Machine Learning and Pattern Recognition (MLPR)

Assignment 2

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In [2]:
```
import math
import imp
from scipy import io
from sklearn.model_selection import KFold
import numpy as np
from matplotlib import pyplot as plt
import time

#or notebook
%matplotlib inline
```

In [3]:
```
import sys
mlprDir = '/home/student/Dropbox/MSc_Artificial_Intelligence/mlpr_Machine_L
earning_Pattern_Recognition/mlpr'
sys.path.append(mlprDir)
```

In [58]:
```
seed = 16011984
```

In [59]:
```
from sklearn.metrics import mean_squared_error
```

In [60]:
```
def getPredictions(X, w, biases):
    return X.dot(w) + biases
```

In [61]:
```
def getRMSE(trueTargets, predictions):
    mse = np.sum((trueTargets - predictions)**2)/len(trueTargets)
    #mse1 = mean_squared_error(trueTargets, predictions)
    #assert mse == mse1
    return math.sqrt(mse)
```

In [5]:
```
ctData = io.loadmat('ct_data.mat', squeeze_me=True) #“squeeze_me=True” so t
haty_train.shapeis(N,)ratherthan(N,1)
ctDataLen = len(ctData)
ctDataLen
```

Out[5]: 9

In [6]:
```
ctData.keys()
```

Out[6]:
```
['X_val',
 'X_train',
 'X_test',
 '__header__',
 '__globals__',
 'y_val',
 'y_train',
 '__version__',
 'y_test']
```

In [12]:
```
assert len(ctData['y_train'].shape) == 1, "the squeeze me = True above has
 failed"
```

In [13]:
```
def convertDictionaryToVariables(dictionary):
    """http://stackoverflow.com/questions/18090672/convert-dictionary-entri
es-into-variables-python"""
    for key,val in dictionary.items():
        exec(key + '=val')
```

In [14]:
```
convertDictionaryToVariables(ctData) # TODO: does not seem to work in pytho
n notebook
```

In [15]:
```
Xtrain, Xval, Xtest, yTrain, yVal, yTest = ctData['X_train'], ctData['X_va
l'], ctData['X_test'], \
    ctData['y_train'], ctData['y_val'], ctData['y_test']
```

In [16]:
```
ctData['__header__']
```

Out[16]:
```
'MATLAB 5.0 MAT-file, written by Octave 4.0.0, 2016-10-30 15:41:35 UTC'
```

In [17]:
```
ctData['__globals__']
```

Out[17]:
```
[]
```

In [18]:
```
ctData['__version__']
```

Out[18]:
```
'1.0'
```

In [19]:
```
Xtrain.shape, yTrain.shape
```

Out[19]:
```
((40754, 384), (40754,))
```

In [20]:
```
Xval.shape, yVal.shape
```

Out[20]:
```
((5785, 384), (5785,))
```

In [21]:
```
Xtest.shape, yTest.shape
```

Out[21]:
```
((6961, 384), (6961,))
```

In [22]:
```
someWhereInTheMiddleOfTraining = range(len(Xtrain)/2,len(Xtrain)/2 + 6)
```

In [23]:
```
Xtrain[someWhereInTheMiddleOfTraining]
```

Out[23]:
```
array([[ 0.      ,  0.      ,  0.      , ...,  0.      ,  0.      , -0.25
 ],
       [ 0.      ,  0.      ,  0.      , ...,  0.963103,  0.      , -0.25
 ],
       [ 0.      ,  0.      ,  0.      , ...,  0.975469,  0.      , -0.25
 ],
       [ 0.      ,  0.      ,  0.      , ...,  0.807768,  0.      , -0.25
 ],
       [ 0.      ,  0.      ,  0.      , ...,  0.      ,  0.      , -0.25
 ],
       [ 0.      ,  0.      ,  0.      , ...,  0.      ,  0.      , -0.25
 ]])
```

In [24]:
```
yTrain[someWhereInTheMiddleOfTraining]
```

Out[24]:
```
array([-0.39463686,  0.37122723,  0.37342168,  0.36903278,  0.33611602,
        0.35147717])
```

In [25]:
```
max(yTrain)
```

Out[25]:
```
2.2265180851800834
```

In [26]:
```
min(yTrain)
```

Out[26]:
```
-1.8679386519531087
```

1a

Verifying that the mean of the training positions in yTrain is zero

In [29]:
```
np.allclose(np.mean(yTrain), 0)
```

Out[29]:
```
True
```

The mean of the 5,785 positions in they_valarray is not zero.

In [30]:
```
yValMean = np.mean(yVal)
yValMean
```

Out[30]:
```
-0.21600850932415991
```

If we gathered a second dataset and computed its mean in the same way, we would get a different mean. For some datasets the mean will be bigger than the underlying true mean, sometimes it will be smaller.
Here we do not have a second dataset and thus we are stuck with that. But we can use the standard deviation to see how much the mean would vary.

In [31]:
```
def getMeanError(arr):
    return np.std(arr)/math.sqrt(len(arr))
```

In [32]:
```
validationMeanError = getMeanError(yVal)
print "The standard error of the validation mean is %f +/- %f" % (yValMean,
 validationMeanError)
```

```
The standard error of the validation mean is -0.216009 +/- 0.012903
```

In [33]:
```
firstPartOfTraining = yTrain[:len(yVal)]
```

In [34]:
```
firstPartOfTrainingMeanError = getMeanError(firstPartOfTraining)
print "The standard error of the first part of training mean is %f +/- %f"
%\
    (np.mean(firstPartOfTraining), firstPartOfTrainingMeanError)
```

```
The standard error of the first part of training mean is -0.442477 +/- 0.011
926
```

Why these standard error bars do not reliably indicate what the average of locations in future CT slice data will be?

Well intuitively the CT scan is a complex process and it involves the complexity of the human body. Here we have less than 60.000 instances in total which is a very small number in comparison with the population. Given that the person is totally still. Because if the person is slightly moving when the CT scan is being operating this will add noise to the data giving slight variations to the inputs thus changing the mean.

We need many more datasets to derive a better mean and have a better approximation of the standard error.

In addition we have taken into account the **assumption that the observations are independent** from each other which might not be the case.

1b

In [35]:
```
def checkIfArrayContainsIdenticalElements(arr):
    assert len(arr) >= 1, "do not call this function if array is empty"
    #reduce(lambda x,y : x if x == y else False, arr) == arr[0]
    return np.all(np.array(arr) == arr[0])
```

In [36]:
```
def identifyRedundantAttributes(dataset):
    """returns a binary mask suggesting the columns where all the instances
 have the same value
    thus contributing zero information"""
    return np.apply_along_axis(checkIfArrayContainsIdenticalElements,
axis=0, arr = dataset)
```

In [37]:
```
redundantAttrs = identifyRedundantAttributes(Xtrain)
redundantAttrs.shape
```

Out[37]:
```
(384,)
```

In [38]:
```
Xtrain.shape
```

Out[38]:
```
(40754, 384)
```

In [39]:
```
def removeRedundantAttrs(dataset, redundantAttributes):
    fixedDataset = np.delete(dataset, np.argwhere(redundantAttributes), axis=1)
    assert len(redundantAttributes[redundantAttributes==True]) == dataset.shape[1] - fixedDataset.shape[1],\
        "%d vs %d" % (len(redundantAttributes[redundantAttributes==True]), dataset.shape[1] - fixedDataset.shape[1])
    return fixedDataset
```

In [40]:
```
Xtr = removeRedundantAttrs(Xtrain, redundantAttrs)
Xtr.shape
```

Out[40]: (40754, 379)

In [41]:
```
Xvalid = removeRedundantAttrs(Xval, redundantAttrs)
Xvalid.shape
```

Out[41]: (5785, 379)

In [42]:
```
Xtesting = removeRedundantAttrs(Xtest, redundantAttrs)
Xtesting.shape
```

Out[42]: (6961, 379)

We have removed the following columns:

In [43]:
```
np.argwhere(redundantAttrs)
```

Out[43]:
```
array([[ 59],
       [ 69],
       [179],
       [189],
       [351]])
```

2

In [36]:
```
alpha = 10
```

In [37]:
```
# We use that only for verification
def closedFormSolutionForRidgeRegression(X, y, l2):
    """eye (I) matrix is modified to not penalize intercept"""
    lenX = len(X)
    H = np.hstack( (np.ones(lenX)[np.newaxis].T, X) )
    eye = np.eye(H.shape[1])
    eyeModified = eye
    eyeModified[0,0] = 0

    #return np.linalg.inv(H.T.dot(H) + l2 * eyeModified).dot(H.T).dot(y)
    #these two are equivalent but the
    return np.linalg.solve(H.T.dot(H) + l2 * eyeModified, H.T.dot(y))
```

In [38]:
```
myWeights = closedFormSolutionForRidgeRegression(Xtr, yTrain, alpha)
myWeights.shape
```

Out[38]: (380,)

In [39]:
```
def augmentTrainingDataWithOnesForBias(X):
    return np.hstack( (np.ones(len(X))[np.newaxis].T, X) )
```

In [40]:
```
H = augmentTrainingDataWithOnesForBias(Xtr)
H.shape
```

Out[40]: (40754, 380)

In [41]:
```
def addRowsForPseudoDataTrick(X, y, l2):
    """http://statweb.stanford.edu/~tibs/sta305files/Rudyregularization.pdf"""
    size = X.shape[1]
    eye = np.eye(size)
    eyeModified = eye
    eyeModified[0,0] = 0
    omega = math.sqrt(l2) * eyeModified
    return np.concatenate( (X, omega), axis=0), np.concatenate((y, np.zeros(size)))
```

In [42]:
```
def fit_linreg(X, yy, alpha):
    inputs, outputs = addRowsForPseudoDataTrick(augmentTrainingDataWithOnesForBias(X), yy, alpha)
    return np.linalg.lstsq(inputs, outputs)[0]
```

In [43]:
```
weights = fit_linreg(Xtr, yTrain, alpha)
```

In [44]:
```
assert np.allclose(myWeights, weights), "means that the two solutions are not identical"
```

In [45]:
```
from ct_support_code import fit_linreg_gradopt
```

In [46]:
```
gradoptFittedWeights, gradoptFittedBias = fit_linreg_gradopt(Xtr, yTrain, alpha)
```

In [47]:
```
gradoptFittedWeights.shape, gradoptFittedBias.shape
```

Out[47]: ((379,), ())

In [48]:
```
gradoptFittedWeightsAndBias = np.concatenate( (
np.array([gradoptFittedBias]), gradoptFittedWeights) )
gradoptFittedWeightsAndBias.shape
```

Out[48]: (380,)

In [49]:
```
np.allclose(gradoptFittedWeightsAndBias, weights)
```

Out[49]: False

In [50]:
```
print "let's print the bias and some weights to see where is the differenc
e, or how big it is"
np.hstack( (gradoptFittedWeightsAndBias[np.newaxis].T,
weights[np.newaxis].T) )[:20]
```

```
let's print the bias and some weights to see where is the difference, or how
 big it is
```

Out[50]:
```
array([[ 0.13824328,  0.13941109],
       [-0.05513268, -0.05512783],
       [-0.10870641, -0.1087216 ],
       [ 0.07951081,  0.07947379],
       [ 0.28194341,  0.28193662],
       [ 0.26014425,  0.26013513],
       [ 0.11940019,  0.11934693],
       [ 0.0142664 ,  0.0142611 ],
       [ 0.23497929,  0.23496813],
       [-0.32012978, -0.32012748],
       [-0.04879251, -0.04877961],
       [-0.04658537, -0.04658515],
       [ 0.05159682,  0.05160122],
       [-0.02323546, -0.02319087],
       [-0.00205468, -0.00202425],
       [-0.0096499 , -0.00962028],
       [ 0.03985583,  0.03987988],
       [ 0.02542174,  0.02538214],
       [ 0.01492785,  0.01503999],
       [-0.10848049, -0.10850978]])
```

In [51]:
```
np.allclose(gradoptFittedWeightsAndBias, weights, atol=1e-2)
```

Out[51]:
```
True
```

We see from the above two cells that the weights including the bias are very close, actually not so close to be considered identical but when we loosened the tolerance we found out that they are very close together as we can observe by eye looking at the values side by side.

