Pract_classification_professor

October 21, 2019

1 Classification

```
Notebook version: 1.1 (Oct 25, 2017)

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Changes: v.1.0 - First version. Python version
         v.1.1 - Updated to sklearn.model_selection. Python 3 compatibility.
```

```
In [1]: # Import some libraries that will be necessary for working with data and displaying pl

        # To visualize plots in the notebook
        %matplotlib inline

        #import matplotlib
        import matplotlib.pyplot as plt
        import numpy as np
        import scipy.io       # To read matlab files
        from sklearn.preprocessing import PolynomialFeatures
        from sklearn import svm

        from sklearn import model_selection

        import pylab
        pylab.rcParams['figure.figsize'] = 9, 7
```

1.1 1. Introduction

In this notebook we will analyze the behavior of logistic regression and support vector machines on the dataset in file `Dataset2D.mat`. We first load the dataset.

```
In [2]: # Load dataset
        matvar = scipy.io.loadmat('Dataset2D.mat')
        Xtrain = matvar['xTrain']
        Xtest = matvar['xTest']
        Xval = matvar['xVal']
```

```
# We must use astype(int) to convert the original target values (which are unsigned in
Ytrain = matvar['yTrain'].astype(int)
Ytest = matvar['yTest'].astype(int)
Yval = matvar['yVal'].astype(int)
```

1.1.1 1.1 Data Preparation.

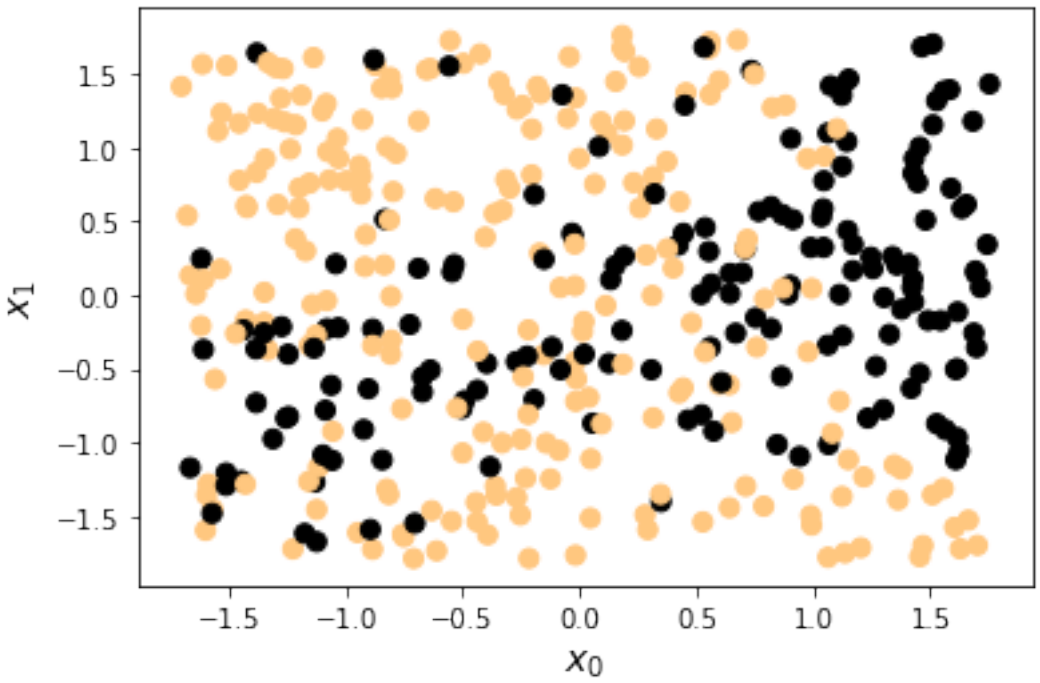
Normalize the dataset. Remind that the same transformation must be applied to training, validation and test data. Store train, validation and test input data in variables `Xtrain`, `Xval` and `Xtest`

