is just 0 for all x.

```
In [ ]: def sigmoid_kernel(X1, X2, eta, nu):
            return np.tanh(eta*X1@X2.T+nu)
In [30]: from sklearn.base import BaseEstimator, RegressorMixin, ClassifierMixin
         class KernelRidgeRegression(BaseEstimator, RegressorMixin):
             """sklearn wrapper for our kernel ridge regression"""
             def __init__(self, kernel="RBF", sigma=1, degree=2, offset=1, 12reg=1, eta=1, nu=1)
                 self.kernel = kernel
                 self.sigma = sigma
                 self.degree = degree
                 self.offset = offset
                 self.12reg = 12reg
                 self.eta = eta
                 self.nu = nu
             def fit(self, X, y=None):
                 This should fit classifier. All the "work" should be done here.
                 if (self.kernel == "linear"):
                     self.k = linear_kernel
                 elif (self.kernel == "RBF"):
                     self.k = functools.partial(RBF_kernel, sigma=self.sigma)
                 elif (self.kernel == "polynomial"):
                     self.k = functools.partial(polynomial_kernel, offset=self.offset, degree=se
                 elif self.kernel == 'sigmoid':
                     self.k = functools.partial(sigmoid_kernel, eta=self.eta, nu=self.nu)
                 else:
                     raise ValueError('Unrecognized kernel type requested.')
                 self.kernel_machine_ = train_kernel_ridge_regression(X, y, self.k, self.l2reg)
                 return self
             def predict(self, X, y=None):
                 try:
                     getattr(self, "kernel_machine_")
                 except AttributeError:
                     raise RuntimeError("You must train classifer before predicting data!")
                 return(self.kernel_machine_.predict(X))
             def score(self, X, y=None):
                 # get the average square error
                 return(((self.predict(X)-y)**2).mean())
In [6]: from sklearn.model_selection import GridSearchCV, PredefinedSplit
```

```
from sklearn.model_selection import ParameterGrid
        from sklearn.metrics import mean_squared_error,make_scorer
        import pandas as pd
        test_fold = [-1]*len(x_train) + [0]*len(x_test) #0 corresponds to test, -1 to train
        predefined_split = PredefinedSplit(test_fold=test_fold)
In [55]: param_grid = [{'kernel': ['RBF'], 'sigma':np.linspace(0.01,1,25), 'l2reg': np.logspace(1
                       {'kernel':['polynomial'],'offset':np.linspace(-5,5,25), 'degree':[2,3,4,5]
                       {'kernel':['linear'],'l2reg': np.linspace(0.1,10,50)}]
         kernel_ridge_regression_estimator = KernelRidgeRegression()
         grid = GridSearchCV(kernel_ridge_regression_estimator,
                             param_grid,
                             cv = predefined_split,
                             scoring = make_scorer(mean_squared_error,greater_is_better = False)
                              ,n_jobs = -1 #should allow parallelism, but crashes Python on my n
                              ,verbose=0
         _ = grid.fit(np.vstack((x_train,x_test)),np.vstack((y_train,y_test)))
In []: pd.set_option('display.max_rows', 20)
        df = pd.DataFrame(grid.cv_results_)
        # Flip sign of score back, because GridSearchCV likes to maximize,
         \textit{\# so it flips the sign of the score if "greater\_is\_better=FALSE" } \\
        df['mean_test_score'] = -df['mean_test_score']
        df['mean_train_score'] = -df['mean_train_score']
        cols_to_keep = ["param_degree", "param_kernel", "param_l2reg" , "param_offset", "param_sigm
                "mean_test_score","mean_train_score"]
        df_toshow = df[cols_to_keep].fillna('-')
        df_toshow = df_toshow.sort_values(by=["mean_test_score"])
```

Perform hyperparameter search and provide a summary of the results for each kernel