This happens because as the algorithm tries to converge 1) maybe the learning rate is not the identical and 2) the threshold for convergence might not be so strict meaning that the provided solutions from the *fit_linreg_gradopt* are good enough for minimizing the error and thus the iterations stop without reaching the true global minimum point.

In addiction taking a look at the implemented code we see that the optimizer is set to iterate at maximum 500 times. This could also be a limitting factor to reach to the absolutely optimal solution.

Note that for the current problem and current dataset the closed form solution is much faster than the gradient descent approach

In [52]:
```
from ct_support_code import linreg_cost
```

In [53]:
```
def getParams(w):
    return w[1:], w[0]
```

In [54]:
```
trainingCostForClosedForm = linreg_cost(getParams(weights), Xtr, yTrain, al
pha)
trainingCostForClosedForm[0]
```

Out[54]:
```
5217.9279636734
```

In [55]:
```
validationCostForClosedForm = linreg_cost(getParams(weights), Xvalid, yVal,
 alpha)
validationCostForClosedForm[0]
```

Out[55]: 1083.2545883098387

The above are the RSS scores, we do not want that because they are not immune to scaling. We want the RMSE

In [59]:
```
trainingRMSEforClosedForm = getRMSE(trueTargets=yTrain, predictions=getPred
ictions(Xtr, weights[1:], weights[0]))
trainingRMSEforClosedForm
```

Out[59]: 0.35566175191574384

In [60]:
```
validationRMSEforClosedForm = getRMSE(trueTargets=yVal, predictions=getPred
ictions(Xvalid, weights[1:], weights[0]))
validationRMSEforClosedForm
```

Out[60]: 0.42000850675140733

Now we can compare the two errors directly and see that the error for training is indeed smaller that the error for the unseen validation data even though the regularization was used

In [61]:
```
w_s = gradoptFittedWeights
b_s = gradoptFittedBias
trainingRMSEforGradientDescent = getRMSE(trueTargets=yTrain, predictions=ge
tPredictions(Xtr,  w_s, b_s))
validationRMSEforGradientDescent = getRMSE(trueTargets=yVal, predictions=ge
tPredictions(Xvalid, w_s, b_s))

trainingRMSEforGradientDescent, validationRMSEforGradientDescent
```

Out[61]: (0.35566091528208404, 0.42000265085266136)

In [62]:
```
np.allclose(np.array([trainingRMSEforClosedForm, validationRMSEforClosedFor
m]),
            np.array([trainingRMSEforGradientDescent, validationRMSEforGradi
entDescent]), atol=1e-5)
```

Out[62]: True

The solution for the gradient descent is almost identical with a tolerance of 1e-5 tot the closed form solution as expected.

In general we are expecting the closed-form solution to always be the truly optimal solution for linear regression.

The closed form solution is not used in practice in many cases because the computation might be very slow in comparison to gradient descent. The more the dimensionality increasing the larger is this issue

3a

In [63]:
```
Xmu = np.mean(Xtr, axis=0)
Xmu.shape
```

Out[63]: (379,)

In [64]:
```
XtrainNorm = Xtr - Xmu
XtrainNorm.shape
```

Out[64]:
```
(40754, 379)
```

In [65]:
```
assert np.all(XtrainNorm[0] == Xtr[0] - Xmu),\
    "just an almost silly assertion to verify that the broadcasting of nump
y is working as expected"
```

In [66]:
```
XvalNorm = Xvalid - Xmu
XvalNorm.shape
```

Out[66]:
```
(5785, 379)
```

Let's first exploit sklearn to easily create a scree plot of the PCA to see really how much is the role of each Principal Component

In [67]:
```
import sklearn.decomposition as deco
```

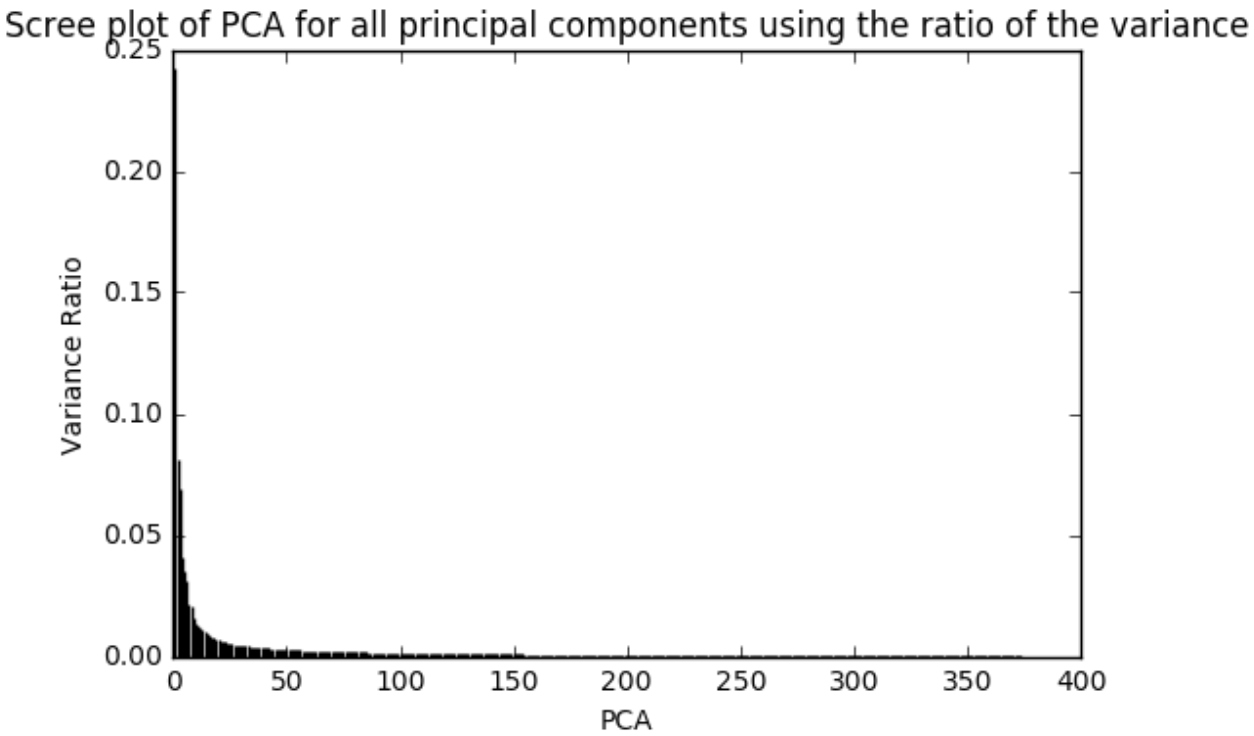
In [68]:
```
pca = deco.PCA(n_components=XtrainNorm.shape[1])
pca
```

Out[68]:
```
PCA(copy=True, iterated_power='auto', n_components=379, random_state=None,
  svd_solver='auto', tol=0.0, whiten=False)
```

In [69]:
```
pca.fit(XtrainNorm)
```

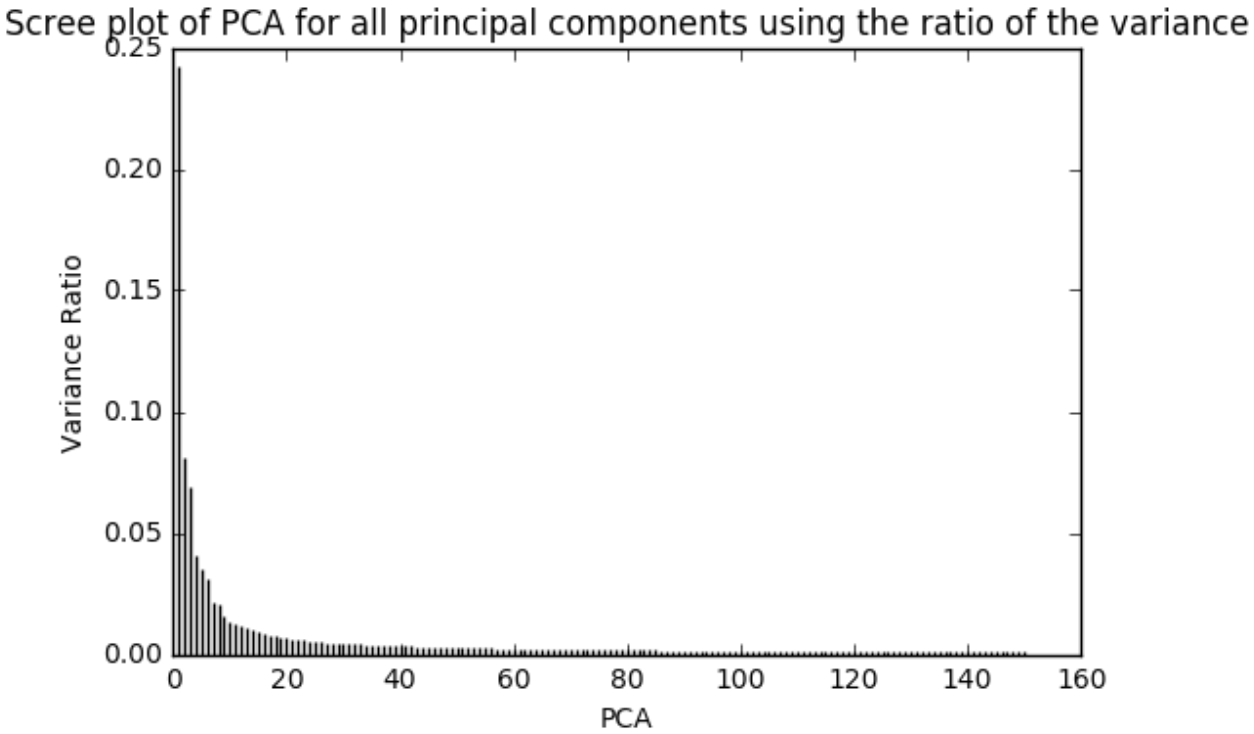
Out[69]:
```
PCA(copy=True, iterated_power='auto', n_components=379, random_state=None,
  svd_solver='auto', tol=0.0, whiten=False)
```