In [3]:
```
# <SOL>
# Data normalization
def normalize(X, mx=None, sx=None):

    # Compute means and standard deviations
    if mx is None:
        mx = np.mean(X, axis=0)
    if sx is None:
        sx = np.std(X, axis=0)

    # Normalize
    X0 = (X-mx)/sx

    return X0, mx, sx

# Normalize data
Xtrain, mx, sx = normalize(Xtrain)
Xval, mx, sx = normalize(Xval, mx, sx)
Xtest, mx, sx = normalize(Xtest, mx, sx)

n_tr = Xtrain.shape[0]
n_val = Xval.shape[0]
n_tst = Xtest.shape[0]

print('The number of training samples is ' + str(n_tr))
print('The number of validation samples is ' + str(n_val))
print('The number of test samples is ' + str(n_tst))
print('The data dimension is ' + str(Xtrain.shape[1]))
# </SOL>

# Check normalization
print(np.mean(Xtrain, axis=0))
print(np.mean(Xval, axis=0))
print(np.mean(Xtest, axis=0))
print(np.std(Xtrain, axis=0))
print(np.std(Xval, axis=0))
print(np.std(Xtest, axis=0))
```

```
The number of training samples is 400
The number of validation samples is 400
The number of test samples is 400
The data dimension is 2
[-3.24185123e-16  2.84217094e-16]
[-0.00966556  0.03965134]
[0.00125431 0.02832642]
[1. 1.]
[0.98064167 1.02630613]
[0.9809003  1.03485737]
```

Visualize the input variables from the training set in a 2-dimensional plot.

```
In [4]: # Data visualization. This works for dimension 2 only.
        if Xtrain.shape[1]==2:
            plt.scatter(Xtrain[:, 0], Xtrain[:, 1], c=Ytrain.flatten(), s=50, cmap='copper')
            plt.xlabel("$x_0$", fontsize=14)
            plt.ylabel("$x_1$", fontsize=14)
        plt.show()
```



1.2 2. Linear Classification with Logistic Regression.

First we will analyze the behavior of logistic regression for this dataset.

1.2.1 2.1. MAP estimator.

Implement a function to compute the MAP estimate of the parameters of a linear logistic regression model with Gaussian prior and a given value of the inverse regularization parameter C. The method should return the estimated parameter and the negative log-likelihood, NLL($\mathbf{w}$). The sintaxis must be `w, NLL = logregFitR(Z_tr, Y_tr, rho, C, n_it)` where

- `Z_tr` is the input training data matrix (one instance per row)
- `Y_tr` contains the labels of corresponding to each row in the data matrix
- `rho` is the learning step
- `C` is the inverse regularizer
- `n_it` is the number of iterations

In [5]:
```
# <SOL>
# Define the logistic function
def logistic(x):
   p = 1.0 / (1 + np.exp(-x))
   return p

# MAP trainer.
def logregFitR(Z_tr, Y_tr, rho, C, n_it):

    # Data dimension
    n_dim = Z_tr.shape[1]

    # Initialize variables
    nll_tr = np.zeros(n_it)
    pe_tr = np.zeros(n_it)
    w = np.random.randn(n_dim,1)

    # Running the gradient descent algorithm
    for n in range(n_it):

        # Compute posterior probabilities for weight w
        p1_tr = logistic(np.dot(Z_tr, w))
        p0_tr = logistic(-np.dot(Z_tr, w))

        # Compute negative log-likelihood
        nll_tr[n] = - np.dot(Y_tr.T, np.log(p1_tr)) - np.dot((1-Y_tr).T, np.log(p0_tr))

        # Update weights
        w = (1-2*rho/C)*w + rho*np.dot(Z_tr.T, Y_tr - p1_tr)

    return w, nll_tr

# Compute predictions for a given model
def logregPredict(Z, w):

    # Compute posterior probability of class 1 for weights w.
```

```
        p = logistic(np.dot(Z, w))

        # Classify
        D = [int(np.round(pn)) for pn in p]

        return p, D

    #</SOL>
```

1.2.2 2.2 Log-likelihood

Compute the MAP estimate for a polynomial regression with degree 5, for C ranging from -0.01 to 100. Sample C uniformly in a log scale, an plot using `plt.semilogx`.

Plot the final value of NLL as a function of C. Can you explain the qualitative behavior of NLL as C grows?

