Lab: Model Selection for Neural Data

Machine learning is a key tool for neuroscientists to understand how sensory and motor signals are encoded in the brain. In addition to improving our scientific understanding of neural phenomena, understanding neural encoding is critical for brain machine interfaces. In this lab, you will use model selection for performing some simple analysis on real neural signals.

Before doing this lab, you should review the ideas in the <u>polynomial model selection demo (./polyfit.ipynb)</u>. In addition to the concepts in that demo, you will learn to:

- · Load MATLAB data
- Formulate models of different complexities using heuristic model selection
- Fit a linear model for the different model orders
- · Select the optimal model via cross-validation

The last stage of the lab uses LASSO estimation for model selection. If you are doing this part of the lab, you should review the concepts in <u>LASSO demonstration (./prostate.ipynb)</u> on the prostate cancer dataset.

Loading the data

The data in this lab comes from neural recordings described in:

Stevenson, Ian H., et al. "Statistical assessment of the stability of neural movement representations." Journal of neurophysiology 106.2 (2011): 764-774 (http://in.physiology.org/content/106/2/764.short)

Neurons are the basic information processing units in the brain. Neurons communicate with one another via *spikes* or *action potentials* which are brief events where voltage in the neuron rapidly rises then falls. These spikes trigger the electro-chemical signals between one neuron and another. In this experiment, the spikes were recorded from 196 neurons in the primary motor cortex (M1) of a monkey using an electrode array implanted onto the surface of a monkey's brain. During the recording, the monkey performed several reaching tasks and the position and velocity of the hand was recorded as well.

The goal of the experiment is to try to *read the monkey*'s *brain*: That is, predict the hand motion from the neural signals from the motor cortex.

We first load the basic packages.

```
In [52]: import numpy as np
import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline
```

The full data is available on the CRCNS website http://crcns.org/data-sets/movements/dream. This website has a large number of great datasets and can be used for projects as well. To make this lab easier, I have pre-processed the data slightly and placed it in the file StevensonV2.mat, which is a MATLAB file. You will need to have this file downloaded in the directory you are working on.

Since MATLAB is widely-used, python provides method for loading MATLAB mat files. We can use these commands to load the data as follows.

```
In [53]: import scipy.io
mat_dict = scipy.io.loadmat('StevensonV2.mat')
```

The returned structure, mat_dict, is a dictionary with each of the MATLAB variables that were saved in the .mat file. Use the .keys() method to list all the variables.

```
In [54]: #TODO
    print(*mat_dict.keys(), sep="\n")

__header__
    __version__
    __globals__
    Publication
    timeBase
    spikes
    time
    handVel
    handPos
    target
    startBins
    targets
    startBinned
```

We extract two variables, spikes and handVel, from the dictionary mat_dict , which represent the recorded spikes per neuron and the hand velocity. We take the transpose of the spikes data so that it is in the form time bins \times number of neurons. For the handVel data, we take the first component which is the motion in the x-direction.

```
In [55]: X0 = mat_dict['spikes'].T
    y0 = mat_dict['handVel'][0,:]
```

The spikes matrix will be a nt x nneuron matrix where nt is the number of time bins and nneuron is the number of neurons. Each entry spikes[k,j] is the number of spikes in time bin k from neuron j. Use the shape method to find nt and nneuron and print the values.

Now extract the time variable from the mat_dict dictionary. Reshape this to a 1D array with nt components. Each entry time[k] is the starting time of the time bin k. Find the sampling time tsamp which is the time between measurements, and ttotal which is the total duration of the recording.

```
In [57]:
         # TODO
         time = mat_dict['time'].squeeze()
         # unnessesarily complicated way to show that timesteps are basically equ
         al in length
         tsamp_arr = time[1:nt] - time[:nt-1]
         tsamp = np.mean(tsamp_arr)
         SE = np.std(tsamp_arr)/np.sqrt(nt-2)
         print(("min\t\max\t\tstd\t\tsE\n" + "{:.5f}\t\t" * 5)
                    .format(np.min(tsamp_arr), np.mean(tsamp_arr),
                           np.max(tsamp_arr), np.std(tsamp_arr),
                            SE))
         print("\ntsamp = {0:} ± {1:.5}\n=> tsamp is basically {0:} s".format(tsa
         mp, SE))
         # get total time
         ttotal = time[-1] - time[0]
         print("\nttotal =", ttotal, "s")
         min
                         mean
                                          max
                                                          std
                                                                          SE
         0.04950
                         0.05000
                                          0.05050
                                                          0.00007
                                                                          0.00000
         tsamp = 0.05 \pm 5.987e-07
         => tsamp is basically 0.05 s
         ttotal = 776.75 s
```