In [70]:
```
fig = plt.figure()
xsize =XtrainNorm.shape[1]
plt.bar( range(1,xsize+1), pca.explained_variance_ratio_, width =
1/(xsize/2) )
plt.title('Scree plot of PCA for all principal components using the ratio o
f the variance')
plt.xlabel('PCA')
plt.ylabel('Variance Ratio')
plt.show()
```



From this first plot it seems that after the 150th Principal Component there is little information. The variance is much less significant in comparison to the first Principal Components. Let's replot

In [71]:
```
fig = plt.figure()
xsize = 150
plt.bar( range(1,xsize+1), pca.explained_variance_ratio_[:xsize], width =
1/(xsize/2) )
plt.title('Scree plot of PCA for all principal components using the ratio o
f the variance')
plt.xlabel('PCA')
plt.ylabel('Variance Ratio')
plt.show()
```



In [72]:
```
from ct_support_code import pca_zm_proj
```

In [73]:
```
V = pca_zm_proj(XtrainNorm)
V.shape
```

Out[73]: (379, 379)

In [74]:
```
K=10
```

In [75]:
```
V = pca_zm_proj(XtrainNorm, K=K).real # we get back complex numbers, not su
re why
V.shape
```

Out[75]: (379, 10)

In [76]:
```
Xtrain10 = XtrainNorm.dot(V)
```

In [77]:
```
Xtrain10.shape
```

Out[77]: (40754, 10)

In [78]:
```
Xvalid10 = XvalNorm.dot(V)
Xvalid10.shape
```

Out[78]: (5785, 10)

In [79]:
```
weights = fit_linreg(Xtrain10, yTrain, alpha)
weights.shape
```

Out[79]: (11,)

In [80]:
```
print "Training Root Mean Square Error with PCA dimensionality reduction to
 K=%d" % K
trainingRMSEpca10 = getRMSE(trueTargets=yTrain,
predictions=getPredictions(Xtrain10, weights[1:], weights[0]))
trainingRMSEpca10
```

```
Training Root Mean Square Error with PCA dimensionality reduction to K=10
```

Out[80]: 0.5724151784607797

In [81]:
```
print "Validation Root Mean Square Error with PCA dimensionality reduction
 to K=%d" % K
validationRMSEpca10 = getRMSE(trueTargets=yVal,
predictions=getPredictions(Xvalid10, weights[1:], weights[0]))
validationRMSEpca10
```

```
Validation Root Mean Square Error with PCA dimensionality reduction to K=10
```

Out[81]: 0.5712708979178774

Both errors are smaller than when using all of the features. Meaning that now we are doing worse in terms of regression but effectively we have a faster system since the matrix multiplication are reduced a lot. So there is a tradeoff here.

We are noticing that the training error has increased in relation to the validation error.
This is happening because unlike before that the model was fitted to the peculiarities of the training data we now have new features, actually we have the best possible linear combinations of our features and we are not using all of them, but only few of them. Therefore it is more unlikely that we are going to overfit to our training data. More possible to underfit instead.

In [82]:
```
K=100
```

In [83]:
```
V = pca_zm_proj(XtrainNorm, K=K).real # we get back complex numbers, not su
re why
V.shape
```

Out[83]: (379, 100)

In [84]:
```
Xtrain100 = XtrainNorm.dot(V)
```

In [85]:
```
Xtrain100.shape
```

Out[85]: (40754, 100)

In [86]:
```
Xvalid100 = XvalNorm.dot(V)
Xvalid100.shape
```

Out[86]: (5785, 100)

In [87]:
```
weights = fit_linreg(Xtrain100, yTrain, alpha)
weights.shape
```

Out[87]: (101,)

In [88]:
```
print "Training Root Mean Square Error with PCA dimensionality reduction to
 K=%d" % K
trainingRMSEpca100 = getRMSE(trueTargets=yTrain,
predictions=getPredictions(Xtrain100, weights[1:], weights[0]))
trainingRMSEpca100
```

```
Training Root Mean Square Error with PCA dimensionality reduction to K=100
```

Out[88]:
```
0.4105637933749981
```

In [89]:
```
print "Validation Root Mean Square Error with PCA dimensionality reduction
 to K=%d" % K
validationRMSEpca100 = getRMSE(trueTargets=yVal,
predictions=getPredictions(Xvalid100, weights[1:], weights[0]))
validationRMSEpca100
```

```
Validation Root Mean Square Error with PCA dimensionality reduction to K=100
```

Out[89]:
```
0.4326955524607758
```

By increasing the number of principal components we are including more information in the model and we see that we have approached the RMSE of the original experiment but with much fewer attributes, only 100 in comparison to 379. Again our computations are going to be faster.

The RMSE of K=100 is smaller, better, than the RMSE for K=10 which is expected because we have included more information in the model. But as we are adding information we see that the training error is deviating from the validation error because these peculiarities of the training data start to re-appear. The gap is still much closer though.

Let's show this for all possible K values

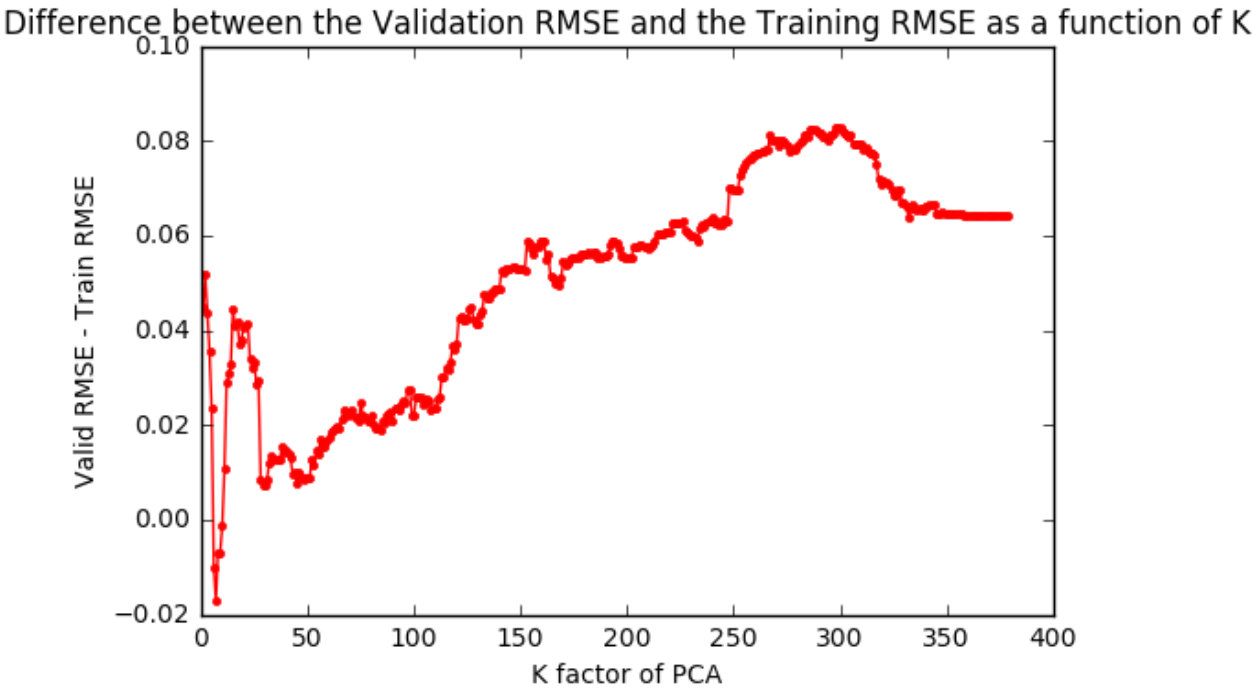
In [108]:
```
Ks = np.arange(1, Xtr.shape[1] + 1)
Ks
```

Out[108]:
```
array([  1,   2,   3,   4,   5,   6,   7,   8,   9,  10,  11,  12,  13,
        14,  15,  16,  17,  18,  19,  20,  21,  22,  23,  24,  25,  26,
        27,  28,  29,  30,  31,  32,  33,  34,  35,  36,  37,  38,  39,
        40,  41,  42,  43,  44,  45,  46,  47,  48,  49,  50,  51,  52,
        53,  54,  55,  56,  57,  58,  59,  60,  61,  62,  63,  64,  65,
        66,  67,  68,  69,  70,  71,  72,  73,  74,  75,  76,  77,  78,
        79,  80,  81,  82,  83,  84,  85,  86,  87,  88,  89,  90,  91,
        92,  93,  94,  95,  96,  97,  98,  99, 100, 101, 102, 103, 104,
       105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117,
       118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130,
       131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143,
       144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156,
       157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169,
       170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182,
       183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195,
       196, 197, 198, 199, 200, 201, 202, 203, 204, 205, 206, 207, 208,
       209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221,
       222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233, 234,
       235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246, 247,
       248, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259, 260,
       261, 262, 263, 264, 265, 266, 267, 268, 269, 270, 271, 272, 273,
       274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285, 286,
       287, 288, 289, 290, 291, 292, 293, 294, 295, 296, 297, 298, 299,
       300, 301, 302, 303, 304, 305, 306, 307, 308, 309, 310, 311, 312,
       313, 314, 315, 316, 317, 318, 319, 320, 321, 322, 323, 324, 325,
       326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 336, 337, 338,
       339, 340, 341, 342, 343, 344, 345, 346, 347, 348, 349, 350, 351,
       352, 353, 354, 355, 356, 357, 358, 359, 360, 361, 362, 363, 364,
       365, 366, 367, 368, 369, 370, 371, 372, 373, 374, 375, 376, 377,
       378, 379])
```

In [109]:
```
def fitAndTrainForPCA(trainNorm, valNorm, trainTargets, valTargets, K, alph
a):
    V = pca_zm_proj(trainNorm, K=K).real # we get back complex numbers, not
 sure why
    Xtrain = trainNorm.dot(V)
    Xvalid = valNorm.dot(V)
    weights = fit_linreg(Xtrain, yTrain, alpha)

    trainRMSE = getRMSE(trueTargets=trainTargets, predictions=getPrediction
s(Xtrain, weights[1:], weights[0]))

    validRMSE = getRMSE(trueTargets=valTargets,
predictions=getPredictions(Xvalid, weights[1:], weights[0]))

    return trainRMSE, validRMSE
```

In [112]:
```
trainRMSEs = np.zeros(len(Ks))
validRMSEs = np.zeros(len(Ks))

for i, K in enumerate(Ks):
    trainRMSE, validRMSE = fitAndTrainForPCA(trainNorm = XtrainNorm, valNor
m=XvalNorm,
                                             trainTargets= yTrain, valTarge
ts= yVal, K=K, alpha=alpha)

    trainRMSEs[i] = trainRMSE
    validRMSEs[i] = validRMSE
```

In [122]:
```
fig = plt.figure()
plt.hold(True)
#plt.plot(Ks, trainRMSEs, 'b.-')
#plt.plot(Ks, validRMSEs, 'g.-')
plt.plot(Ks, validRMSEs - trainRMSEs, 'r.-')
plt.hold(False)
plt.xlabel('K factor of PCA')
plt.ylabel('Valid RMSE - Train RMSE')
plt.title('Difference between the Validation RMSE and the Training RMSE as
 a function of K')
plt.show()
```



From the above plot we get what we expecting. At the beginning using only a few princinpal components we have lost lots of information, we have underfitted a lot and the way the model can perform on the validation and the training data is not easily predictable.