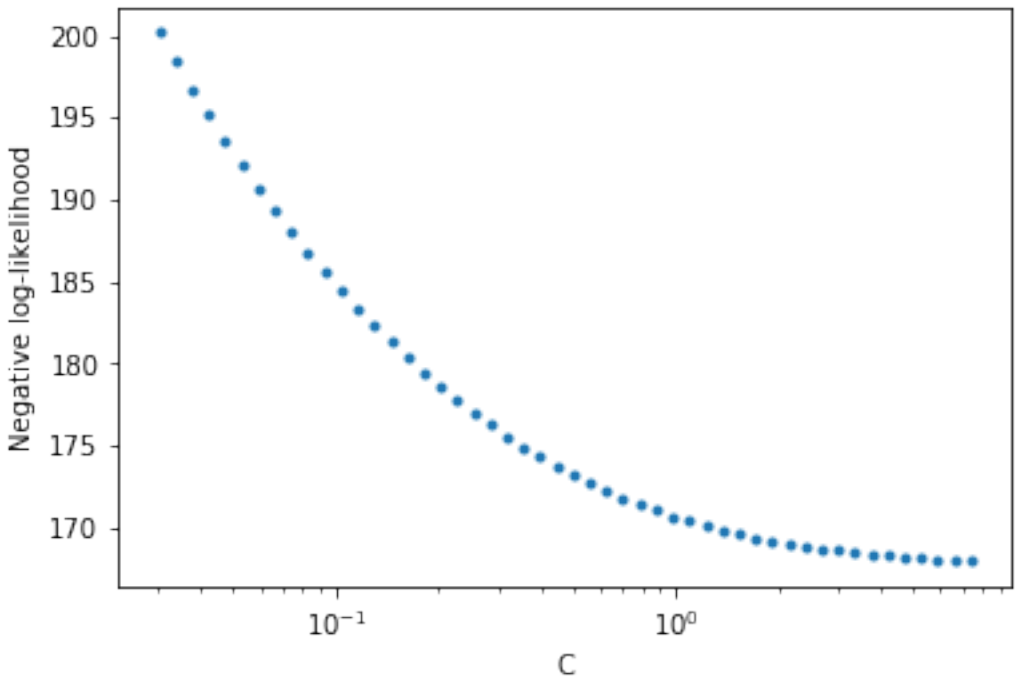
The plot may show some oscillation because of the random noise introduced by random initializations of the learning algoritm. In order to smooth the results, you can initialize the random seed right before calling the `logregFitR` method, using

```
np.random.seed(3)
```

```
In [6]: # <SOL>
        # Set parameters
        nC = 50

        logC = np.linspace(-3.5, 2, num=nC)
        C_all = np.exp(logC)
        n_it = 2000
        rho = 0.001

        # Compute Z_tr
        poly = PolynomialFeatures(degree=5)
        Z_tr = poly.fit_transform(Xtrain)

        # Normalize columns (this is useful to make algorithms more stable).)
        Zn, mz, sz = normalize(Z_tr[:,1:])
        Z_tr = np.concatenate((np.ones((n_tr, 1)), Zn), axis=1)

        # Compute Z_val
        Z_val = poly.fit_transform(Xval)
        Zn, mz, sz = normalize(Z_val[:,1:], mz, sz)
        Z_val = np.concatenate((np.ones((n_val,1)), Zn), axis=1)

        dim = Z_tr.shape[1]
        L = np.zeros((nC, 1))
        w_all = np.zeros((nC, dim))

        # Train models
```