## **Best params for RBF**

```
In [57]: df_toshow[df_toshow.param_kernel=='RBF'].head()
            param_degree param_kernel param_l2reg param_offset param_sigma \
Out [57]:
         1
                                  RBF
                                          1.000023
                                                                    0.05125
         26
                                  RBF
                                          3.359892
                                                                    0.05125
         2
                                  RBF
                                          1.000023
                                                                     0.0925
         4
                                  RBF
                                          1.000023
                                                                      0.175
         3
                                  RBF
                                          1.000023
                                                                    0.13375
             mean_test_score mean_train_score
         1
                    0.015609
                                      0.018215
         26
                    0.025470
                                      0.031895
         2
                    0.026406
                                      0.029071
         4
                    0.028863
                                      0.040367
         3
                    0.028890
                                      0.034944
```

### **Best params for Polynomial Kernel**

```
In [58]: df_toshow[df_toshow.param_kernel=='polynomial'].head()
```

Out[58]:		param_degree	param_ke	rnel	param_	12reg	param_o	ffset	param_sigma	\
3	3042	6	polynomial polynomial polynomial polynomial		0.	05125	2.	08333	-	
3	3069	6			0.	09250	2.	91667	-	
3	8095	6			0.	13375	3.	33333	-	
3	3121	6			0.	17500		3.75	-	
3	8096	6	polynomial		0.	13375		3.75	-	
mean_test_score mean_train_score										
3	3042	0.032453			0.049113					
3	8069	0.032	0.032517		0.048018					
3	8095	0.032	2600		0.04869	9				

0.048877

0.046910

### **Best params for Linear**

3121

3096

```
In [59]: df_toshow[df_toshow.param_kernel=='linear'].head()
```

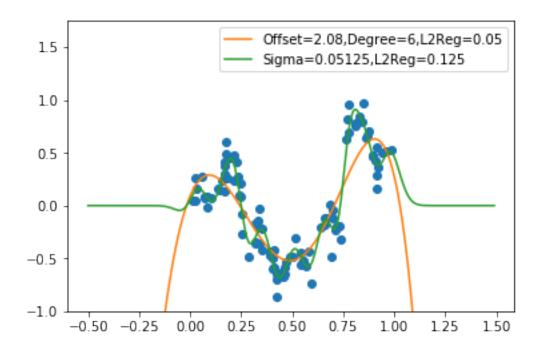
0.032672

0.032692

3646	-	linear	4.342857	-	-
	mean_test_score	mean train	n scoro		
	mean_test_score	mean_train	u_score		
3644	0.16451	0	.206561		
3643	0.16451	0	. 206556		
3645	0.16451	0	. 206567		
3642	0.16451	0	. 206551		
3646	0.16451	0	. 206572		

Plot the best fitting prediction functions using the polynomial and RBF kernels.

```
In [60]: ## Plot the best polynomial and RBF fits you found
        plot_step = .01
         xpts = np.arange(-.5 , 1.5, plot_step).reshape(-1,1)
         plt.plot(x_train,y_train,'o')
         #Plot best polynomial fit
         offset= 2.08
         degree = 6
         12reg = 0.05
         k = functools.partial(polynomial_kernel, offset=offset, degree=degree)
         f = train_kernel_ridge_regression(x_train, y_train, k, 12reg=12reg)
         label = "Offset="+str(offset)+", Degree="+str(degree)+", L2Reg="+str(12reg)
         plt.plot(xpts, f.predict(xpts), label=label)
         #Plot best RBF fit
         sigma = 0.05125
         12reg= 0.125000
         k = functools.partial(RBF_kernel, sigma=sigma)
         f = train_kernel_ridge_regression(x_train, y_train, k, 12reg=12reg)
         label = "Sigma="+str(sigma)+",L2Reg="+str(12reg)
         plt.plot(xpts, f.predict(xpts), label=label)
         plt.legend(loc = 'best')
         plt.ylim(-1, 1.75)
         plt.show()
```



The RBF kernel fits the data much better. Another thing to note is that outside the domain of x values that the model saw, it predicts approximately 0 while the polynomial kernel quickly goes to  $-\infty$  on both ends. This means that most likely, the RBF would perform better with predicting new data that fell outside the range of observed values.