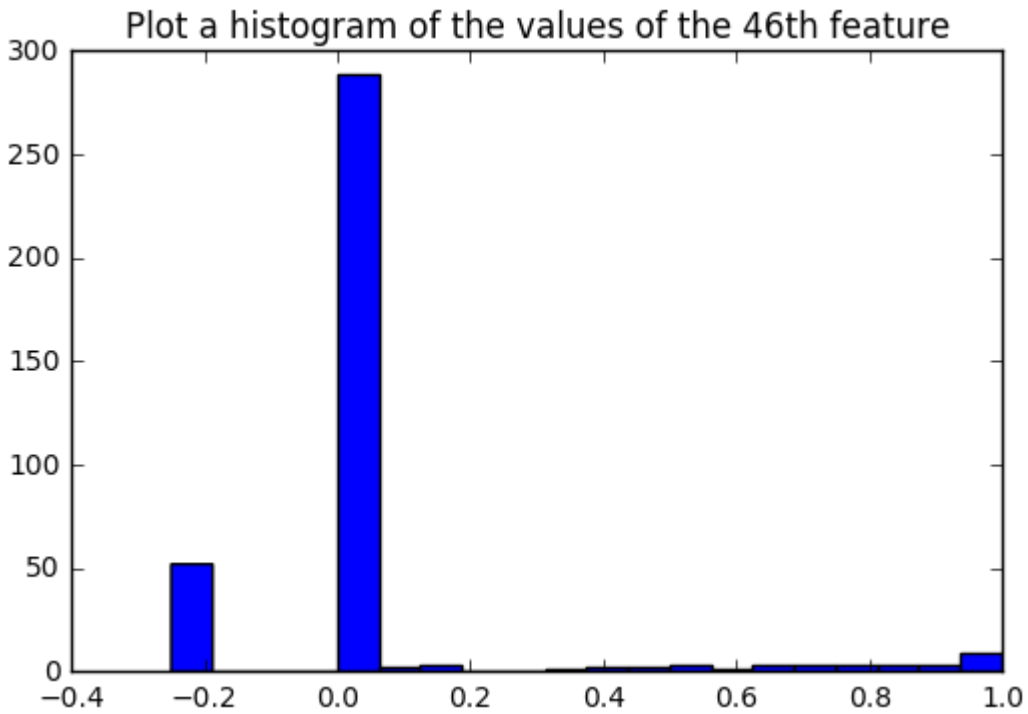
However when there are enough principal components and further the validation error has an increasingly larger difference from the training error because the model contains more complexity and can more easily fit the training data but it fails to work as well on the validation data.

This trend stops when we have included most of the principal components because these add little information to the model and thus the difference between the training RMSE and the validation RMSE remains constant

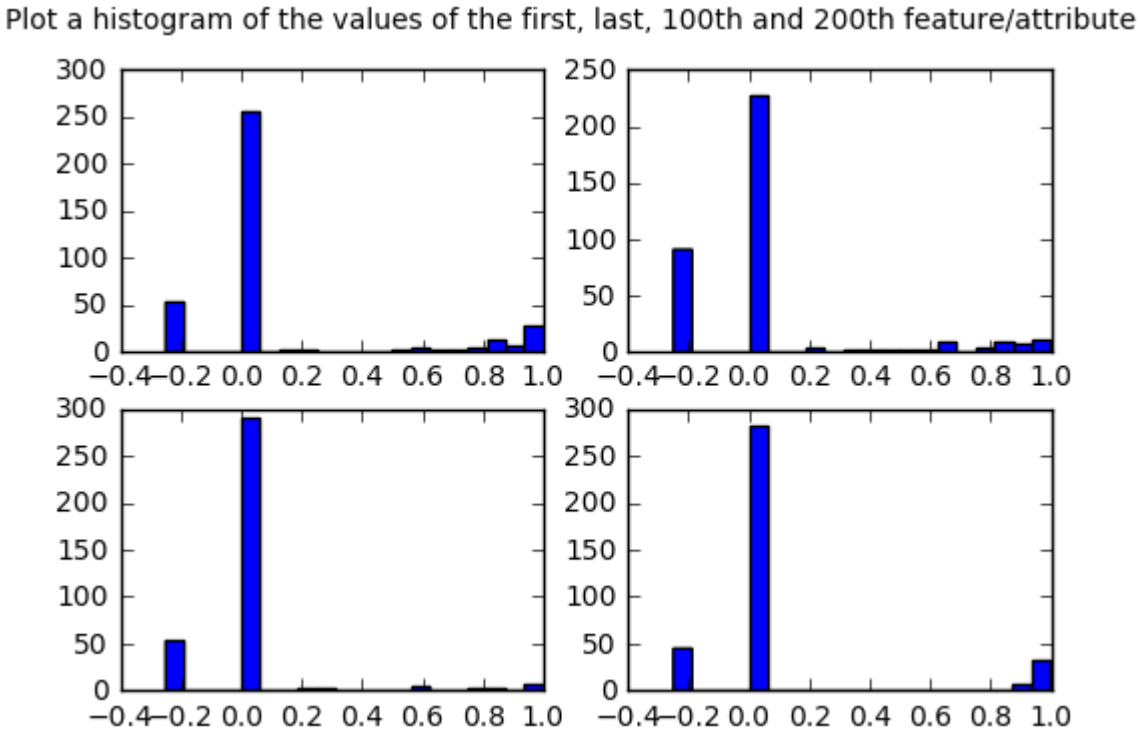
3b

In [90]:
```
#Plot a histogram of the values of the 46th feature (index 45 in python).
index = 45
plt.hist(Xtr[index],bins=20)
plt.title('Plot a histogram of the values of the 46th feature')
```

Out[90]: <matplotlib.text.Text at 0x7f4483f2d0d0>



In [98]:
```
fig, axes = plt.subplots(nrows=2, ncols=2)
plt.suptitle("Plot a histogram of the values of the first, last, 100th and
 200th feature/attribute")
ax0, ax1, ax2, ax3 = axes.flat
ax0.hist(Xtr[0],bins=20)
ax1.hist(Xtr[-1],bins=20)
ax2.hist(Xtr[100],bins=20)
ax3.hist(Xtr[200],bins=20)
print
```



By plotting these randomly selected plots and the plot with index 45, above, we notice that lots of features are near to zero and -0.25

In [113]:
```
totalElements = Xtr.shape[0] * Xtr.shape[1]
```

In [114]:
```
target = -0.25
```

In [115]:
```
count = len(Xtr[Xtr==target])
count
```

Out[115]:
```
2297040
```

In [116]:
```
print "The fraction of the values in training matrix that are equal to %f i
s %f" %\
    (target, float(count) / float(totalElements))
```

```
The fraction of the values in training matrix that are equal to -0.250000 is
 0.148716
```

In [117]:
```
target = 0
```

In [118]:
```
count = len(Xtr[Xtr==target])
count
```

Out[118]:
```
10163563
```

In [119]:
```
print "The fraction of the values in training matrix that are equal to %d i
s %f" %\
    (target, float(count) / float(totalElements))
```

```
The fraction of the values in training matrix that are equal to 0 is 0.65801
6
```

In [120]:
```
aug_fn = lambda X : np.hstack([X, X==0, X<0])
```

In [121]:
```
Xtr_augmented = aug_fn(Xtr)
```

In [122]:
```
Xtr_augmented.shape
```

Out[122]:
```
(40754, 1137)
```

In [123]:
```
weights = fit_linreg(Xtr_augmented, yTrain, alpha)
weights.shape
```

Out[123]:
```
(1138,)
```

In [124]:
```
trainingRMSEbinaryAugmentation = getRMSE(trueTargets=yTrain, predictions=ge
tPredictions(Xtr_augmented, weights[1:], weights[0]))
trainingRMSEbinaryAugmentation
```

Out[124]:
```
0.3178319185485654
```

In [125]:
```
Xvalid_binary_aug = aug_fn(Xvalid)
Xvalid_binary_aug.shape
```

Out[125]:
```
(5785, 1137)
```

In [126]:
```
testingRMSEbinaryAugmentation = getRMSE(trueTargets=yVal, predictions=getPr
edictions(Xvalid_binary_aug, weights[1:], weights[0]))
testingRMSEbinaryAugmentation
```

Out[126]:
```
0.3770058378403649
```

We notice that after applying the binary augmentation (which tripled the number of our attributes though) we managed to achieve a lower RMSE for both the training and validation error

The error goes down, thus the model improves, because all of those zeros present in the input array when multiplied by the weights they "kill" the weights and the model becomes inflexible.

One more reason is that the negative values seem like a special category which is treated like a number. By making it binary we treat it as we would treat binary categories in linear regression. We do the same thing with you the zero, treating it as a category.
In other words we did the same thing as if we had three categories for each attribute A, B and C and we wanted to encode them with one-hot-encoding. Where here the A is zero, B is our special negative value and C is anything else. Recall that in one hot encoding you throw away one of the three columns because it is redundant.

The above means there is not really a linear relationship between our data and our outputs/targets variables. Meaning that the non-linearities introduced by converting the matrix X to binary data with X==0 and X < 0 derived more useful representation.