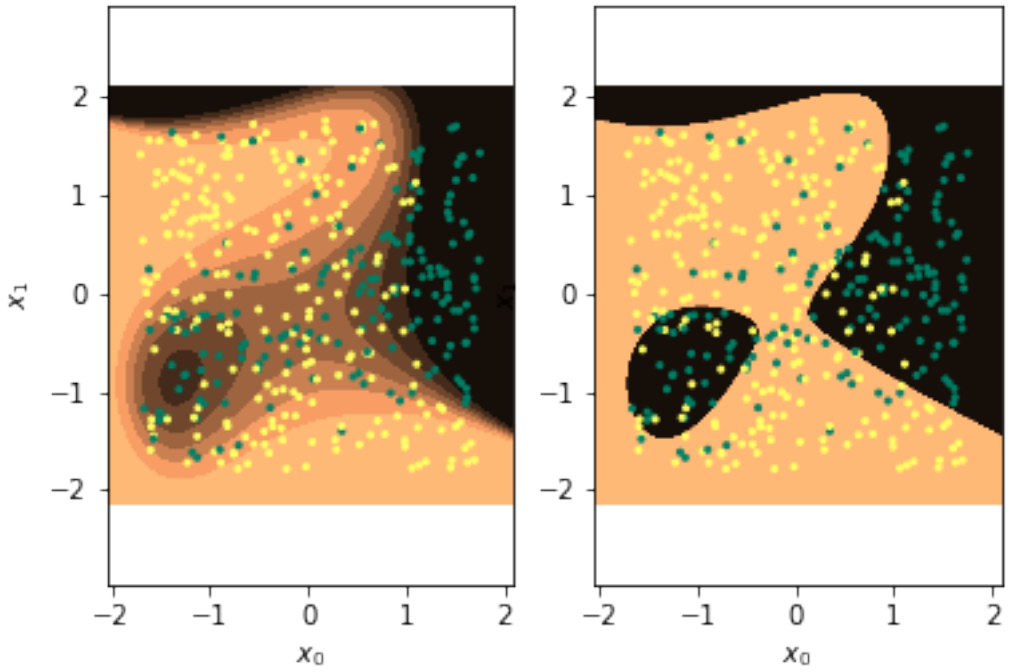
```
    for k, C in enumerate(C_all):

        np.random.seed(3)
        w, L_all = logregFitR(Z_tr, Ytrain, rho, C, n_it)

        L[k] = L_all[-1]
        w_all[k] = w.T

    plt.figure()
    plt.semilogx(C_all, L, '.')
    plt.xlabel('C')
    plt.ylabel('Negative log-likelihood')

    print("As C grows, the regularization effect dissapears, and the fit method minimizes N
    # </SOL>
```

```
As C grows, the regularization effect dissapears, and the fit method minimizes NLL.
```



In [7]:
```
# This is a plot for the last value of C used in the code above.

if Xtrain.shape[1]==2:

    # Create a regtangular grid.
    x_min, x_max = Xtrain[:, 0].min(), Xtrain[:, 0].max()
```

```
y_min, y_max = Xtrain[:, 1].min(), Xtrain[:, 1].max()
dx = x_max - x_min
dy = y_max - y_min
h = dy /400
xx, yy = np.meshgrid(np.arange(x_min - 0.1 * dx, x_max + 0.1 * dx, h),
                     np.arange(y_min - 0.1 * dx, y_max + 0.1 * dy, h))
X_grid = np.array([xx.ravel(), yy.ravel()]).T

# Compute Z_grid
Z_grid = poly.fit_transform(X_grid)
n_grid = Z_grid.shape[0]
Zn, mz, sz = normalize(Z_grid[:,1:], mz, sz)
Z_grid = np.concatenate((np.ones((n_grid,1)), Zn), axis=1)

# Compute the classifier output for all samples in the grid.
pp, dd = logregPredict(Z_grid, w)
pp = pp.reshape(xx.shape)

# Paint output maps
plt.figure()
pylab.rcParams['figure.figsize'] = 8, 4  # Set figure size
for i in [1, 2]:
    ax = plt.subplot(1,2,i)
    ax.set_xlabel('$x_0$')
    ax.set_ylabel('$x_1$')
    ax.axis('equal')
    if i==1:
        ax.contourf(xx, yy, pp, cmap=plt.cm.copper)
    else:
        ax.contourf(xx, yy, np.round(pp), cmap=plt.cm.copper)
    ax.scatter(Xtrain[:, 0], Xtrain[:, 1], c=Ytrain.flatten(), s=4, cmap='summer')

plt.show()
```