The Bayes prediction function is

$$f^* = E(Y|X) = f(x)$$

The risk of this function is

$$R(f^*) = E[l(f^*(x), y)]$$

$$= E[(f^*(x) - f(x) - \epsilon)^2]$$

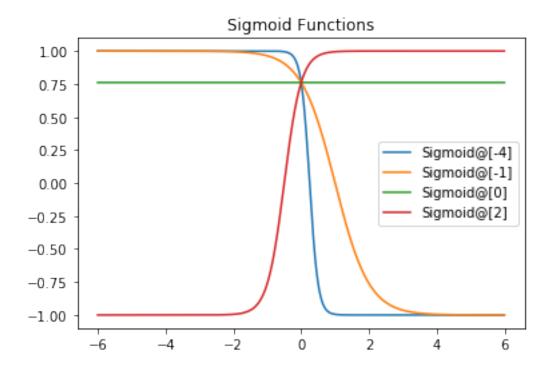
$$= E[(f(x) - f(x) - \epsilon)^2]$$

$$= E[\epsilon^2]$$

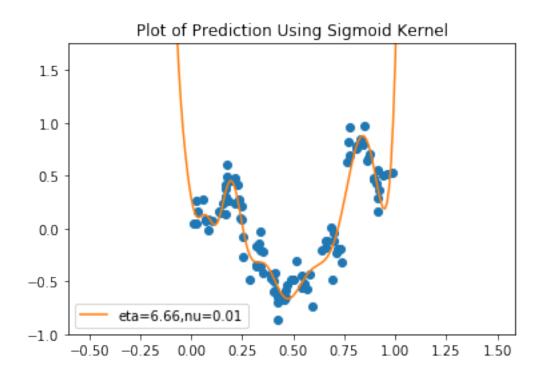
$$= Var(\epsilon)$$

$$= 0.1^2$$

Attempt to improve performance by using different kernel functions.



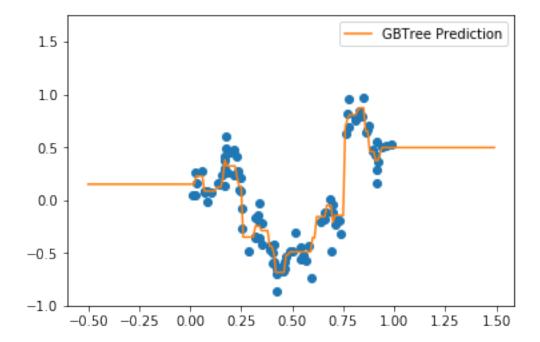
```
kernel_ridge_regression_estimator = KernelRidgeRegression()
         grid = GridSearchCV(kernel_ridge_regression_estimator,
                             param_grid,
                             cv = predefined_split,
                             scoring = make_scorer(mean_squared_error,
                                                   greater_is_better = False)
                             n_{jobs} = -1
                             ,verbose=0
         _ = grid.fit(np.vstack((x_train,x_test)),np.vstack((y_train,y_test)))
In [64]: df2 = pd.DataFrame(grid.cv_results_)
         # Flip sign of score back, because GridSearchCV likes to maximize,
         # so it flips the sign of the score if "greater_is_better=FALSE"
         df2['mean_test_score'] = -df2['mean_test_score']
         df2['mean_train_score'] = -df2['mean_train_score']
         cols_to_keep = ["param_eta", "param_nu", "mean_test_score",
                         "mean_train_score", "param_12reg"]
         df2 = df2[cols_to_keep]
         df2 = df2.sort_values(by=["mean_test_score"])
         df2.head()
Out [64]:
             param_eta
                         param_nu mean_test_score mean_train_score param_12reg
        900
                6.66667
                              0.01
                                          0.020141
                                                             0.025288
         901
                6.66667
                        0.016681
                                          0.020214
                                                             0.025650
                                                                            1e-07
               6.66667 0.0278256
                                          0.020612
                                                             0.026430
         902
                                                                            1e-07
         1354
                     10 0.0774264
                                          0.021767
                                                             0.025143
                                                                            1e-07
         1362
                     10 0.0278256
                                          0.021950
                                                             0.024905 1.3895e-07
In [65]: plot_step = .01
        xpts = np.arange(-.5 , 1.5, plot_step).reshape(-1,1)
        plt.plot(x_train,y_train,'o')
         #Plot best sigmoid fit
        eta = 6.66
        nu= 0.01
         12reg = 1e-7
        k = functools.partial(sigmoid_kernel, eta=eta, nu=nu)
        f = train_kernel_ridge_regression(x_train, y_train, k, 12reg=12reg)
         label = "eta="+str(eta)+",nu="+str(nu)
        plt.plot(xpts, f.predict(xpts), label=label)
        plt.legend(loc = 'best')
        plt.ylim(-1, 1.75)
        plt.title("Plot of Prediction Using Sigmoid Kernel")
        plt.show()
```