3. extra step to see how the binary data behave on their own

In [106]:
```
aug_fn = lambda X : np.hstack([X==0, X<0])
```

In [100]:
```
Xtr_augmented = aug_fn(Xtr)
```

In [101]:
```
Xtr_augmented.shape
```

Out[101]: (40754, 758)

In [102]:
```
weights = fit_linreg(Xtr_augmented, yTrain, alpha)
weights.shape
```

Out[102]: (759,)

In [103]:
```
trainingRMSEbinaryAugmentation = getRMSE(trueTargets=yTrain, predictions=ge
tPredictions(Xtr_augmented, weights[1:], weights[0]))
trainingRMSEbinaryAugmentation
```

Out[103]: 0.36229540203307875

In [104]:
```
Xvalid_binary_aug = aug_fn(Xvalid)
Xvalid_binary_aug.shape
```

Out[104]: (5785, 758)

In [105]:
```
testingRMSEbinaryAugmentation = getRMSE(trueTargets=yVal, predictions=getPr
edictions(Xvalid_binary_aug, weights[1:], weights[0]))
testingRMSEbinaryAugmentation
```

Out[105]: 0.40197102810499635

From this extra experiment we realize when keeping the binary data alone we have lost some information and we have done worse by removing the original attributes. 0.40 error is larger than 0.37 from the previous experiment, speaking about the validation RMSE.

This is expected since we have removed information.

However it is interesting to note that even though the original matrix is missing the categorization of X==0 and X < 0 to binary values still works better than keeping only the original matrix. Recall that when used linear regression on the original X data (no augmentation or pca or other transformation) then the validation RMSE was 0.42 which is larger than 0.40.

4. Inverted Classification Tasks

In [104]:
```
from ct_support_code import minimize_list, logreg_cost
```

In [105]:
```
K = 10 # number of thresholded classification problems to fit
```

In [106]:
```
mx = np.max(yTrain)
mx
```

Out[106]: 2.2265180851800834

In [107]:
```
mn = np.min(yTrain)
mn
```

Out[107]:
```
-1.8679386519531087
```

In [108]:
```
hh = (mx-mn)/(K+1)
hh
```

Out[108]:
```
0.3722233397393811
```

In [109]:
```
thresholds = np.linspace(mn+hh, mx-hh, num=K, endpoint=True)
thresholds
```

Out[109]:
```
array([-1.49571531, -1.12349197, -0.75126863, -0.37904529, -0.00682195,
        0.36540139,  0.73762473,  1.10984807,  1.48207141,  1.85429475])
```

In [110]:
```
def fitLogisticRegression(X, yy, alpha):
    D = X.shape[1]
    args = (X, yy, alpha)
    init  = (np.zeros(D), np.array(0)) #initialize weights and biases to ze
ro and start from there
    #init  = (np.zeros(D), 0) #actually same thing
    ww, bb = minimize_list(logreg_cost, init, args)
    return ww, bb
```

In [111]:
```
paramsCollection = []
```

In [112]:
```
for kk in range(K):
    labels = yTrain > thresholds[kk]
    #labels (boolean) and labels*1 (which is ones and zeros) has the same b
ehavior in python
    params = fitLogisticRegression(Xtr, labels, alpha)
    paramsCollection.append(params)
```

In [113]:
```
def logisticRegression(X, w, b):
    X = np.hstack((np.ones((len(X), 1)),X))
    w = np.concatenate((np.array([b]), w))
    return 1 / (1 + np.exp(- X.dot(w)))
```

In [114]:
```
#just initialising with -1 to make sure that if we see a zero or an one it
 comes from the logistic regression and
#not because of our initialization
probsTrain = -np.ones((len(Xtr),K))
```

In [115]:
```
for i, params in enumerate(paramsCollection):
    probsTrain[:, i] = logisticRegression(X= Xtr, w=params[0], b=params[1])
```

In [116]:
```
probsTrain.shape
```

Out[116]:
```
(40754, 10)
```

In [117]:
```
probsTrain[:5, :]
```

Out[117]:
```
array([[  9.96793793e-01,   7.71478616e-02,   8.35548478e-04,
          3.34252213e-04,   8.82304343e-04,   3.81492646e-04,
          1.47085018e-04,   2.59552076e-05,   1.00197970e-06,
          2.85093492e-06],
       [  9.97196504e-01,   3.65736517e-02,   5.55120134e-04,
          6.93762470e-04,   3.12478303e-03,   4.50276758e-04,
          2.91632804e-04,   3.34887243e-05,   2.77678011e-06,
          4.55765983e-06],
       [  9.97595483e-01,   3.78427978e-02,   5.41703673e-04,
          9.14565893e-04,   3.81475234e-03,   4.28759522e-04,
          2.26465379e-04,   2.69257117e-05,   3.73049278e-06,
          4.58520602e-06],
       [  9.97866754e-01,   5.84546716e-02,   3.66980495e-04,
          5.90636557e-04,   8.42530012e-04,   1.88923319e-04,
          9.91816112e-05,   1.91489189e-05,   8.32376037e-06,
          3.82256053e-06],
       [  9.97709884e-01,   5.49115080e-02,   3.59104887e-04,
          4.97237521e-04,   9.58534312e-04,   1.97973117e-04,
          8.85213826e-05,   1.57358347e-05,   7.92454692e-06,
          3.47352856e-06]])
```

Now let's fit a regularized linear regression model (alpha = 10) to our transformed 10-dimensional training set

In [118]:
```
alpha = 10
alpha
```

Out[118]:
```
10
```

In [119]:
```
weights = fit_linreg(probsTrain, yTrain, alpha)
weights.shape
```

Out[119]:
```
(11,)
```

In [120]:
```
ww_5 = weights[1:].copy() #just storing the weights for question 5
bb_5 = weights[0].copy()
```

In [121]:
```
trainingRMSE = getRMSE(trueTargets=yTrain, predictions=getPredictions(probs
Train, weights[1:], weights[0]))
print "Training RMSE for our reduced by the classification via logistic reg
ression we used above is"
trainingRMSE
```

```
Training RMSE for our reduced by the classification via logistic regression
 we used above is
```

Out[121]:
```
0.13799833707562892
```

In [122]:
```
#just initialising with -1 to make sure that if we see a zero or an one it
 comes from the logistic regression and
#not because of our initialization
probsVal = -np.ones((len(Xvalid),K))
for i, params in enumerate(paramsCollection):
    probsVal[:, i] = logisticRegression(X=Xvalid, w=params[0], b=params[1])
```

In [123]:
```
testingRMSE = getRMSE(trueTargets=yVal,
predictions=getPredictions(probsVal, weights[1:], weights[0]))
print "Testing RMSE for our reduced by the classification via logistic regr
ession we used above is"
testingRMSE
```

```
Testing RMSE for our reduced by the classification via logistic regression w
e used above is
```

Out[123]:
```
0.25151779052868917
```

We see here that we have improved the model a lot by doing this simple 10 different classifications of the data. The RMSE of both training and validation sets have been improved. We tried to reduce the dimensionality with PCA. However the PCA can only do a (or I must say the best) linear combination of out features. It does that to give a projection of the data on the hyperplane which is parallel to where the variance of the data is maximum. But still we must consider that the best thing that it can do is do a linear combination of the features.
By doing logistic regression we have imposed some non-linearities which obviously were appropriate for the current data and the RMSE is lower than before.

5. Small Neural Network

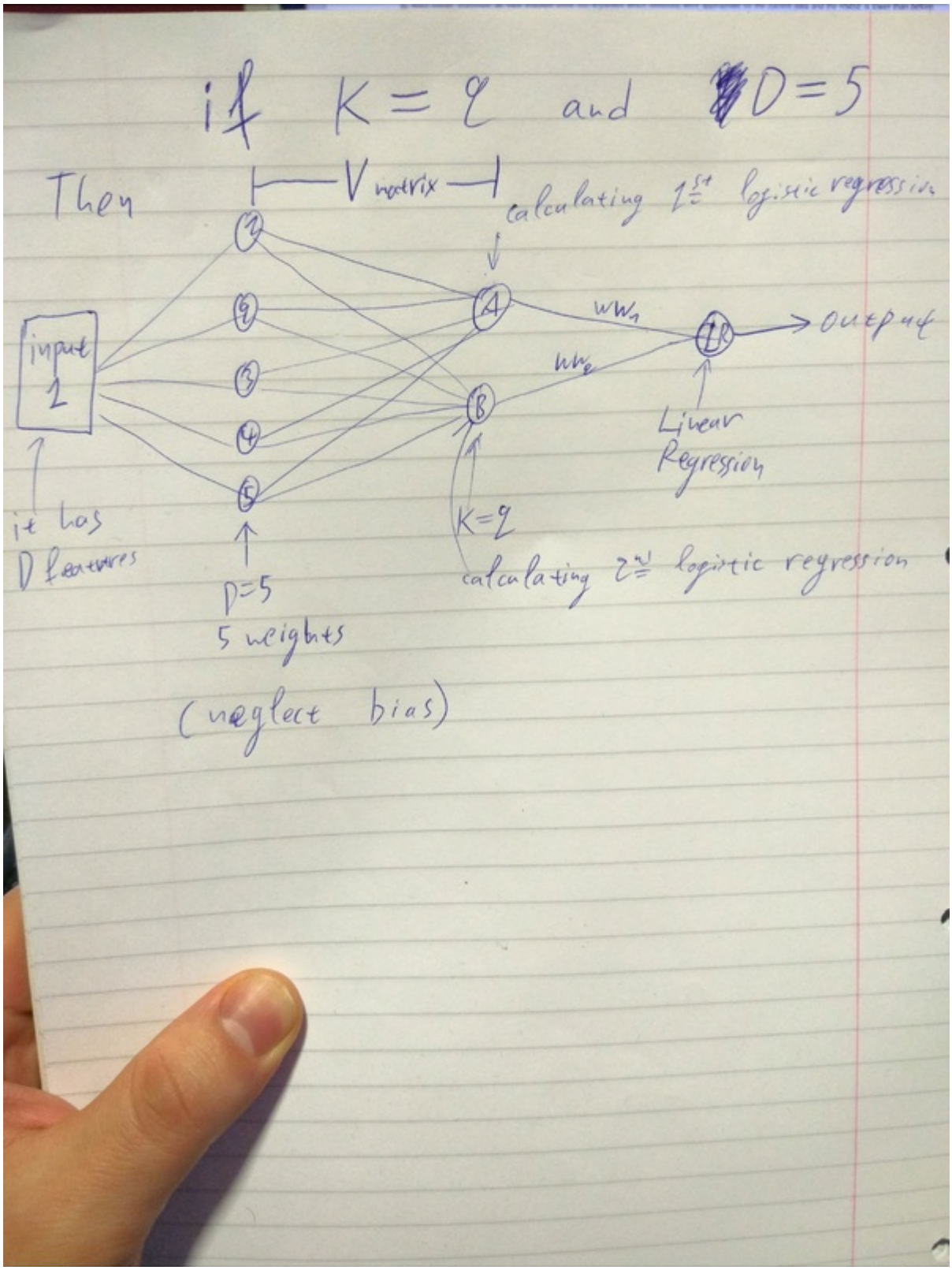
In [50]:
```
alpha = 10
```

In [51]:
```
rng = np.random.RandomState(seed=seed)
```

In [52]:
```
from ct_support_code import nn_cost, minimize_list
```

We understand here that we have not done full back propagation and therefore we have fitted the two layers of this model separately.