Linear fitting on all the neurons

First divide the data into training and test with approximately half the samples in each. Let Xtr and ytr denote the training data and Xts and yts denote the test data.

```
In [58]: from sklearn import preprocessing
         n_train = int(nt/2)
         n_test = nt-n_train
         Xs = preprocessing.scale(X0)
         XY0 = np.hstack((Xs, y0[:, None]))
         np.random.shuffle(XY0)
         Xshuf = XY0[:, :X0.shape[1]]
         yshuf = XY0[:, X0.shape[1]]
         Xtr = Xshuf[:n_train]
         ytr = yshuf[:n train]
         Xts = Xshuf[n train:]
         yts = yshuf[n_train:]
         print("Xtr={}\nytr={}\nXts={}\nyts={}\".format(Xtr.shape, ytr.shape,
         Xts.shape, yts.shape))
         print("Train:\tmean={:.4}\tstd={:.4}\".format(np.mean(Xtr), np.std(Xtr)))
         print("Test:\tmean={:.4}\tstd={:.4}".format(np.mean(Xts), np.std(Xts)))
         Xtr=(7768, 196)
         ytr=(7768,)
         Xts=(7768, 196)
         yts=(7768,)
         Train: mean=-0.001513 std=1.001
         Test:
                 mean=0.001513
                                 std=0.9935
         /usr/local/lib/python3.6/site-packages/sklearn/utils/validation.py:429:
         DataConversionWarning: Data with input dtype uint8 was converted to flo
         at64 by the scale function.
           warnings.warn(msg, DataConversionWarning)
```

Now, we begin by trying to fit a simple linear model using *all* the neurons as predictors. To this end, use the sklearn.linear_model package to create a regression object, and fit the linear model to the training data.

```
In [59]: # import sklearn.linear_model
    from sklearn import linear_model

# TODO
    model = linear_model.LinearRegression()
    model.fit(Xtr, ytr)
Out[59]: LinearRegression(copy_X=True, fit_intercept=True, n_jobs=1, normalize=F alse)
```

Measure and print the normalized RSS on the test data.

```
In [60]: from sklearn.metrics import r2_score
         # TODO
         y_hat_tr = model.predict(Xtr)
         RSSn_tr = (np.mean((y_hat_tr - ytr)**2))/(np.std(ytr)**2)
         rsq tr = r2_score(ytr, y_hat_tr)
         print(("R^2 = {:.4}").format(rsq_tr))
         print(("The normalized RSStr = {:.4}").format(RSSn_tr))
         y_hat_ts = model.predict(Xts)
         RSSn_ts = (np.mean((y_hat_ts - yts)**2))/(np.std(yts)**2)
         rsq ts = r2 score(yts, y hat ts)
         print(("\nR^2 = {:.4}").format(rsq_ts))
         print(("The normalized RSSts = {:.4}").format(RSSn ts))
         R^2 = 0.5272
         The normalized RSStr = 0.4728
         R^2 = -2.747e + 20
         The normalized RSSts = 2.747e+20
```

You should see that the test error is enormous -- the model does not generalize to the test data at all.

Linear Fitting with Heuristic Model Selection

The above shows that we need a way to reduce the model complexity. One simple idea is to select only the neurons that individually have a high correlation with the output.