This didn't improve the test score over using RBF (RBF=0.015, Sigmoid=0.02). However it still fits the data very well.

Use any machine learning model to get the best performance you can.

```
In [7]: from sklearn.ensemble import GradientBoostingRegressor
        from sklearn.model_selection import RandomizedSearchCV
        from scipy.stats import randint
        from scipy.stats.distributions import uniform
        param_dist = {'learning_rate': uniform(0.01,1),
                      'n_estimators': randint(1,50),
                      'min_samples_leaf': randint(1,5),
                      'max_depth': randint(2,5)}
        grid = RandomizedSearchCV(GradientBoostingRegressor(),
                                    param_dist,
                                     cv = predefined_split,
                                     scoring = make_scorer(mean_squared_error,
                                                           greater_is_better = False)
                                     ,n_{jobs} = -1
                                     ,verbose=0
                                     , n_iter=500
        _ = grid.fit(np.vstack((x_train,x_test)),np.vstack((y_train,y_test)))
In [73]: pd.set_option('display.max_rows', 20)
         df2 = pd.DataFrame(grid.cv_results_)
         # Flip sign of score back, because GridSearchCV likes to maximize,
         # so it flips the sign of the score if "greater_is_better=FALSE"
         df2['mean_test_score'] = -df2['mean_test_score']
         df2['mean_train_score'] = -df2['mean_train_score']
         cols_to_keep = ["param_learning_rate", "param_n_estimators",
                         "param_min_samples_leaf", 'param_max_depth',
                         "mean_test_score", "mean_train_score"]
         df_toshow2 = df2[cols_to_keep].fillna('-')
         df_toshow2 = df_toshow2.sort_values(by=["mean_test_score"])
         df_toshow2.head()
Out [73]:
              param_learning_rate param_n_estimators param_min_samples_leaf
         99
                         0.270287
                                                    25
                                                                              3
         308
                         0.086171
                                                    43
                                                                              2
         355
                         0.211756
                                                    43
                                                                              1
         64
                                                    24
                                                                              2
                         0.218163
         9
                                                                              2
                         0.082174
                                                    30
              param_max_depth mean_test_score mean_train_score
         99
                            4
                                      0.394587
                                                         0.032204
         308
                            4
                                      0.395288
                                                         0.054924
         355
                            4
                                      0.395995
                                                         0.008076
         64
                            4
                                      0.407881
                                                         0.039017
                                      0.408592
         9
                                                         0.088934
```



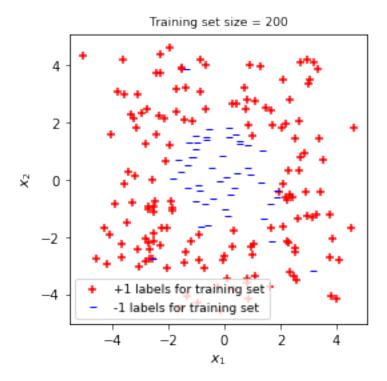
Usign gradient boosted trees resulted in an improved test score over RBF SVF. (RBF=0.15, GBT=0.013)