So here we are building a model with two layers or to be more explicit we build a model with a single layer neural network plus a linear regression layer



In [53]:
```
def getRandomParams(D, K, factor = 1e-1):
    """D dimensionality of inputs, K dimensionality of outputs"""
    factor = factor / math.sqrt(K) #to make it robust against the dimension
ality of our hidden layer
    ww = rng.randn(K) * factor
    bb = rng.randn(1) * factor
    V =  rng.randn(K, D) * factor
    bk = rng.randn(K)

    return (ww, bb, V, bk)
```

In [54]:
```
initialParams = getRandomParams(D=Xtr.shape[1], K=10)
for initialParam in initialParams:
    print initialParam.shape
```

```
(10,)
(1,)
(10, 379)
(10,)
```

In [55]:
```
fittedParams = minimize_list(nn_cost, initialParams, (Xtr, yTrain, alpha))
```

In [56]:
```
for fittedParam in fittedParams:
    print fittedParam.shape
```

```
(10,)
(1,)
(10, 379)
(10,)
```

In [62]:
```
rmse = getRMSE(trueTargets=yTrain,predictions=nn_cost(fittedParams, Xtr))
print "printing Root Mean Square Error for some random initial weights"
rmse
```

```
printing Root Mean Square Error for some random initial weights
```

Out[62]:
```
0.1007315344759879
```

5a

Let's try and initialize the model a few times with random parameters that derive from the standard normal distribution multiplied with different factors

In [63]:
```
factors = np.logspace(-2, 2, 5)
factors
```

Out[63]:
```
array([  1.00000000e-02,   1.00000000e-01,   1.00000000e+00,
         1.00000000e+01,   1.00000000e+02])
```

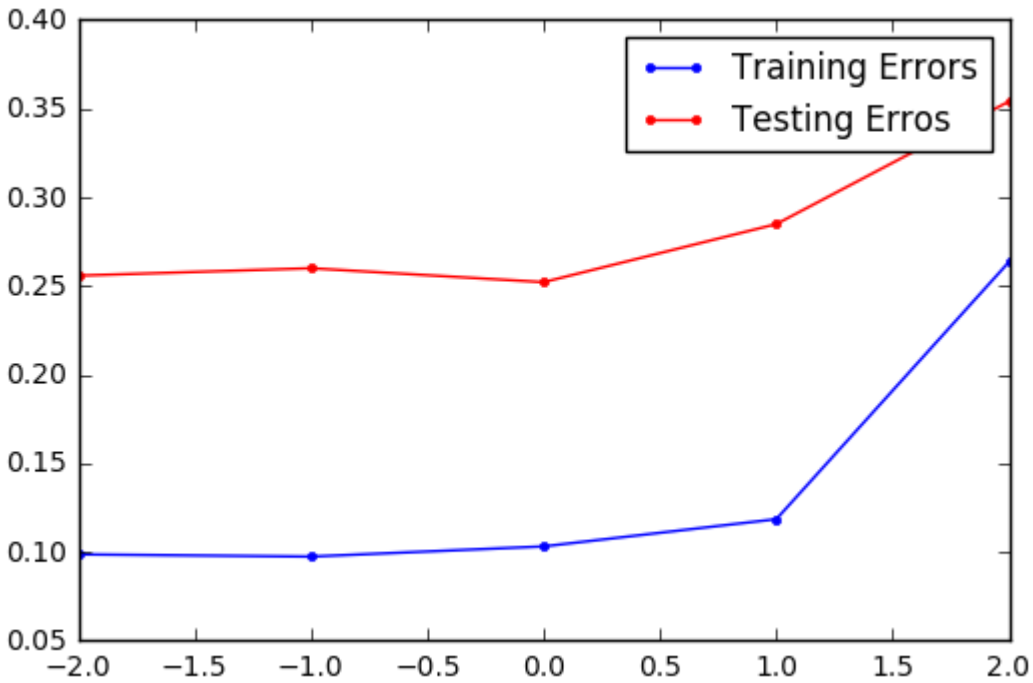
In [72]:
```
def fitAndScore(factor, K=10):
    fittedParams = minimize_list(nn_cost,
getRandomParams(D=Xtr.shape[1],K=K,factor=factor), (Xtr,yTrain,alpha))
    return (
        getRMSE(trueTargets=yTrain,predictions=nn_cost(fittedParams, Xtr)),
        getRMSE(trueTargets=yVal,predictions=nn_cost(fittedParams, Xvalid))
    )
```

In [65]:
```
scores = []

for factor in factors:
    scores.append(
        fitAndScore(factor)
    )
```

```
ct_support_code.py:201: RuntimeWarning: overflow encountered in exp
  P = 1 / (1 + np.exp(-A)) # N,K
```

In [66]:
```
trainErrors = [s[0] for s in scores]
testingErrors = [s[1] for s in scores]
```

In [67]:
```
fig = plt.figure()
plt.hold(True)
plt.plot(np.log10(factors), trainErrors, 'b.-')
plt.plot(np.log10(factors),testingErrors, 'r.-')
plt.hold(False)
plt.legend(['Training Errors', 'Testing Erros'])
plt.show()
```



From the plot above we see that the randomly initially weights give a non-high-variance RMSE ~0.1 for training and ~0.25 for validation but when the weights are very high the sigmoids of the neural network saturate and we get a very bad RMSE

Let's take the mean, max and min RMSE of both training and validation set for the above experiment excluding the value when the saturation occured

In [68]:
```
trainErrorsFixed = trainErrors[:-1]
```

In [69]:
```
minTrainRMSE, maxTrainRMSE, meanTrainRMSE = min(trainErrorsFixed), max(trai
nErrorsFixed), np.mean(trainErrorsFixed)
minTrainRMSE, maxTrainRMSE, meanTrainRMSE
```

Out[69]:
```
(0.097470394334065, 0.1185664570251758, 0.10449261805654335)
```

In [70]:
```
testingErrorsFixed = testingErrors[:-1]
```

In [71]:
```
minTestRMSE, maxTestRMSE, meanTestRMSE = min(testingErrorsFixed), max(testi
ngErrorsFixed), np.mean(testingErrorsFixed)
minTestRMSE, maxTestRMSE, meanTestRMSE
```

Out[71]:
```
(0.25218178203992786, 0.28493189766215743, 0.26324682846348935)
```

5b

Let's try and use the weights from the question 4 as the initial parameters and see if this training layer by layer is useful for initialization (paramsCollection)

In [142]:
```
len(paramsCollection) #TODO refactor params collection to make it into a ma
trix to have it ready for question 5
```

Out[142]: 10

In [143]:
```
bk = np.array([p[1] for p in paramsCollection]) #get biases from params col
lection
```

In [144]:
```
D = Xtr.shape[1]
```

In [145]:
```
V = np.zeros((K, D))
V.shape
```

Out[145]: (10, 379)

In [146]:
```
weightsFromParamsCollection = [p[0] for p in paramsCollection]
```

In [147]:
```
for i, w in enumerate(weightsFromParamsCollection):
    V[i, :] = w
```

In [148]:
```
V[:5,:10]
```

Out[148]:
```
array([[-0.1804373 ,  0.16753387,  0.0861282 , -0.05835337, -0.27254156,
         0.01045983,  0.09169777,  0.14772877,  0.1130179 ,  0.01292211],
       [ 0.23818631, -0.0037519 ,  0.08939135, -0.28249096,  0.46947222,
         0.2428821 , -0.20053769,  0.5639093 ,  0.19279334,  0.02279842],
       [-0.34090875, -0.01084626,  0.15612231,  0.53620278,  1.43310226,
         0.39290399, -0.01777887,  0.16203922, -0.77345654, -0.17547967],
       [-0.47333174, -0.64860932, -0.14091801,  1.33454083,  1.45991401,
         0.16763888,  0.25495831,  0.81614697, -0.70309945, -0.27338187],
       [-0.41188558, -0.61319485, -0.0988138 ,  1.30113018,  1.34673323,
         0.33154783, -0.46113265,  0.59379654, -0.94065742, -0.32934864]])
```

In [149]:
```
def getInitialNeuralNetworkState():
    return (ww_5.copy(), bb_5.copy(), V.copy(), bk.copy())
```

In [150]:
```
fittedParams = minimize_list(nn_cost, getInitialNeuralNetworkState(), (Xtr,
 yTrain, alpha))
train_question4_RMSE = getRMSE(trueTargets=yTrain, predictions=nn_cost(fitt
edParams, Xtr)),
testing_question4_RMSE = getRMSE(trueTargets=yVal, predictions=nn_cost(fitt
edParams, Xvalid))
```

In [151]:
```
train_question4_RMSE
```

Out[151]: (0.10026697346626232,)

In [152]:
```
testing_question4_RMSE
```

Out[152]: 0.2613245639516538

We followed a procedure for pretraining / initialization which is called Layer-by-Layer cross-entropy training. In our case it does not seem to yield any amazing results even though the training error is below the mean of the previous experiment and the testing error is slighly above the mean of the previous experiment.

We can only conclude that this methodology is not bad and is guaranteed some good results but not optimal.
We see that initialization with some random values we were able to find a better local (if not global) minima.

6. What's Next?

Here we are going to implement a larger neural network with ten times more neurons. Let's see if we have an improved performance with 100 neurons

```
In [153]: trainError, testError = fitAndScore(1e-3, K=100)

In [154]: trainError
Out[154]: 0.09935530492176238

In [155]: testError
Out[155]: 0.26360266742658284
```

With 100 neurons the system became much more computationally intensive. It took much longer to complete the process and the result was not an amazing one.

We notice that the training error has decreased a little bit but the testing error has not changed significantly than the previous experiments.

The increased number of neurons means that the system has more flexibility to derive more features because the logistic regressions to only K=10 might not be enough to capture the complexity of the data and thus some information is lost in this dimensionality reduction.

Extra idea

One more idea worth trying is to improve the performance by optimizing the regularization variable lambda (or alpha as we have called it in this assignment). We might also want to do a k-fold cross validation by combining the training and validation data and use as test the testing dataset.

Note that for this part of the answer we are using K=10 neurons

```
In [156]: Xtr.shape, Xvalid.shape, Xtesting.shape
Out[156]: ((40754, 379), (5785, 379), (6961, 379))

In [157]: yTrain.shape, yVal.shape, yTest.shape
Out[157]: ((40754,), (5785,), (6961,))
```

In [158]:
```
Xall = np.concatenate( (Xtr, Xvalid), axis=0 )
assert Xall.shape[0] == Xtr.shape[0] + Xvalid.shape[0] and Xall.shape[1] ==
 Xtr.shape[1]
Xall.shape
```

Out[158]:
```
(46539, 379)
```

In [159]:
```
yAll = np.concatenate( (yTrain, yVal), axis=0 )
assert yAll.shape[0] == yTrain.shape[0] + yVal.shape[0]
yAll.shape
```

Out[159]:
```
(46539,)
```

Let's do a 10-fold cross validation

In [160]:
```
k = 10
```

In [161]:
```
kFold = KFold(n_splits=k, shuffle=True, random_state=seed) #be aware this b
ehaves differently for different versions of scipy
```

In [162]:
```
print "let's print all the sizes of the different combinations of the k fol
d cross validation"
for a, b in kFold.split(Xall):
    print a.shape
    print b.shape
```

```
let's print all the sizes of the different combinations of the k fold cross
 validation
(41885,)
(4654,)
(41885,)
(4654,)
(41885,)
(4654,)
(41885,)
(4654,)
(41885,)
(4654,)
(41885,)
(4654,)
(41885,)
(4654,)
(41885,)
(4654,)
(41885,)
(4654,)
(41886,)
(4653,)
```

In [163]:
```
np.log10(alpha)
```

Out[163]:
```
1.0
```

In [164]:
```
numOfPossibleAlphas = 5
shift = (numOfPossibleAlphas-1)/2
shift
```

Out[164]:
```
2
```

In [165]:
```
alphas = np.logspace(np.log10(alpha) - shift, np.log10(alpha) + shift, num
= numOfPossibleAlphas)
print alphas.shape
alphas
```

```
(5,)
```

Out[165]:
```
array([  1.00000000e-01,   1.00000000e+00,   1.00000000e+01,
         1.00000000e+02,   1.00000000e+03])
```

In [166]:
```
print "This is the initial neural network state as computed from the previo
us exercises"
for item in getInitialNeuralNetworkState():
    print item.shape
```

```
This is the initial neural network state as computed from the previous exerc
ises
(10,)
()
(10, 379)
(10,)
```

In [173]:
```
def fitNeuralNetwork(trainInputs, trainTargets, validInputs, validTargets,
alpha):
    fittedParams = minimize_list(nn_cost, getInitialNeuralNetworkState(),
(trainInputs, trainTargets, alpha))
    trainRMSE = getRMSE(trueTargets=trainTargets, predictions=nn_cost(fitte
dParams, trainInputs)),
    validRMSE = getRMSE(trueTargets=validTargets, predictions=nn_cost(fitte
dParams, validInputs))
    return fittedParams, trainRMSE, validRMSE
```

In [174]:
```
resultsShape = (k, len(alphas))
resultsShape
```

Out[174]:
```
(10, 5)
```

In [175]:
```
trainErrors = np.zeros(resultsShape)
validationErrors = np.zeros(resultsShape)
```

In [177]:
```
def doCrossValidation(alpha, i):
    for j, (trainIndices, validationIndices) in
enumerate(kFold.split(Xall)):
        fittedParams, trainRMSE, validRMSE = fitNeuralNetwork(
            trainInputs=Xall[trainIndices],
trainTargets=yAll[trainIndices],
            validInputs=Xall[validationIndices], validTargets = yAll[valida
tionIndices], alpha=alpha
        )

        assert len(trainRMSE) == 1
        trainErrors[j, i] = trainRMSE[0]
        validationErrors[j, i] = validRMSE
```

In [178]:
```
def fitAndValidateForMultipleAlphas(alphas):
    for i, alpha in enumerate(alphas):
        doCrossValidation(alpha, i)
```

In [179]:
```
trainErrors = np.zeros(resultsShape)
validationErrors = np.zeros(resultsShape)
run_start_time = time.time()
fitAndValidateForMultipleAlphas(alphas) #long running script because we nee
d to run the neural network 50 times
run_time = time.time() - run_start_time
run_time
```

Out[179]: 1160.1132969856262

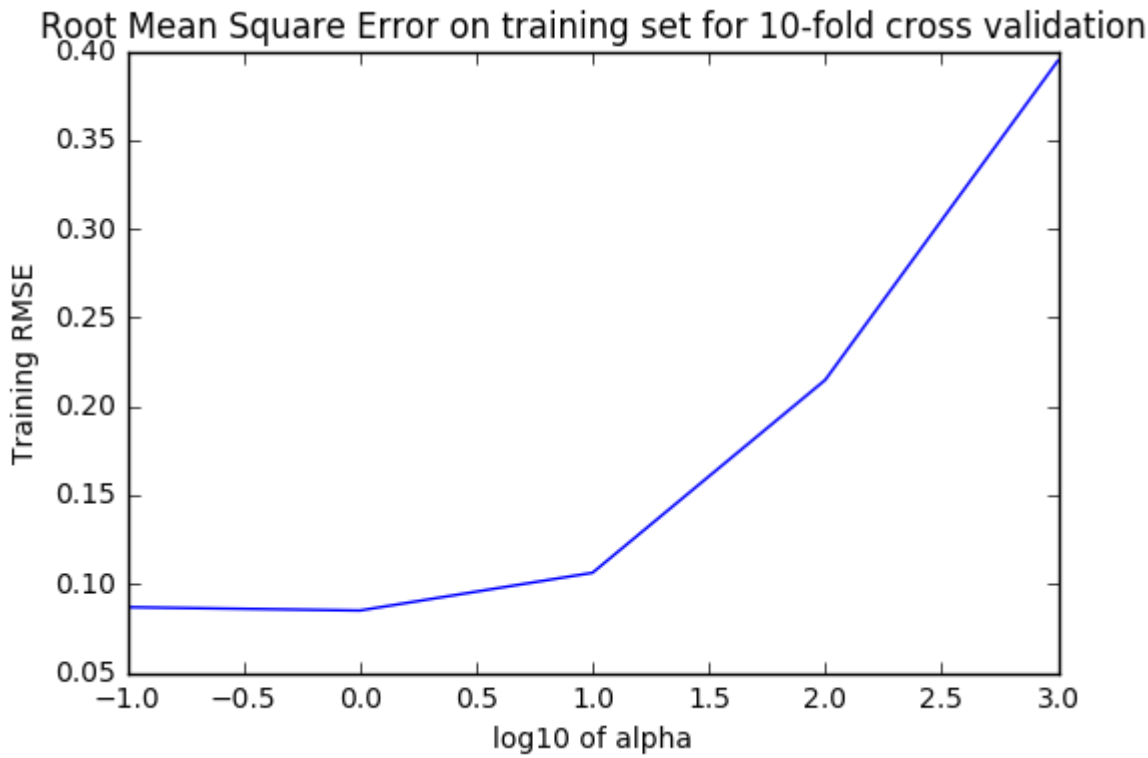
In [180]:
```
trainMeanRMSEs = np.mean(trainErrors, axis=0)
trainMeanRMSEs.shape
```

Out[180]: (5,)

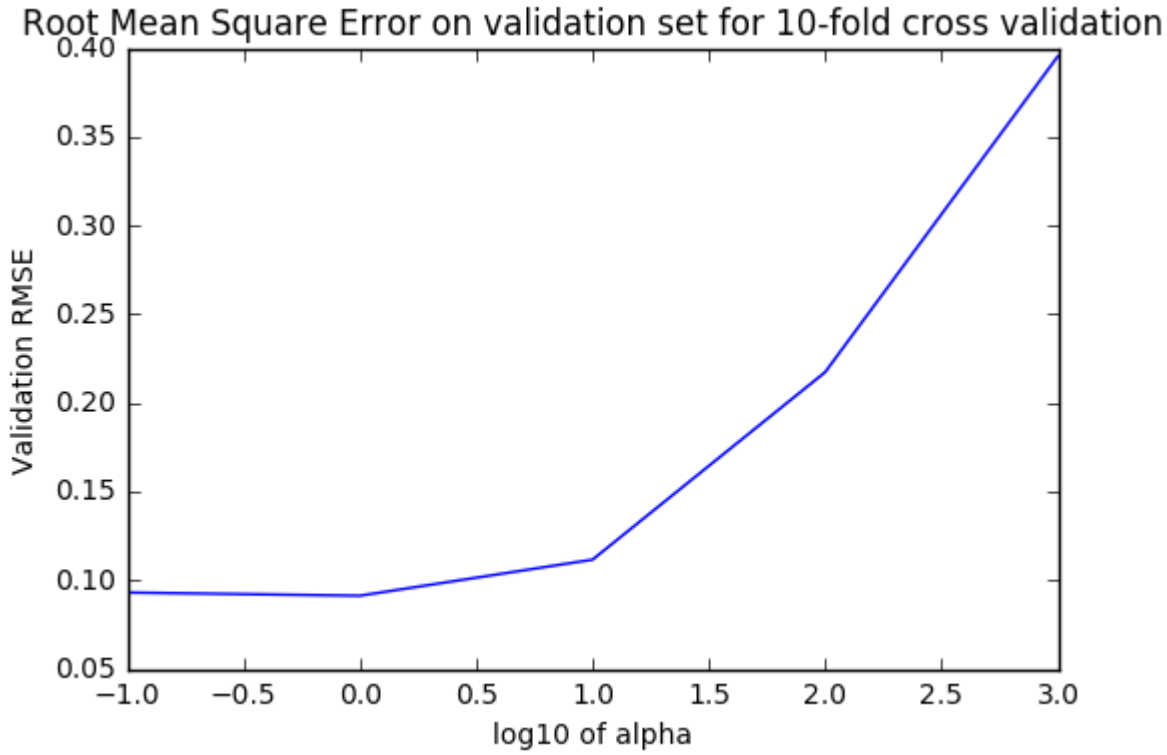
In [181]:
```
validationMeanRMSEs = np.mean(validationErrors, axis=0)
validationMeanRMSEs.shape
```

Out[181]: (5,)

In [182]:
```
fig = plt.figure()
plt.plot(np.log10(alphas), trainMeanRMSEs)
plt.title('Root Mean Square Error on training set for %d-fold cross validat
ion' % k,
          fontsize=12)
plt.ylabel('Training RMSE')
plt.xlabel('log10 of alpha')
plt.show()
```



In [183]:
```
fig = plt.figure()
plt.plot(np.log10(alphas), validationMeanRMSEs)
plt.title('Root Mean Square Error on validation set for %d-fold cross valid
ation' % k,
          fontsize=12)
plt.ylabel('Validation RMSE')
plt.xlabel('log10 of alpha')
plt.show()
```