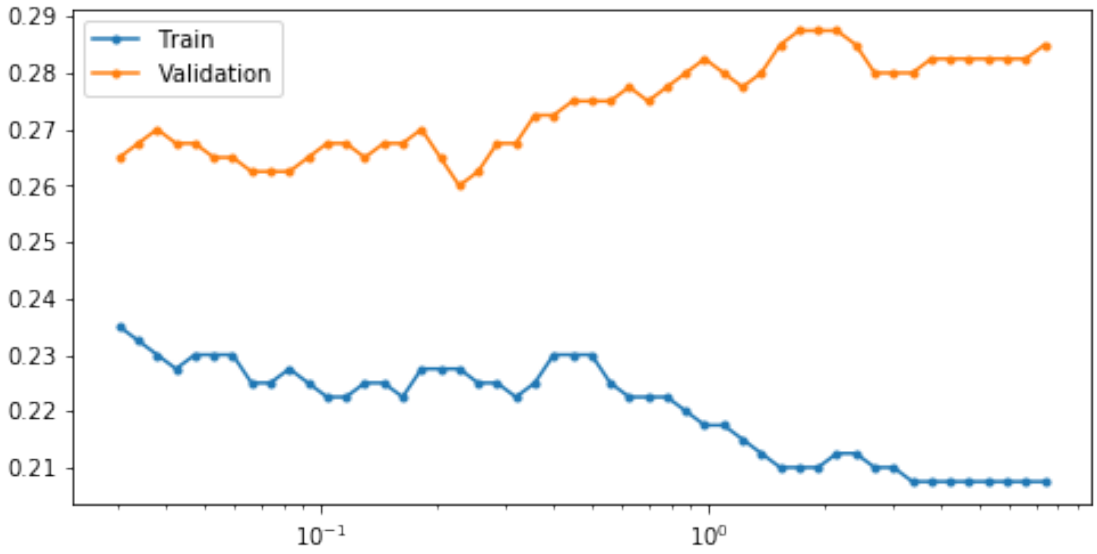
1.2.3 2.3. Training and test errors.

Plot the training and validation error rates as a function of C. Compute the value of C minimizing the validation error rate.

```
In [8]: # <SOL>
        # Train models
        pe_tr = np.zeros((nC, 1))
        pe_val = np.zeros((nC, 1))

        for k, C in enumerate(C_all):

            p_tr, D_tr = logregPredict(Z_tr, w_all[k])
            p_val, D_val = logregPredict(Z_val, w_all[k])

            # Compute error rates
            E_tr = D_tr!=Ytrain.T
            E_val = D_val!=Yval.T

            # Error rates
            pe_tr[k] = np.mean(E_tr)
            pe_val[k] = np.mean(E_val)

        plt.figure()
```

```
        plt.semilogx(C_all, pe_tr, '.-', label='Train')
        plt.semilogx(C_all, pe_val, '.-', label='Validation')
        plt.legend(loc='best')

        print("The optimal value of C is {0}".format(C_all[np.argmin(pe_val)]))

        # </SOL>
```

```
The optimal value of C is 0.22773062069049685
```



1.3 3. Non-linear classification with Support Vector Machines

In this section we will train an SVM with Gaussian kernels. In this case, we will select parameter C of the SVM by cross-validation.

1.3.1 3.1. Dataset preparation.

Join the training and validation datasets in a single input matrix `X_tr2` and a single label vector `Y_tr2`

```
In [9]: # <SOL>
        X_tr2 = np.concatenate((Xtrain, Xval), axis = 0)
        Y_tr2 = np.concatenate((Ytrain, Yval), axis = 0)
        # </SOL>
```

1.3.2 3.2. Cross validated error estimate

Apply a 10-fold cross validation procedure to estimate the average error rate of the SVM for $C = 1$ and γ (which is the kernel width) equal to 5.

```
In [10]: # <SOL>
         n_folds = 10
         C = 1
         gamma = 5
         n_samples = X_tr2.shape[0]

         kf = model_selection.KFold(n_splits=n_folds)
         pe_val = 0
         clf = svm.SVC(kernel='rbf', C=C, gamma=1)
         for tr_index, val_index in kf.split(X_tr2):
             Xcv_tr, Xcv_val = X_tr2[tr_index], X_tr2[val_index]
             Ycv_tr, Ycv_val = Y_tr2[tr_index], Y_tr2[val_index]

             clf.fit(Xcv_tr, np.ravel(Ycv_tr))

             pe_val += 1.0 - clf.score(Xval, Yval)

         pe_val = pe_val/n_folds
         print("The average error rate is {0}".format(pe_val))
         # </SOL>
```

```
The average error rate is 0.24225
```

1.3.3 3.3. Influence of C.

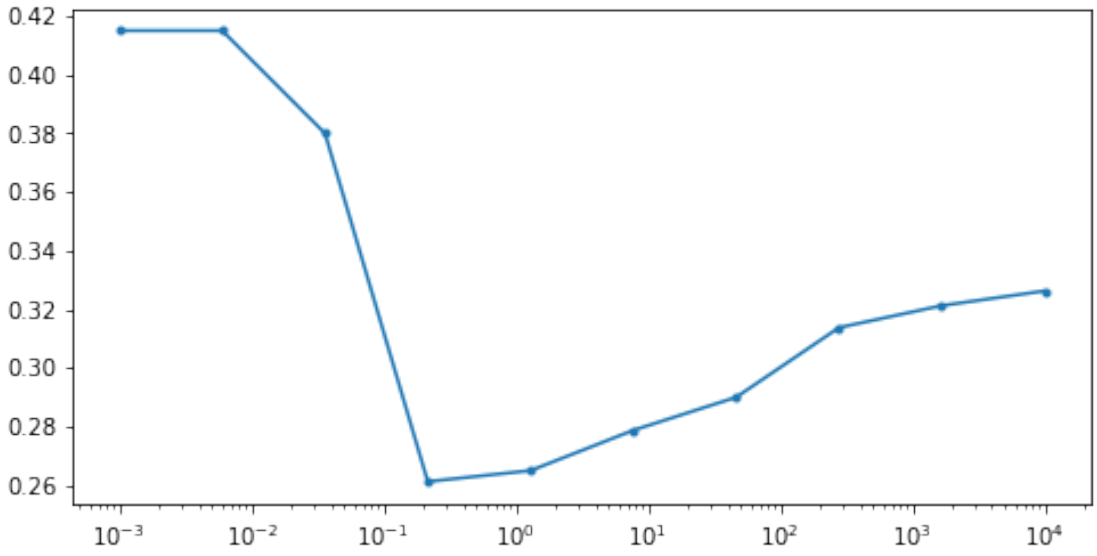
Repeate exercise 3.2 for $\gamma = 5$ and different values of C, ranging from 10^{-3} to 10^4, obtained by uniform sampling in a logarithmic scale. Plot the average number of errors as function of C.

Note that fitting the SVM may take some time, specially for the largest values of C.

```
In [11]: # <SOL>
         C_all = np.logspace(-3, 4, 10)
         n_folds = 10

         n_samples = X_tr2.shape[0]
         kf = model_selection.KFold(n_splits=n_folds)

         gamma = 5
         pe_val = np.zeros((len(C_all),1))

         for k, C in enumerate(C_all):
             print("C = {0}".format(C))

             clf = svm.SVC(kernel='rbf', C=C, gamma=gamma)

             for tr_index, val_index in kf.split(X_tr2):
                 Xcv_tr, Xcv_val = X_tr2[tr_index], X_tr2[val_index]
                 Ycv_tr, Ycv_val = Y_tr2[tr_index], Y_tr2[val_index]
```

```
            clf.fit(Xcv_tr, np.ravel(Ycv_tr))

            pe_val[k] += 1.0 - clf.score(Xcv_val, Ycv_val)

        pe_val[k] = pe_val[k]/n_folds

    # Put the result into a color plot
    plt.figure()
    plt.semilogx(C_all, pe_val,'.-')
    plt.show()
    # </SOL>
```

```
C = 0.001
C = 0.005994842503189409
C = 0.03593813663804628
C = 0.21544346900318845
C = 1.291549665014884
C = 7.742636826811269
C = 46.41588833612782
C = 278.2559402207126
C = 1668.100537200059
C = 10000.0
```



1.3.4 3.3. Hyperparameter optimization.

Compute the value of C minimizing the validation error rate.

```
In [12]: # <SOL>
         C_opt = C_all[np.argmin(pe_val)]
         print("The optimal value of C in the explored range is {0}".format(C_opt))
         # </SOL>
```

```
The optimal value of C in the explored range is 0.21544346900318845
```

1.3.5 3.4. Test error

Evaluate the classifier performance using the test data, for the selected hyperparameter values.

```
In [13]: # <SOL>
         clf = svm.SVC(kernel='rbf', C=C_opt, gamma=gamma)
         clf.fit(X_tr2, np.ravel(Y_tr2))
         pe_tst = 1.0 - clf.score(Xtest, Ytest)
         print("The test error for the selected model is {0}".format(pe_tst))
         # </SOL>
```

```
The test error for the selected model is 0.20499999999999996
```