## 6.4 Kernalized Support Vector Machines with Kernalized Pegasos

#### 6.4.1

Load the SVM training and test data from the zip file. Plot the training data using the code supplied. Are the data linearly separable? Quadratically separable? What if we used some RBF kernel?

```
In [69]: # Load and plot the SVM data
         #load the training and test sets
         data_train,data_test = np.loadtxt("svm-train.txt"),np.loadtxt("svm-test.txt")
         x_train, y_train = data_train[:,0:2], data_train[:,2].reshape(-1,1)
         x_test, y_test = data_test[:,0:2], data_test[:,2].reshape(-1,1)
         #determine predictions for the training set
         yplus = np.ma.masked_where(y_train[:,0]<=0, y_train[:,0])</pre>
         xplus = x_train[~np.array(yplus.mask)]
         yminus = np.ma.masked_where(y_train[:,0]>0, y_train[:,0])
         xminus = x_train[~np.array(yminus.mask)]
         #plot the predictions for the training set
         figsize = plt.figaspect(1)
         f, (ax) = plt.subplots(1, 1, figsize=figsize)
         pluses = ax.scatter (xplus[:,0], xplus[:,1], marker='+', c='r',
                              label = '+1 labels for training set')
         minuses = ax.scatter (xminus[:,0], xminus[:,1], marker=r'$-$', c='b',
                               label = '-1 labels for training set')
         ax.set_ylabel(r"$x_2$", fontsize=11)
         ax.set_xlabel(r"$x_1$", fontsize=11)
         ax.set_title('Training set size = %s'% len(data_train), fontsize=9)
         ax.axis('tight')
         ax.legend(handles=[pluses, minuses], fontsize=9)
         plt.show()
```



The data is not linearly or quadratically seperable. However, an RBF kernel could separate it,

```
In [70]: # Code to help plot the decision regions
         # (Note: This ode isn't necessarily entirely appropriate for the questions asked. So the
         sigma=1
         k = functools.partial(RBF_kernel, sigma=sigma)
         f = train_soft_svm(x_train, y_train, k, ...)
         #determine the decision regions for the predictions
         x1_min = min(x_test[:,0])
         x1_{max} = max(x_{test}[:,0])
         x2_{min} = min(x_{test}[:,1])
         x2_max= max(x_test[:,1])
         h=0.1
         xx, yy = np.meshgrid(np.arange(x1_min, x1_max, h),
                              np.arange(x2_min, x2_max, h))
         Z = f.predict(np.c_[xx.ravel(), yy.ravel()])
         Z = Z.reshape(xx.shape)
         #determine the predictions for the test set
         y_bar = f.predict (x_test)
         yplus = np.ma.masked_where(y_bar<=0, y_bar)</pre>
         xplus = x_test[~np.array(yplus.mask)]
         yminus = np.ma.masked_where(y_bar>0, y_bar)
         xminus = x_test[~np.array(yminus.mask)]
         #plot the learned boundary and the predictions for the test set
         figsize = plt.figaspect(1)
         f, (ax) = plt.subplots(1, 1, figsize=figsize)
         decision =ax.contourf(xx, yy, Z, cmap=plt.cm.coolwarm, alpha=0.8)
         pluses = ax.scatter (xplus[:,0], xplus[:,1], marker='+', c='b',
                              label = '+1 prediction for test set')
         minuses = ax.scatter (xminus[:,0], xminus[:,1], marker=r'$-$', c='b',
                               label = '-1 prediction for test set')
         ax.set_ylabel(r"$x_2$", fontsize=11)
         ax.set_xlabel(r"$x_1$", fontsize=11)
         ax.set_title('SVM with RBF Kernel: training set size = %s'% len(data_train), fontsize=9
         ax.axis('tight')
         ax.legend(handles=[pluses, minuses], fontsize=9)
         plt.show()
        NameError
                                                   Traceback (most recent call last)
        <ipython-input-70-2d02ee1ae610> in <module>
          4 sigma=1
```

```
5 k = functools.partial(RBF_kernel, sigma=sigma)
----> 6 f = train_soft_svm(x_train, y_train, k, ...)
7
8 #determine the decision regions for the predictions
```

NameError: name 'train\_soft\_svm' is not defined