From the two graphs above we understand that we need to explore for smaller values of alpha

In [184]:
```
alphas = np.logspace(-3, 1, num=5)
alphas
```

Out[184]:
```
array([  1.00000000e-03,   1.00000000e-02,   1.00000000e-01,
         1.00000000e+00,   1.00000000e+01])
```

In [185]:
```
trainErrors = np.zeros(resultsShape)
validationErrors = np.zeros(resultsShape)
run_start_time = time.time()
fitAndValidateForMultipleAlphas(alphas) #long running script because we nee
d to run the neural network 50 times
run_time = time.time() - run_start_time
run_time
```

Out[185]:
```
1274.1242611408234
```

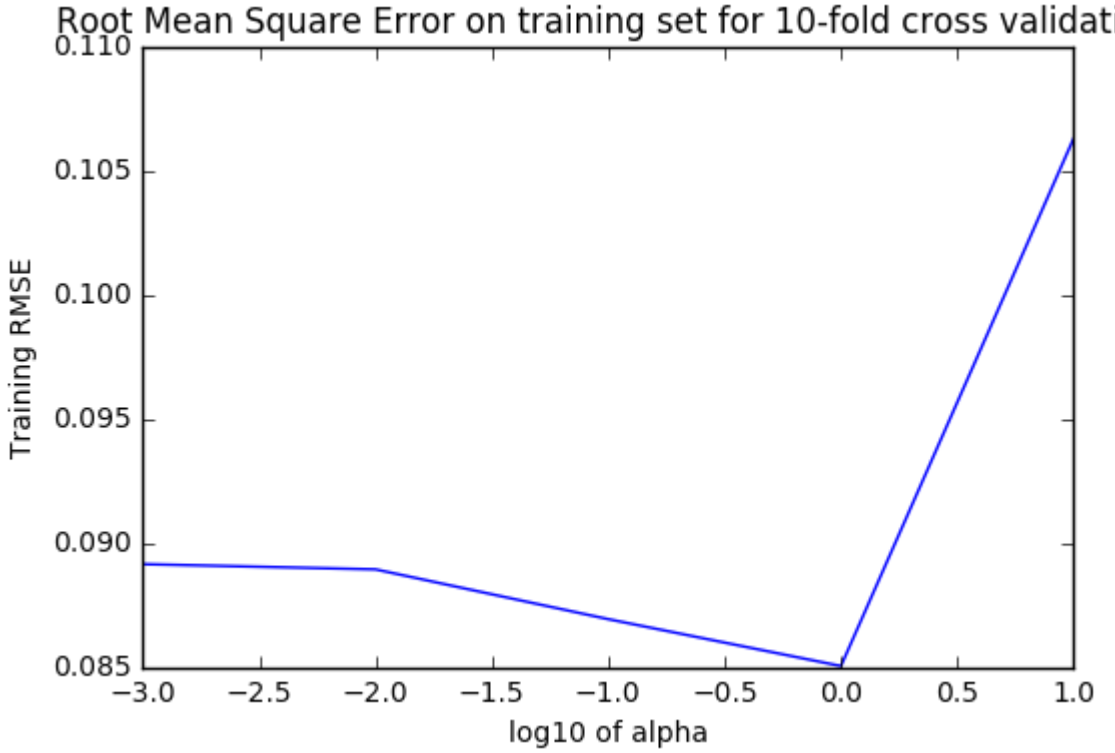
In [186]:
```
trainMeanRMSEs = np.mean(trainErrors, axis=0)
trainMeanRMSEs.shape
```

Out[186]:
```
(5,)
```

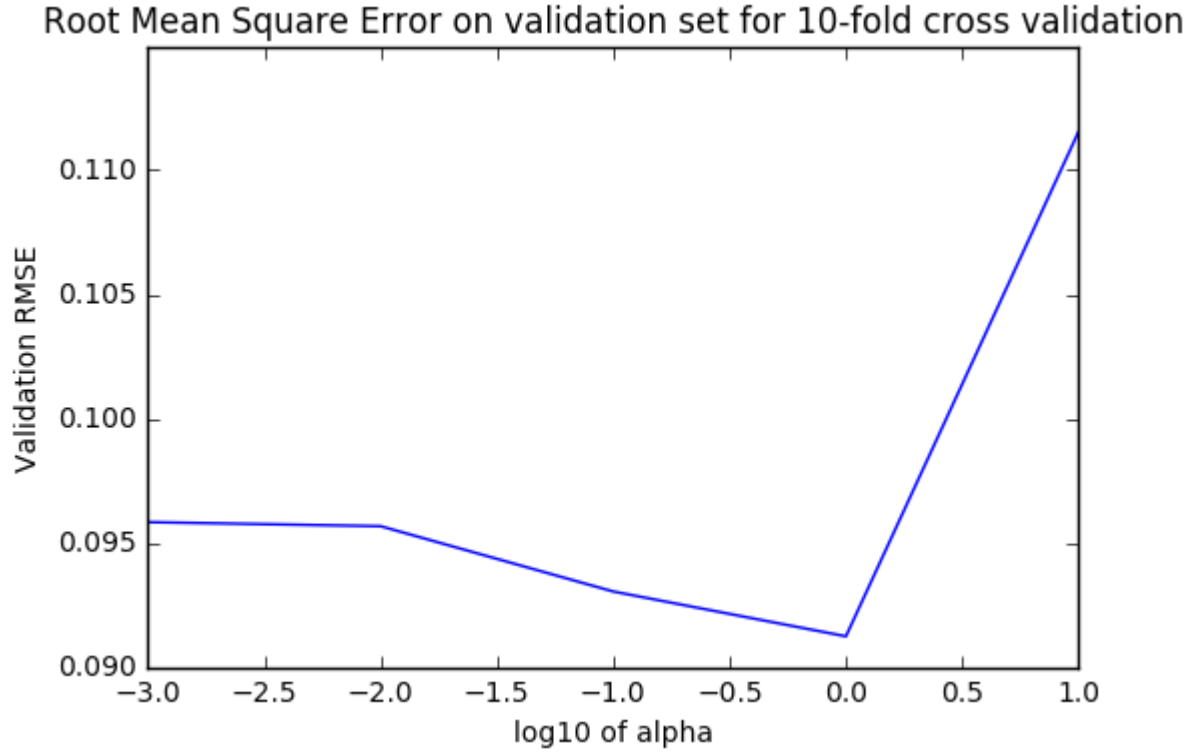
In [187]:
```
validationMeanRMSEs = np.mean(validationErrors, axis=0)
validationMeanRMSEs.shape
```

Out[187]:
```
(5,)
```

In [188]:
```
fig = plt.figure()
plt.plot(np.log10(alphas), trainMeanRMSEs)
plt.title('Root Mean Square Error on training set for %d-fold cross validat
ion' % k,
          fontsize=12)
plt.ylabel('Training RMSE')
plt.xlabel('log10 of alpha')
plt.show()
```



In [189]:
```
fig = plt.figure()
plt.plot(np.log10(alphas), validationMeanRMSEs)
plt.title('Root Mean Square Error on validation set for %d-fold cross valid
ation' % k,
          fontsize=12)
plt.ylabel('Validation RMSE')
plt.xlabel('log10 of alpha')
plt.show()
```



In [190]:
```
print "the best RMSE is achieved by alpha:"
bestAlpha = alphas[np.argmin(validationMeanRMSEs)]
bestAlpha
```

```
the best RMSE is achieved by alpha:
```

Out[190]:
```
1.0
```

We are going to retrain the neural network using the entire dataset based on this alpha and then we are going to test on the testing set which is unseen data we have not worked with before in this assignment

In [191]:
```
fittedParams, trainRMSE, testRMSE = fitNeuralNetwork(trainInputs=Xall, trai
nTargets=yAll,
                                                     validInputs=Xtesting,
validTargets=yTest, alpha=bestAlpha)
```

In [192]:
```
print "training RMSE for the neural network with optimal alpha is"
trainRMSE
```

```
training RMSE for the neural network with optimal alpha is
```

Out[192]:
```
(0.08385678969088153,)
```

In [193]:
```
print "testing RMSE for the neural network with optimal alpha is"
testRMSE
```

```
testing RMSE for the neural network with optimal alpha is
```

Out[193]:
```
0.2949036328213312
```

Let's compare the above values with the simple case where we had the alpha = 10

In [194]:
```
fittedParams, trainRMSE_alpha10, testRMSE_alpha10 = fitNeuralNetwork(trainI
nputs=Xall, trainTargets=yAll,
                                                      validInputs=Xtesting,
validTargets=yTest, alpha=10)
```

In [199]:
```
print "training RMSE for the neural network with alpha 10 is"
trainRMSE_alpha10
```

```
training RMSE for the neural network with alpha 10 is
```

Out[199]:
```
(0.10395701898016467,)
```

In [198]:
```
print "testing RMSE for the neural network with alpha 10 is"
testRMSE_alpha10
```

```
testing RMSE for the neural network with alpha 10 is
```

Out[198]:
```
0.28177834079572883
```

The training error is reduced when choosing the optimal alpha for training: ~0.083 < ~0.104

But the testing error in the unseen data is lower when training data used the alpha=10 as we used in previous exercises

We are going to repeat the previous two fit-and-RMSE of the neural network but this time we are going to use the training set as the training set and the validation set as testing set in order to be able and compare with the results of previous exercises

In [200]:
```
fittedParams, trainRMSE, testRMSE = fitNeuralNetwork(trainInputs=Xtr, train
Targets=yTrain,
                                                      validInputs=Xvalid, va
lidTargets=yVal, alpha=bestAlpha)

print "training RMSE for the neural network with optimal alpha is"
print trainRMSE
print
print "testing RMSE for the neural network with optimal alpha is"
print testRMSE
```

```
training RMSE for the neural network with optimal alpha is
(0.07919593358323644,)

testing RMSE for the neural network with optimal alpha is
0.240008558659
```

In [201]:
```
fittedParams, trainRMSE_alpha10, testRMSE_alpha10 = fitNeuralNetwork(trainI
nputs=Xtr, trainTargets=yTrain,
                                                      validInputs=Xvalid, va
lidTargets=yVal, alpha=10)

print "training RMSE for the neural network with alpha 10 is"
print trainRMSE_alpha10
print
print "testing RMSE for the neural network with alpha 10 is"
print testRMSE_alpha10
```

```
training RMSE for the neural network with alpha 10 is
(0.10026697346626232,)

testing RMSE for the neural network with alpha 10 is
0.261324563952
```

Note the last cell are just the results of the last run of the previous exercise, exercise 5, put again here for easier comparison

So as a conclusion we see that the training error is reduced and so is the validation error which means that cross-validation was a reliable procedure to output the best alpha parameter to use for regularization

In [ ]: