

```
In [1]: %load_ext autoreload
        %autoreload 2

        import numpy as np
        np.random.seed(0)
        import mltools as ml
        import matplotlib.pyplot as plt    # use matplotlib for plotting with inline plots
        %matplotlib inline
```

P1: Linear Regression

First, we'll load the data, and split it into training and evaluation blocks:

```
In [2]: curve = np.genfromtxt("data/curve80.txt",delimiter=None)
        # print curve.shape
        X = curve[:,0]          # extract features
        X = X[:,np.newaxis]     # force X to be shape (M,1)
        Y = curve[:,1]          # extract target values
        # print X.shape, Y.shape # check shapes
        Xt,Xe,Yt,Ye = ml.splitData(X,Y,0.75)
```

1.1

```
In [3]: print(Xt.shape, Xe.shape, Yt.shape, Ye.shape)

(60, 1) (20, 1) (60,) (20,)
```

1.2

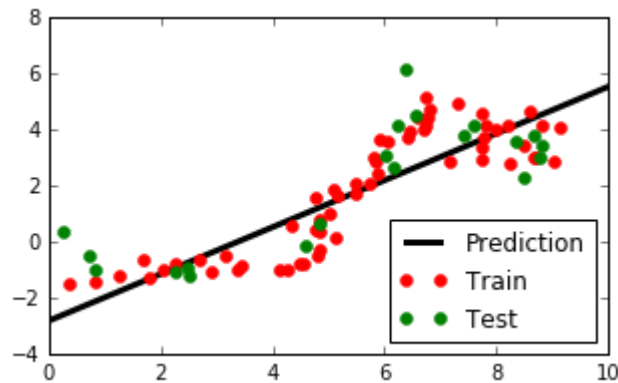
Now, let's train a simple linear regression model on the training data, and plot the training data, evaluation data, and our linear fit:

```
In [4]: import mltools.linear

lr = ml.linear.linearRegress(Xt,Yt, reg=0) # init and train the model
# to plot the prediction, we'll evaluate our model at a dense set of location
s:
xs = np.linspace(0,10,200)
xs = xs[:,np.newaxis]
ys = lr.predict(xs)

plt.rcParams['figure.figsize'] = (5.0, 3.0)
lines = plt.plot(xs,ys,'k-',Xt,Yt,'r.',Xe,Ye,'g.', linewidth=3,markersize=12)

plt.legend(['Prediction','Train','Test'],loc='lower right');
```



```
In [5]: print(lr.theta)
# verify y-intercept is around theta0 and the slope is increasing like theta1

[[-2.82765049  0.83606916]]
```

```
In [6]: print("MSE (Train) = ", lr.mse(Xt,Yt))
print("MSE (Test) = ", lr.mse(Xe,Ye))
```

```
MSE (Train) =  1.12771195561
MSE (Test) =  2.24234920301
```

1.3 Polynomial features

As mentioned in the homework, you can create additional features manually, e.g.,

```
In [7]: Xt2 = np.zeros((Xt.shape[0],2))
print (Xt2.shape)
print (Xt.shape)
Xt2[:,0] = Xt[:,0]
Xt2[:,1] = Xt[:,0]**2
print (Xt2[0:6,:])    # Look at a few data points to check:

(60, 2)
(60, 1)
[[ 3.4447005  11.86596153]
 [ 4.7580645  22.63917779]
 [ 6.4170507  41.17853969]
 [ 5.7949309  33.58122414]
 [ 7.7304147  59.75931143]
 [ 7.8225806  61.19276724]]
```

or, you can create them using the provided "fpoly" function:

```
In [8]: import mltools.transforms as xform
Xt2 = xform.fpoly(Xt,2, bias=False)
print (Xt2[0:6,:])    # Look at the same data points -- same values

[[ 3.4447005  11.86596153]
 [ 4.7580645  22.63917779]
 [ 6.4170507  41.17853969]
 [ 5.7949309  33.58122414]
 [ 7.7304147  59.75931143]
 [ 7.8225806  61.19276724]]
```

Now, let's try fitting a linear regression model using different numbers of polynomial features of x:

```

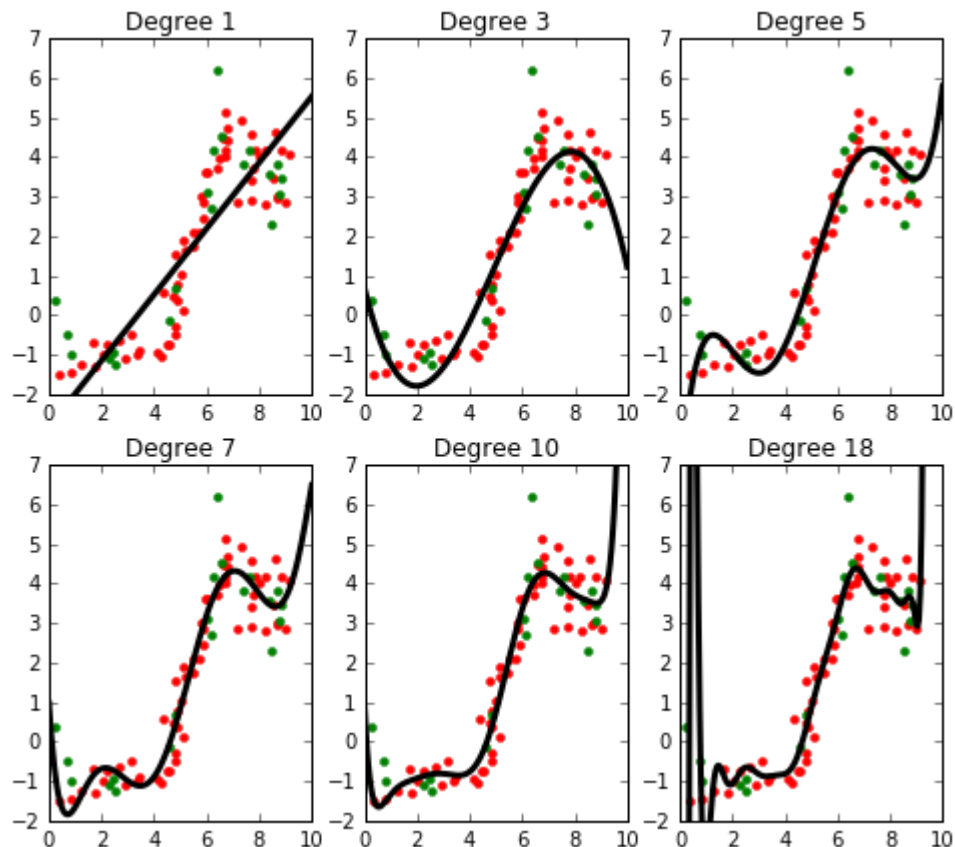
In [16]: degrees = np.array(range(0,19))
learners = [ [] ]*len(degrees)
errT = np.zeros((len(degrees),))
errV = np.zeros((len(degrees),))

plt.rcParams['figure.figsize'] = (8.0, 7.0)
fig, ax = plt.subplots(2,3)
axFlat = [a for row in ax for a in row] # 2x3 subplots as simple list
i = 0
for degree in degrees:
    XtP = xform.fpoly(Xt, degree, bias=False) # generate polynomial features
    up to degree d
    XtP, params = xform.rescale(XtP) # normalize scale & save transform parameters
    def Phi(X): return xform.rescale(xform.fpoly(X,degree,bias=False),params)
    [0] # and define feature transform f'n
    learners[degree] = ml.linear.linearRegress( Phi(Xt), Yt )

    if degree in [1,3,5,7,10,18]:
        axFlat[i].plot(Xt,Yt,'r.','g.',markersize=8)
        axFlat[i].set_title("Degree {}".format(degree))
        axisSize = axFlat[i].axis()
        axFlat[i].plot(xs,learners[degree].predict(Phi(xs)),'k-',linewidth=3)
        axFlat[i].axis(axisSize) # restore original Y-range
        i += 1

errT[degree] = learners[degree].mse(Phi(Xt),Yt)
errV[degree] = learners[degree].mse(Phi(Xe),Ye)

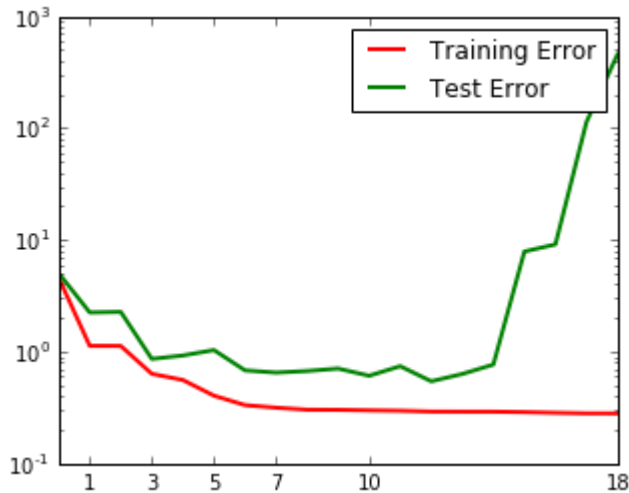
```



Finally, let's plot the training and test error as a function of the polynomial degree we used:

```
In [17]: plt.rcParams['figure.figsize'] = (5.0, 4.0)

plt.semilogy(degrees, errT, 'r-', degrees, errV, 'g-', linewidth=2);
plt.xticks([1, 3, 5, 7, 10, 18])
plt.legend(['Training Error', 'Test Error'], loc='upper right');
```



From this particular plot, it looks like degree 12 is the lowest validation error, and hence the model to pick (based on this information), although probably one could argue for anything between about 6 and 14.

If you only plot the degrees that were included in the question, the answer would be 7 or 10.

P2: Cross-validation

Cross validation is another method of model complexity assessment. We use it only to determine the correct setting of complexity parameters ("hyperparameters"), such as how many and which features to use, or parameters like "k" in KNN, for which training error alone provides little information. In particular, cross validation will not produce a model -- only a setting of the parameter values that cross-validation thinks will lead to a model with low test error.

2.1

We imagine that we do not have our "test" data X_E, Y_E , that we used for assessment in the previous problem, and will try to assess the quality of fit of our polynomial regressions using only the "training" data X_T, Y_T . To this end, we split (again) the data multiple times, one for each of the K partitions (nFolds in the code), and repeat our entire training and evaluation procedure on each split:

```

In [28]: def xval_err(nFolds, degree):
    err = np.zeros(nFolds)
    for iFold in range(nFolds):
        # Extract the ith cross-validation fold (training/validation split)
        [Xti,Xvi,Yti,Yvi] = ml.crossValidate(Xt,Yt,nFolds,iFold)

        # Build the feature transform on these training data
        XtiP = xform.fpoly(Xti, d, bias=False)
        XtiP,params = xform.rescale(XtiP)
        Phi = lambda X: xform.rescale(xform.fpoly(X,d,bias=False),params)[0]

        # Create and train the model, and save the error for this degree & split:
        lr = ml.linear.linearRegress( Phi(Xti), Yti )
        # Now, to estimate the test performance of each degree, take the average error across the folds:
        err[iFold] = lr.mse( Phi(Xvi),Yvi )
    return np.mean(err)

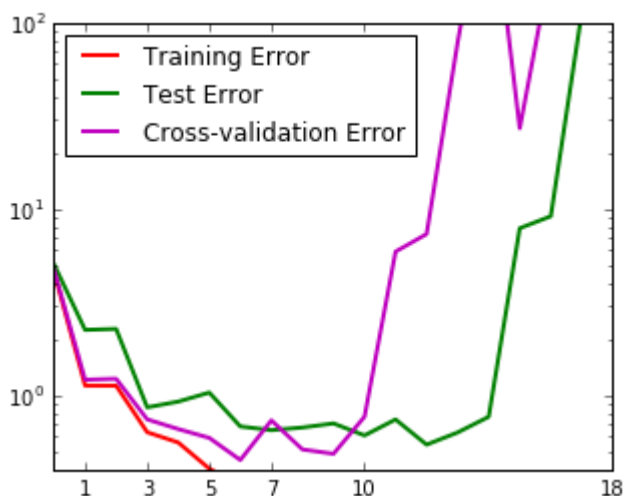
nFolds = 5
errX = np.zeros(len(degrees))

# Run over all degrees, and each fold for each degree
for i,d in enumerate(degrees):
    errX[i] = xval_err(nFolds, d)

plt.rcParams['figure.figsize'] = (5.0, 4.0)

plt.semilogy(degrees,errT,'r-',      # training error (from P1)
              degrees,errV,'g-',      # validation error (from P1)
              degrees,errX,'m-',      # cross-validation estimate of validation error
              linewidth=2);
plt.legend(['Training Error','Test Error', 'Cross-validation Error'], loc='upper left');
plt.xticks([1,3,5,7,10,18])
plt.axis([0,18,4e-1,1e2]);

```



2.2

Initially, the resulting plot shows a pretty similar characterization of performance as a function of degree to the validation data used in the previous problem (which, remember, we didn't access in this problem). A noticeable difference is that moderate to high degrees begin to degrade the performance (and begin overfitting) earlier than in the previous problem -- mainly, this is due to the 20% decrease in training data within our cross-validation process, which causes slightly lower degrees to begin overfitting.

(If you like, you can plot a learning curve to see how performance is changing for these degrees as a function of the number of training data.)

This illustrates how cross-validation can be used for model selection, and is a good surrogate when you do not have additional validation/test data.

2.3

Given the plot above, the lowest cross-validation error is at 6, but 8 or 9 would be reasonable choices as well. Amongst the choice of degrees mentioned in the question, either of 5, 7, or 10 would be reasonable answers.

2.4

```

In [33]: # pick the polynomial degree
d = 7
nFolds_list = [2,3,4,5,6,10,12,15]
errC = np.zeros(len(nFolds_list))

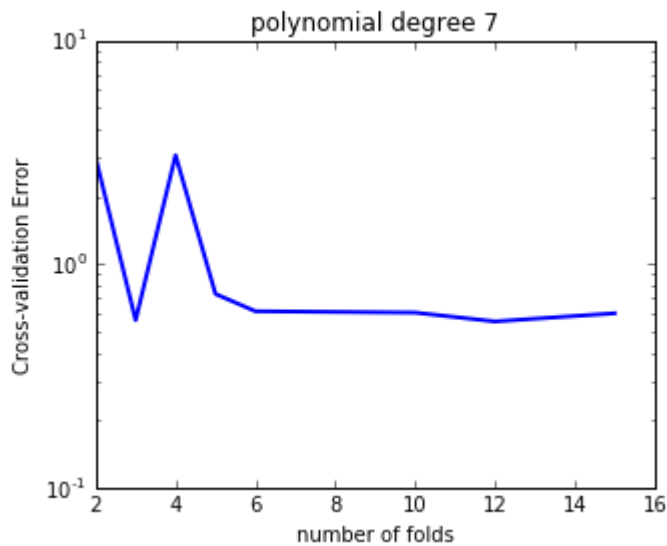
for i,nFolds in enumerate(nFolds_list):
    errC[i] = xval_err(nFolds, d)

plt.rcParams['figure.figsize'] = (5.0, 4.0)

plt.semilogy(nFolds_list,errC,'b-',
             linewidth=2);
plt.xlabel('number of folds')
plt.ylabel('Cross-validation Error')
plt.title('polynomial degree {}'.format(d))

```

Out[33]: <matplotlib.text.Text at 0x7fdb135f0278>



This plot shows a really high error at a few number of folds, and a low error with a high number of folds. This can be explained by the fact that the amount of data available for training is increasing as we increase the number of folds, i.e. since each block is M/K , and number of blocks used is $(K-1)$, the amount of data available for training in each fold is $(K-1)M/K$. For small K , this is much smaller than with large K .

The spikes you see are because you are averaging over fewer folds in the early part of the graph. So if you get an unfortunate split, since you are only averaging over K errors, that split has a large effect on the cross-validation error.