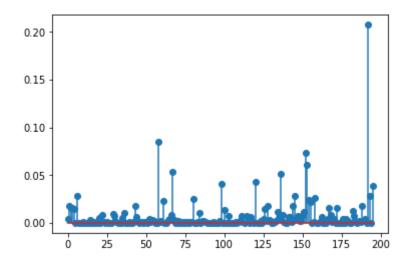
Write code which computes the coefficient of determination, R_k^2 , for each neuron k. Plot the R_k^2 values.

You can use a for loop over each neuron, but if you want to make efficient code try to avoid the for loop and use python broadcasting (../Basics/numpy_axes_broadcasting.ipynb).

```
In [61]: # TODO
# Rsq = ...
# plt.stem(...)
model = linear_model.LinearRegression()
rsq = np.zeros(Xtr.shape[1])
for i in range(Xtr.shape[1]):
    x = Xtr[:, i].reshape(-1, 1)
    model.fit(x, ytr)
    y_hat = model.predict(x)
    rsq[i] = r2_score(ytr, y_hat)

plt.stem(rsq)
```

Out[61]: <Container object of 3 artists>



We see that many neurons have low correlation and can probably be discarded from the model.

Use the np.argsort() command to find the indices of the d=100 neurons with the highest R_k^2 value. Put the d indices into an array Isel. Print the indices of the neurons with the 10 highest correlations.

The neurons with the ten highest R^2 values are:

idx	R^2
192	0.2076
58	0.0853
152	0.0736
153	0.0613
67	0.0536
136	0.0512
120	0.0431
98	0.0406
195	0.0392
193	0.0286

Fit a model using only the d neurons selected in the previous step and print both the test RSS per sample and the normalized test RSS.

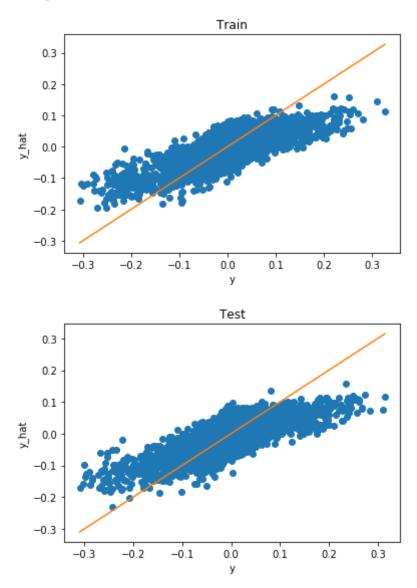
```
In [63]: # TODO
         X tr_sel = Xtr[:,Isel[:d]]
         X_ts_sel = Xts[:,Isel[:d]]
         model.fit(X_tr_sel, ytr )
         y_hat_tr = model.predict(X_tr_sel)
         y_hat_ts = model.predict(X_ts_sel)
         RSSper_samp_tr = np.mean((y_hat_tr - ytr) ** 2)
         RSSnorm tr = np.mean((y_hat_tr - ytr) ** 2) / (np.std(ytr)**2)
         RSSper_samp_ts = np.mean((y hat_ts - yts) ** 2)
         RSSnorm ts = np.mean((y hat ts - yts) ** 2) / (np.std(yts)**2)
         rsq_tr = r2_score(ytr, y_hat_tr)
         rsq ts = r2 score(yts, y hat ts)
         print("TRAIN: R^2= {:.4}, RSSper_samp={:.4}, RSSnorm={:.4}"
                   .format(rsq tr, RSSper samp tr, RSSnorm tr))
         print("TEST: R^2={:.4}, RSSper_samp={:.4}, RSSnorm={:.4}"
                   .format(rsq ts, RSSper samp ts, RSSnorm ts))
```

TRAIN: R^2= 0.5096, RSSper_samp=0.001489, RSSnorm=0.4904 TEST: R^2=0.5195, RSSper_samp=0.001529, RSSnorm=0.4805

Create a scatter plot of the predicted vs. actual hand motion on the test data. On the same plot, plot the line where yts_hat = yts.

```
In [64]: # TODO
         plt.plot(ytr, y_hat_tr, 'o')
         ax = plt.gca()
         lims = [
             np.min([np.min(y_hat_tr), np.min(ytr)]), # min of both axes
             np.max([np.max(y hat tr), np.max(ytr)]), # max of both axes
         ]
         plt.plot(lims, lims)
         plt.title("Train")
         plt.xlabel("y")
         plt.ylabel("y_hat")
         plt.figure()
         ax = plt.gca()
         lims = [
             np.min([np.min(y hat ts), np.min(yts)]), # min of both axes
             np.max([np.max(y_hat_ts), np.max(yts)]), # max of both axes
         ]
         plt.plot(yts, y hat ts, 'o')
         plt.plot(lims, lims)
         plt.title("Test")
         plt.xlabel("y")
         plt.ylabel("y_hat")
         # limits = [-6, 6]
         # plt.plot(limits, limits)
         # axes = plt.gca()
         # axes.set_xlim(limits)
         # axes.set ylim(limits)
```

Out[64]: <matplotlib.text.Text at 0x1185cf320>



Using K-fold cross validation for the optimal number of neurons

In the above, we fixed d=100. We can use cross validation to try to determine the best number of neurons to use. Try model orders with d=10,20,...,190. For each value of d, use K-fold validation with 10 folds to estimate the test RSS. For a data set this size, each fold will take a few seconds to compute, so it may be useful to print the progress.

```
In [65]: import sklearn.model_selection
         # Create a k-fold object
         nfold = 10
         kf = sklearn.model selection.KFold(n splits=nfold,shuffle=True)
         # Model orders to be tested
         dtest = np.arange(10,200,10)
         nd = len(dtest)
         # TODO.
         model = linear_model.LinearRegression()
         # Loop over the folds
         RSSts = np.zeros((nd,nfold))
         for isplit, Ind in enumerate(kf.split(Xtr)):
             # Get the training data in the split
             Itr, Its = Ind
             x_cv_tr = Xtr[Itr]
             y_cv_tr = ytr[Itr]
             x_cv_ts = Xtr[Its]
             y_cv_ts = ytr[Its]
             for it, d in enumerate(dtest):
                 # Fit data on training data
                 model.fit(x_cv_tr[Isel[:d]], y_cv_tr[Isel[:d]])
                 # Measure RSS on test data
                 y hat = model.predict(x cv ts)
                 RSSts[it,isplit] = np.mean((y_hat-y_cv_ts)**2)
               print(("{:.2f} "*19).format(*RSSts[:,isplit]))
               print("fold#","{}:".format(isplit), ("{:.2}\t"*19).format(*RSSts
         [:,isplit]))
```

Compute the RSS test mean and standard error and plot them as a function of the model order d using the plt.errorbar() method.

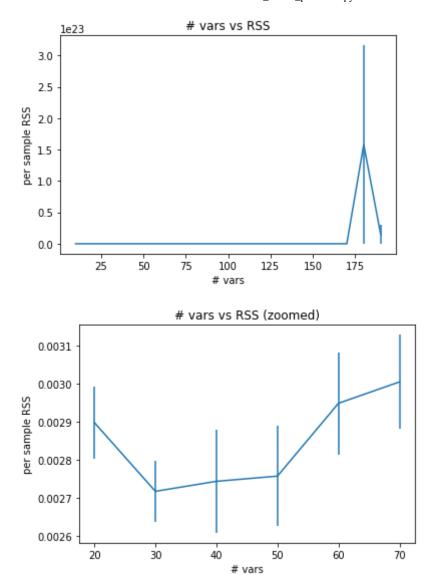
```
In [72]: # TODO
         # print(RSSts.shape)
         means = np.mean(RSSts, axis=1)
         stdErrs = np.std(RSSts, axis=1)/np.sqrt(nfold-1)
         idx = np.argsort(means)
         print("# vars\tRSS/sample\tstdErr")
         print("\n".join(["{:3d}\t{:.3}\t\t{:.3}\".format(*row) for row in zip(dte
         st[idx], means[idx], stdErrs[idx])]))
         targetRSS = means[idx][0]+stdErrs[idx][0]
         print("\n\n RSS) = min(RSS) + SE = {:.4} + {:.4} =
         {:.4}".format(means[idx][0], stdErrs[idx][0], targetRSS))
         print("So we need to find # vars such that the corrisponding RSS is less
          than {:.4}\n".format(targetRSS))
         print("\n".join(["{:3d}\t{:.3}\t{}".format(*row) for row in zip(dtest, m
         eans, means<targetRSS)]))</pre>
         # plt.plot(dtest, means)
         # plt.plot(dtest, means, 'o')
         plt.errorbar(dtest, means, yerr=stdErrs)
         plt.title("# vars vs RSS")
         plt.xlabel("# vars")
         plt.ylabel("per sample RSS")
         plt.figure()
         plt.title("# vars vs RSS (zoomed)")
         #1, r = 0, 5
         # plt.errorbar(dtest[1:r], means[1:r], yerr=stdErrs[1:r])
         # plt.xlabel("# vars")
         # plt.ylabel("per sample RSS")
         1, r = 1, 7
         # plt.figure()
         plt.errorbar(dtest[l:r], means[l:r], yerr=stdErrs[l:r])
         plt.xlabel("# vars")
         plt.ylabel("per sample RSS")
         #1, r = 10, 15
         # plt.figure()
         # plt.errorbar(dtest[1:r], means[1:r], yerr=stdErrs[1:r])
         # plt.xlabel("# vars")
         # plt.ylabel("per sample RSS")
         #1, r = 15, 20
         # plt.figure()
         # plt.errorbar(dtest[1:r], means[1:r], yerr=stdErrs[1:r])
         # plt.xlabel("# vars")
         # plt.ylabel("per sample RSS")
```

```
# vars
        RSS/sample
                          stdErr
 30
        0.00272
                          7.99e-05
 40
        0.00274
                          0.000135
 50
        0.00276
                          0.000131
 20
        0.0029
                          9.36e-05
                          0.000134
 60
        0.00295
 70
        0.003
                          0.000123
 10
        0.0031
                          0.000115
 80
        0.00321
                          0.000145
 90
        0.00358
                          0.000193
100
        0.00423
                          0.000291
110
        0.00529
                          0.000423
120
        0.00673
                          0.000458
130
        0.00889
                          0.000598
140
        0.0132
                          0.00136
150
        0.0309
                          0.00562
170
        0.0379
                          0.0112
                          0.0816
160
        0.288
190
        1.47e+22
                                   1.47e+22
180
        1.58e+23
                                   1.58e+23
```

Target RSS = min(RSS)+SE = 0.002718+7.992e-05 = 0.002798So we need to find # vars such that the corrisponding RSS is less than 0.002798

```
10
        0.0031 False
 20
        0.0029 False
 30
        0.00272 True
        0.00274 True
 40
        0.00276 True
 50
 60
        0.00295 False
 70
        0.003
                False
 80
        0.00321 False
 90
        0.00358 False
100
        0.00423 False
110
        0.00529 False
120
        0.00673 False
130
        0.00889 False
140
        0.0132 False
150
        0.0309 False
160
        0.288
                False
170
        0.0379 False
180
        1.58e+23
                         False
190
        1.47e+22
                         False
```

Out[72]: <matplotlib.text.Text at 0x115c882e8>



Find the optimal order using the one standard error rule. Print the optimal value of d and the mean test RSS per sample at the optimal d.

```
In [73]: # TODO
         RSSmeans = np.mean(RSSts, axis=1)
         stdErrs = np.std(RSSts, axis=1)/np.sqrt(nfold-1)
         minidx = np.argmin(means)
         target = RSSmeans[minidx]+stdErrs[minidx]
         d = np.min(dtest[RSSmeans < target])</pre>
         model = linear model.LinearRegression()
         print(Xtr[:, Isel[:10]].shape)
         model.fit(Xtr[:, Isel[:10]], ytr)
         y_hat_tr = model.predict(Xtr[:, Isel[:10]])
         RSS_tr = np.mean((ytr-y_hat_tr)**2)
         Rsq tr = r2 score(ytr, y hat tr)
         RSS_ts = np.mean((yts-y_hat_ts)**2)
         Rsq_ts = r2_score(yts, y_hat_ts)
         print("The optimal value of d is {}.".format(d))
         print("The train and test RSS/sample vales are {:.4} and {:.4} respectiv
         ely.".format(RSS_tr, RSS_ts))
         (7768, 10)
         The optimal value of d is 30.
         The train and test RSS/sample vales are 0.001862 and 0.001529 respectiv
         ely.
In [74]: model = linear model.LinearRegression()
         X subset tr = Xtr[:, Isel[:d]]
         X_subset_ts = Xts[:, Isel[:d]]
         model.fit(X_subset_tr, ytr)
         print(X_subset_tr.shape)
         y hat tr = model.predict(X subset tr)
         y_hat_ts = model.predict(X_subset_ts)
         Rsq_tr = r2_score(ytr, y_hat_tr)
         Rsq_ts = r2_score(yts, y_hat_ts)
         print("Train R^2 = {}".format(Rsq_tr))
         print("Test R^2 = {}".format(Rsq_ts))
         # print(("{} R^2 = {}\n"*2).format(["Train", Rsq tr, "Test", Rsq ts]))
         (7768, 30)
         Train R^2 = 0.4394042849266767
         Test R^2 = 0.4558766373353268
```

Using LASSO regression

Instead of using the above heuristic to select the variables, we can use LASSO regression.

First use the preprocessing.scale method to standardize the data matrix x0. Store the standardized values in xs. You do not need to standardize the response. For this data, the scale routine may throw a warning that you are converting data types. That is fine.

```
In [75]: from sklearn import preprocessing
# TODO
Xs = preprocessing.scale(X0)

/usr/local/lib/python3.6/site-packages/sklearn/utils/validation.py:429:
DataConversionWarning: Data with input dtype uint8 was converted to flo at64 by the scale function.
    warnings.warn(msg, _DataConversionWarning)
```

Now, use the LASSO method to fit a model. Use cross validation to select the regularization level alpha. Use alpha values logarithmically spaced from 1e-5 to 0.1, and use 10 fold cross validation.

Plot the mean test RSS and test RSS standard error with the plt.errorbar plot.

```
In [77]: # TODO

mean_RSS_each_fold_and_alpha = model.mse_path_
print(mean_RSS_each_fold_and_alpha.shape)

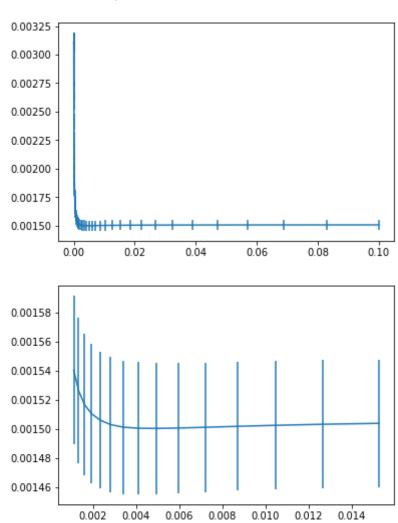
mean_RSS_each_alpha = np.mean(mean_RSS_each_fold_and_alpha, axis=1)
std_err_each_alpha = np.std (mean_RSS_each_fold_and_alpha, axis=1) /
np.sqrt(nfolds-1)

plt.errorbar(alphas, mean_RSS_each_alpha, yerr=std_err_each_alpha)

plt.figure()
a, b = 25, 40
plt.errorbar(alphas[a:b], mean_RSS_each_alpha[a:b], yerr=std_err_each_alpha[a:b])

(50, 10)
```

Out[77]: <Container object of 3 artists>



Find the optimal alpha and mean test RSS using the one standard error rule.

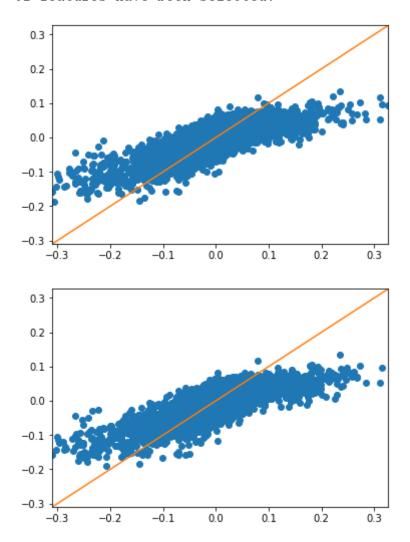
```
In [78]: # TODO
         mean RSS each fold and alpha = model.mse path
         mean RSS each alpha = np.mean(mean RSS each fold and alpha, axis=1)
         std_err_each_alpha = np.std (mean RSS_each fold and alpha, axis=1) /
         np.sqrt(nfolds-1)
         # print(*["{:03.3}\t\t{:05.6f}\n".format(*row) for row in zip(alphas, me
         an RSS each alpha)])
         minidx = np.argmin(mean_RSS_each_alpha)
         # print(minidx)
         # print(mean_RSS_each_alpha[33])
         # print(mean RSS each alpha <= mean RSS each alpha[33])</pre>
         target = mean RSS each alpha[minidx]+std err each alpha[minidx]
         opt_alpha idx = np.argmax(alphas[mean_RSS_each_alpha < target])</pre>
                                                                              # cho
         ose the biggest alpha => simpler model
         opt alpha = alphas[opt alpha idx]
         opt alpha RSS = mean RSS each alpha[opt alpha idx]
         print("The optimal value of d is using the one standard error rule is al
         pha={:.5f} with RSS={:.4f}."
                    .format(opt alpha, mean RSS each alpha[opt alpha idx]))
         print("As opposed to alpha = {:.5f} with RSS={:.4f} without using the ru
         le."
                    .format(model.alpha , mean RSS each alpha[minidx]))
```

The optimal value of d is using the one standard error rule is alpha=0.00091 with RSS=0.0016. As opposed to alpha = 0.00020 with RSS=0.0015 without using the rule.

Using the optimal alpha, recompute the predicted response variable on the whole data. Plot the predicted vs. actual values.

```
In [79]: # TODO
         new model = linear model.Lasso(alpha=opt alpha)
         # new model = linear model.Lasso(alpha=0.01)
         n = len(Xs) // 2
         Xtr = Xs[n:]
         ytr = y0[n:]
         Xtr = Xs[:n]
         ytr = y0[:n]
         new_model.fit(Xtr, ytr)
         y_hat_tr = new_model.predict(Xtr)
         limits = [np.min([np.min(y hat tr), np.min(ytr)]), np.max([np.max(y hat
         tr), np.max(ytr)])]
         plt.figure()
         plt.plot(ytr,y_hat_tr, 'o')
         plt.plot(limits, limits)
         axes = plt.gca()
         axes.set_xlim(limits)
         axes.set_ylim(limits)
         y hat ts = new model.predict(Xts)
         plt.figure()
         plt.plot(yts, y_hat_ts, 'o')
         plt.plot(limits, limits)
         axes = plt.gca()
         axes.set xlim(limits)
         axes.set ylim(limits)
         print("R^2 Train = ", r2_score(ytr, y_hat_tr))
         print("R^2 Test = ", r2_score(yts, y_hat_ts))
         print(np.sum(new model.coef != 0), "features have been selected.")
```

R^2 Train = 0.507501380223 R^2 Test = 0.514930508264 82 features have been selected.



More Fun

You can play around with this and many other neural data sets. Two things that one can do to further improve the quality of fit are:

- Use more time lags in the data. Instead of predicting the hand motion from the spikes in the previous time, use the spikes in the last few delays.
- Add a nonlinearity. You should see that the predicted hand motion differs from the actual for high
 values of the actual. You can improve the fit by adding a nonlinearity on the output. A polynomial fit
 would work well here.

You do not need to do these, but you can try them if you like.

In []: