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STA561 - Probabilistic Machine Learning
Kaggle Competition Writeup

Import libraries

In [2]:

```
import pandas as pd
from sklearn.cross_validation import train_test_split
from sklearn.ensemble import RandomForestRegressor
from sklearn.metrics import mean_squared_error
from sklearn import decomposition
from sklearn.linear_model import Lasso
from sklearn.svm import SVR
import matplotlib.pyplot as plt
from sklearn.metrics import r2_score
from sklearn.metrics import mean_absolute_error
%matplotlib inline
from sklearn.linear_model import BayesianRidge
from sklearn.preprocessing import PolynomialFeatures
import numpy as np
from sklearn.neural_network import MLPRegressor
import time
import warnings
import pylab
warnings.filterwarnings('ignore')
```

Read in data and perform minor preprocessing

In [3]:

```
# Read in training and test data
train_tmp = pd.read_csv('pml_train.csv')
test_tmp = pd.read_csv('pml_test_features.csv')

# Drop the loss col temporarily in order to merge data frames
loss = train_tmp['loss']
train_tmp.drop(labels=['loss'], axis=1,inplace = True)

# Cat the training and test in order to convert categorical vars to dummies
frames = [train_tmp,test_tmp]
data_tmp = pd.concat(frames)

# Convert categorical features to dummy vars
data_dummy = pd.get_dummies(data_tmp)

# Split back in to train and test
train_size = len(train_tmp['id'])
train = data_dummy.iloc[0:train_size,:]
test = data_dummy.iloc[train_size:,:]
```

Exploratory analysis and Feature Reduction

In [4]:

```
# Get some summary stats
train.describe()
```

Out[4]:

	id	cont1	cont2	cont3	cont4	c
count	131822.00000	131822.000000	131822.000000	131822.000000	131822.000000	1
mean	65910.50000	0.493342	0.507205	0.499348	0.491129	0
std	38053.87793	0.187592	0.207240	0.202093	0.211094	0
min	0.00000	0.000016	0.001149	0.002634	0.176921	0
25%	32955.25000	0.344779	0.358319	0.336963	0.327354	0
50%	65910.50000	0.475784	0.555782	0.527991	0.452887	0
75%	98865.75000	0.623912	0.681761	0.634224	0.652072	0
max	131821.00000	0.984975	0.862654	0.944251	0.952482	0

8 rows × 1154 columns

In [5]:

```
# Drop the categorical features that have very few instances (<10000)
cols_to_drop = []
for i in range(len(train.iloc[1])):
    if (np.count_nonzero(train.iloc[:,i]) < 10000):
        cols_to_drop = np.append(cols_to_drop,i)
train.drop(train.columns[cols_to_drop.astype(int)],axis=1,inplace = True)
test.drop(test.columns[cols_to_drop.astype(int)],axis=1,inplace = True)

# Move the loss to column 0
train.insert(0, 'loss', loss)

# randomly partition data into train_sub (80%) and cross_val (20%) sets
train_sub,cross_val = train_test_split(train, test_size=.2)
```

In [ ]:

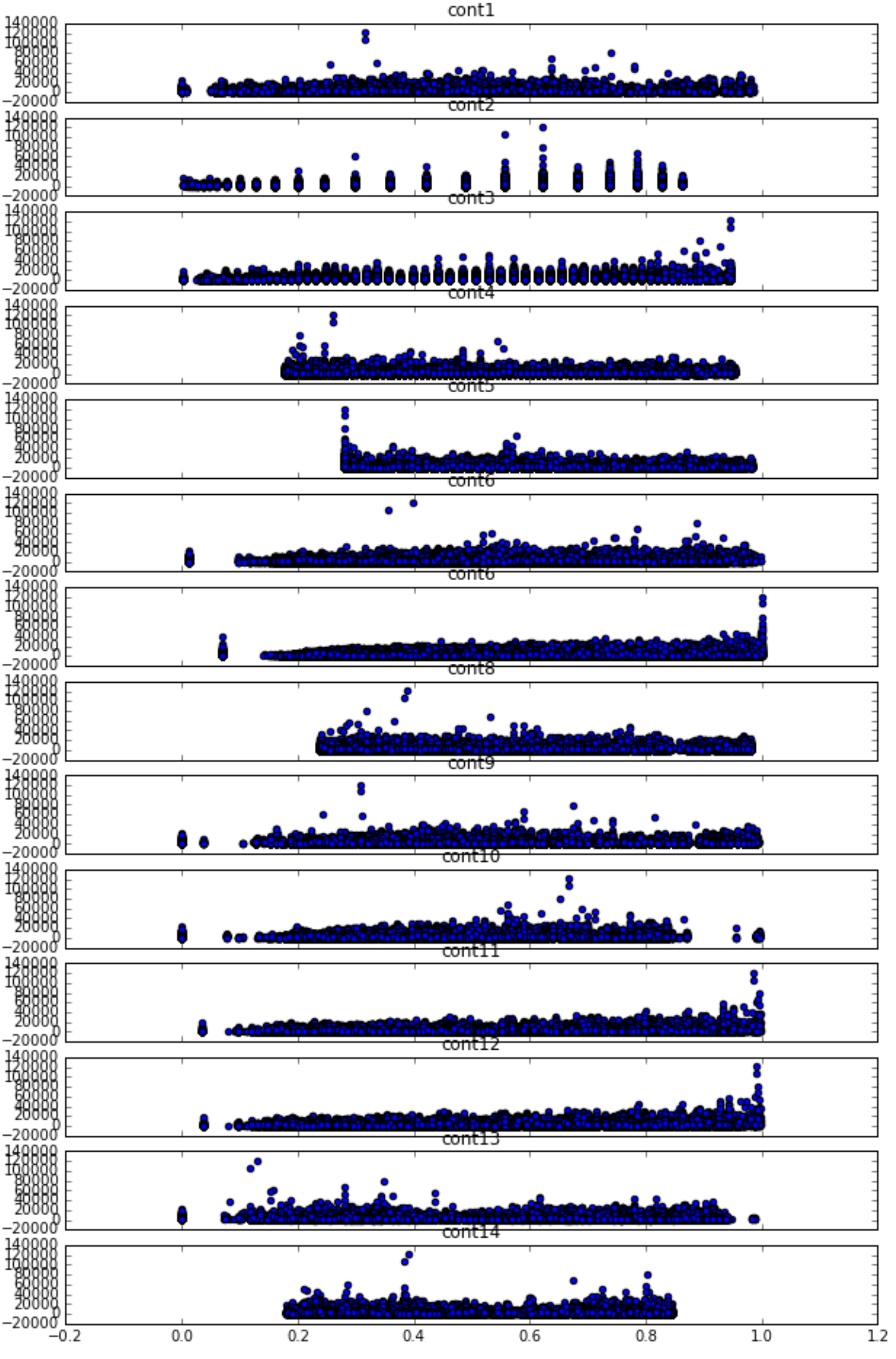
```
len(train.iloc[1])
```

In [6]:

```
# Scatter plot of continuous vars
fig_size = plt.rcParams["figure.figsize"]
fig_size[0] = 10
fig_size[1] = 16
plt.rcParams["figure.figsize"] = fig_size

f, (ax1, ax2, ax3, ax4, ax5, ax6, ax7, ax8, ax9, ax10, ax11, ax12, ax13, ax14) = p
lt.subplots(14, sharex=True, sharey=True)
ax1.scatter(train['cont1'],train['loss'])
f, (ax1).title.set_text('cont1')
ax2.scatter(train['cont2'],train['loss'])
f, (ax2).title.set_text('cont2')
ax3.scatter(train['cont3'],train['loss'])
f, (ax3).title.set_text('cont3')
ax4.scatter(train['cont4'],train['loss'])
f, (ax4).title.set_text('cont4')
ax5.scatter(train['cont5'],train['loss'])
f, (ax5).title.set_text('cont5')
ax6.scatter(train['cont6'],train['loss'])
f, (ax6).title.set_text('cont6')
ax7.scatter(train['cont7'],train['loss'])
f, (ax7).title.set_text('cont6')
ax8.scatter(train['cont8'],train['loss'])
f, (ax8).title.set_text('cont8')
ax9.scatter(train['cont9'],train['loss'])
f, (ax9).title.set_text('cont9')
ax10.scatter(train['cont10'],train['loss'])
f, (ax10).title.set_text('cont10')
ax11.scatter(train['cont11'],train['loss'])
f, (ax11).title.set_text('cont11')
ax12.scatter(train['cont12'],train['loss'])
f, (ax12).title.set_text('cont12')
ax13.scatter(train['cont13'],train['loss'])
f, (ax13).title.set_text('cont13')
ax14.scatter(train['cont14'],train['loss'])
f, (ax14).title.set_text('cont14')
```

Out[6]:

```
(<matplotlib.figure.Figure at 0x11633b3c8>, None)
```

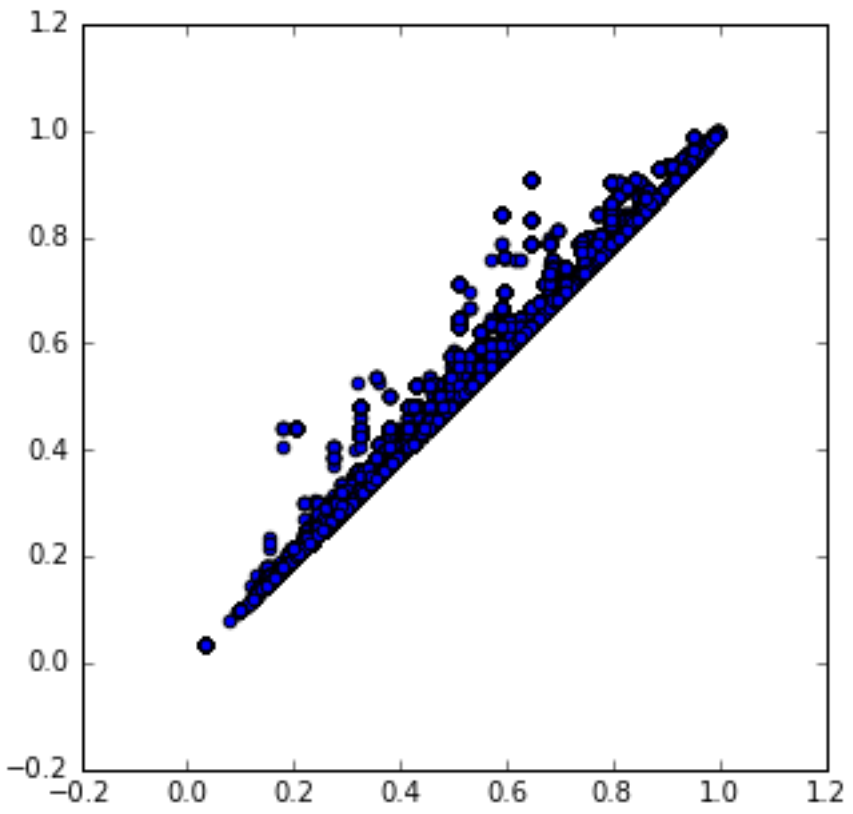

cont1
cont2
cont3
cont4
cont5
cont6
cont7
cont8
cont9
cont10
cont11
cont12
cont13
cont14
140000
120000
100000
80000
60000
40000
20000
0
−20000
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
1.2

Some features seem highly correlated

In [7]:

```
# Plot two variables against eachother that seem correlated
fig_size = plt.rcParams["figure.figsize"]
fig_size[0] = 5
fig_size[1] = 5
plt.rcParams["figure.figsize"] = fig_size
plt.scatter(train['cont11'],train['cont12'])
# Determine correlation r2 between the two variables
r2 = r2_score(train['cont11'],train['cont12'])
print('cont11 and cont12 are highly correlated with r2 score of %f' %r2)
# PCA should take care of these but lets drop one of them just in case
train.drop(labels=['cont11'], axis=1,inplace = True)
train_sub.drop(labels=['cont11'], axis=1,inplace = True)
cross_val.drop(labels=['cont11'], axis=1,inplace = True)
test.drop(labels=['cont11'], axis=1,inplace = True)
```

```
cont11 and cont12 are highly correlated with r2 score of 0.988691
```



PCA to perform dimensionality reduction and take care of correlated features

In [8]:

```
# PCA
pca= decomposition.PCA(n_components=75)
train_pca = pca.fit_transform(train.iloc[:,2:])
train_sub_pca = pca.transform(train_sub.iloc[:,2:])
cross_val_pca = pca.transform(cross_val.iloc[:,2:])
test_pca = pca.transform(test.iloc[:,1:])
```

Random Forest Model

In [9]:

```
# Random Forest Regression
#rf = RandomForestRegressor(n_estimators = 100, criterion='mse',min_samples_leaf=1
0,max_features = 100, random_state = 3)
rf = RandomForestRegressor(n_estimators = 100, criterion='mse',min_samples_split=4
0,min_samples_leaf=20,max_features = 40, random_state = 3)
#rf = RandomForestRegressor(n_estimators = 5, criterion='mse',min_samples_leaf=15,
max_features = 100)

start_time = time.time()
# train the model
rf.fit(train_sub.iloc[:,2:],train_sub.iloc[:,0])
#rf.fit(train_sub_pca,train_sub.iloc[:,0])
elapsed_time = time.time() - start_time
print('Model trained in  %f seconds' % elapsed_time)

# predict the loss for training and cross validation
loss_pred_train = rf.predict(train_sub.iloc[:,2:])
#loss_pred_train = rf.predict(train_sub_pca)
MAE_train = mean_absolute_error(train_sub.iloc[:,0],loss_pred_train)
print('MAE on training set = %f' % MAE_train)

loss_pred_cv = rf.predict(cross_val.iloc[:,2:])
#loss_pred_cv = rf.predict(cross_val_pca)
MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)
print('MAE on cross validation set = %f' % MAE_cv)
```

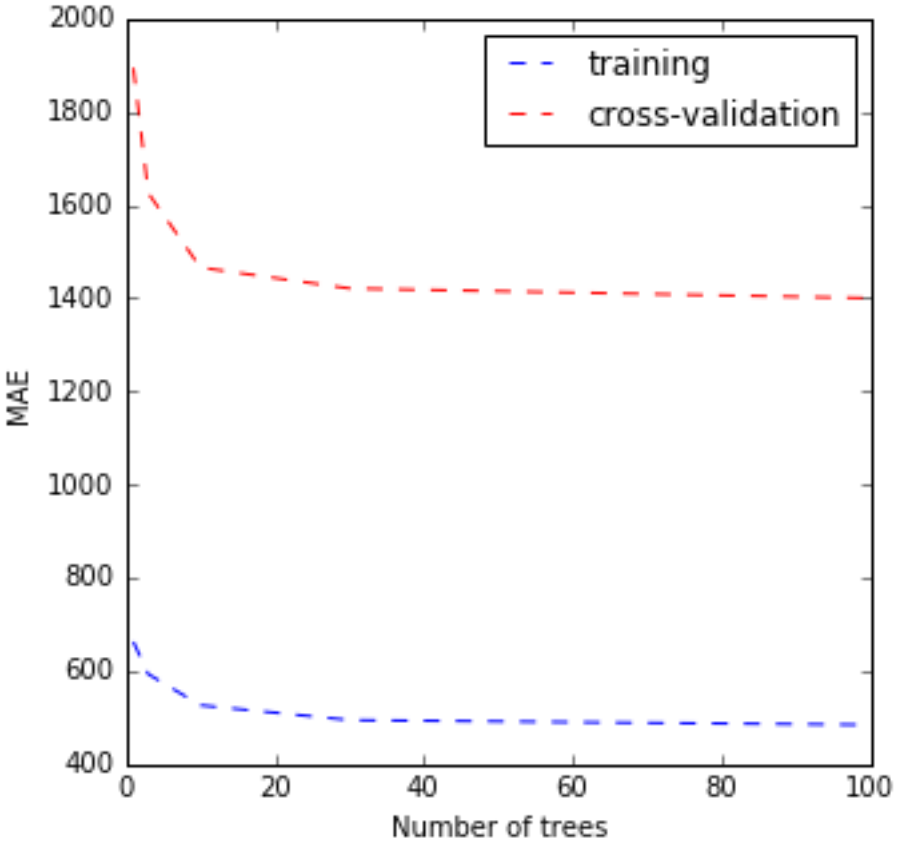
```
Model trained in  49.237059 seconds
MAE on training set = 1146.780570
MAE on cross validation set = 1249.461602
```

In [10]:

```
# Choose Number of Trees
trees = [1,3,10,30,100]
train_error_all = []
cv_error_all = []
size = 1000;
for i in range(len(trees)):
    rf = RandomForestRegressor(n_estimators = trees[i], random_state = 3)
    rf.fit(train_sub.iloc[:size,2:],train_sub.iloc[:size,0])
    loss_pred_train = rf.predict(train_sub.iloc[:size,2:])
    MAE_train = mean_absolute_error(train_sub.iloc[:size,0],loss_pred_train)
    loss_pred_cv = rf.predict(cross_val.iloc[:,2:])
    MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)

    train_error_all = np.append(train_error_all,MAE_train)
    cv_error_all = np.append(cv_error_all,MAE_cv)

pylab.plot(trees,train_error_all,'b--',label='training')
pylab.plot(trees,cv_error_all,'r--',label='cross-validation')
pylab.legend(loc='upper right')
pylab.xlabel('Number of trees')
pylab.ylabel('MAE')
```

Out[10]:

```
<matplotlib.text.Text at 0x118fdd0f0>
```

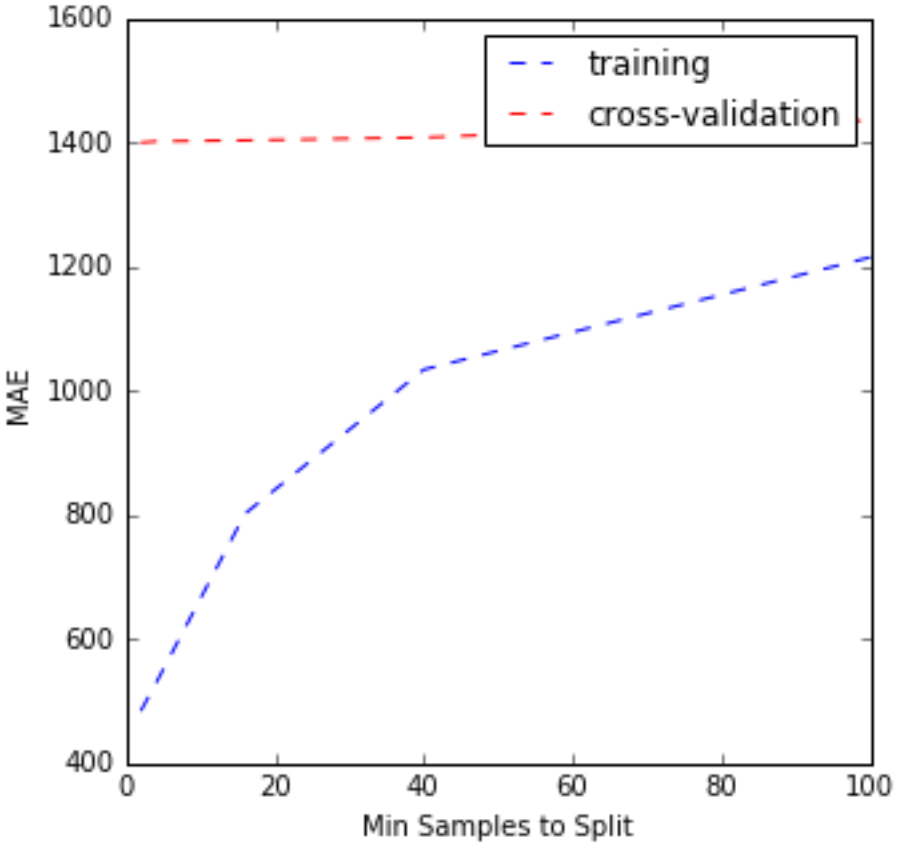


In [11]:

```
# Choose Min Samples to Split
splits = [2,4,16,40,100]
train_error_all = []
cv_error_all = []
size = 1000;
for i in range(len(trees)):
    rf = RandomForestRegressor(n_estimators = 100, min_samples_split=splits[i], ra
ndom_state = 3)
    rf.fit(train_sub.iloc[:size,2:],train_sub.iloc[:size,0])
    loss_pred_train = rf.predict(train_sub.iloc[:size,2:])
    MAE_train = mean_absolute_error(train_sub.iloc[:size,0],loss_pred_train)
    loss_pred_cv = rf.predict(cross_val.iloc[:,2:])
    MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)

    train_error_all = np.append(train_error_all,MAE_train)
    cv_error_all = np.append(cv_error_all,MAE_cv)

pylab.plot(splits,train_error_all,'b--',label='training')
pylab.plot(splits,cv_error_all,'r--',label='cross-validation')
pylab.legend(loc='upper right')
pylab.xlabel('Min Samples to Split')
pylab.ylabel('MAE')
```

Out[11]:

```
<matplotlib.text.Text at 0x1162bdfd0>
```

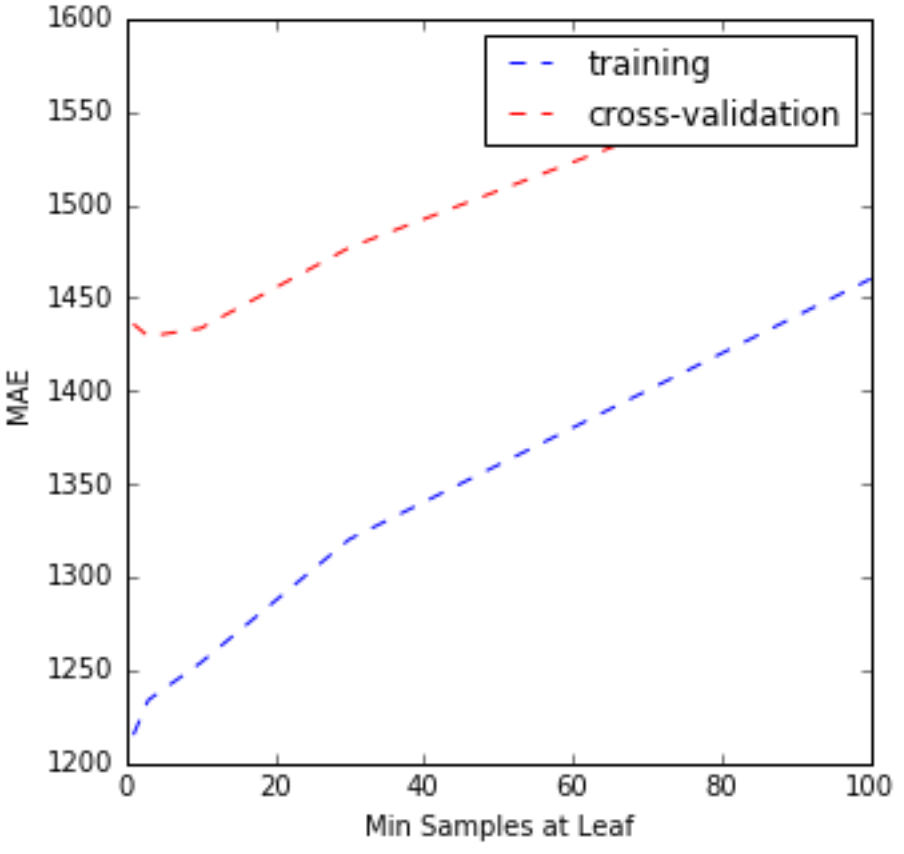


In [12]:

```
# Choose Min Samples at Leaf
leaf = [1,3,10,30,100]
train_error_all = []
cv_error_all = []
size = 1000;
for i in range(len(trees)):
    rf = RandomForestRegressor(n_estimators = 100, min_samples_split=100,min_sampl
es_leaf=leaf[i], random_state = 3)
    rf.fit(train_sub.iloc[:size,2:],train_sub.iloc[:size,0])
    loss_pred_train = rf.predict(train_sub.iloc[:size,2:])
    MAE_train = mean_absolute_error(train_sub.iloc[:size,0],loss_pred_train)
    loss_pred_cv = rf.predict(cross_val.iloc[:,2:])
    MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)

    train_error_all = np.append(train_error_all,MAE_train)
    cv_error_all = np.append(cv_error_all,MAE_cv)

pylab.plot(leaf,train_error_all,'b--',label='training')
pylab.plot(leaf,cv_error_all,'r--',label='cross-validation')
pylab.legend(loc='upper right')
pylab.xlabel('Min Samples at Leaf')
pylab.ylabel('MAE')
```

Out[12]:

```
<matplotlib.text.Text at 0x116774080>
```

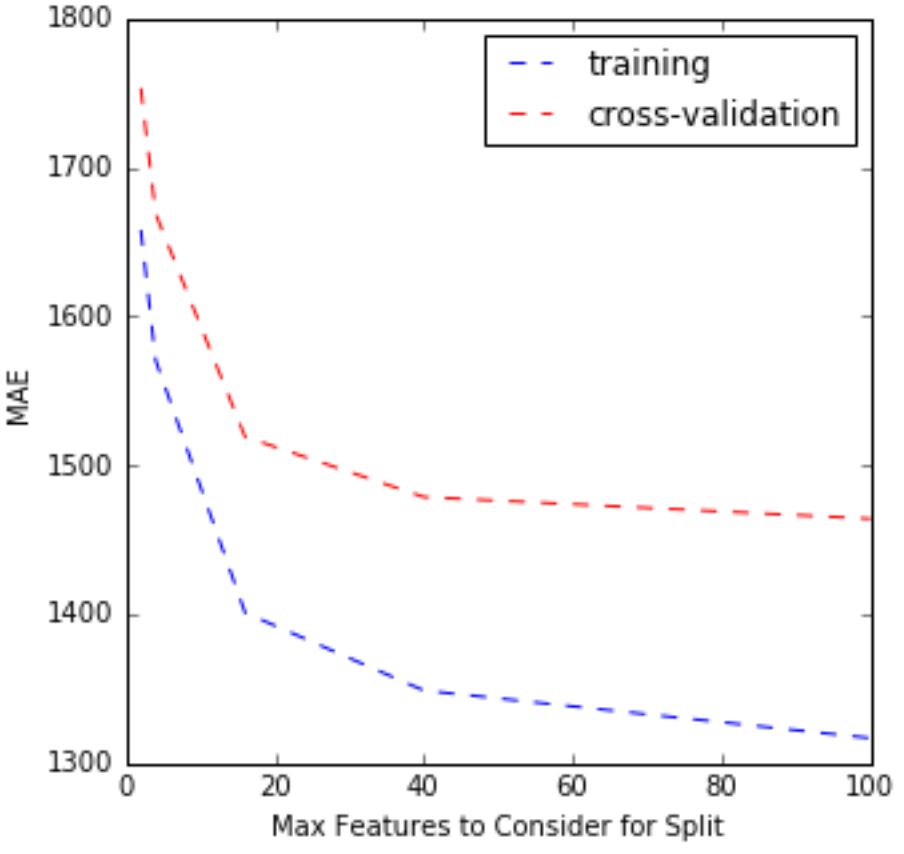


In [13]:

```
# Choose Max Features to consider
feat = [2,4,16,40,100]
train_error_all = []
cv_error_all = []
size = 1000;
for i in range(len(trees)):
    rf = RandomForestRegressor(n_estimators = 100, min_samples_split=100,min_sampl
es_leaf=20,max_features = feat[i], random_state = 3)
    rf.fit(train_sub.iloc[:size,2:],train_sub.iloc[:size,0])
    loss_pred_train = rf.predict(train_sub.iloc[:size,2:])
    MAE_train = mean_absolute_error(train_sub.iloc[:size,0],loss_pred_train)
    loss_pred_cv = rf.predict(cross_val.iloc[:,2:])
    MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)

    train_error_all = np.append(train_error_all,MAE_train)
    cv_error_all = np.append(cv_error_all,MAE_cv)

pylab.plot(feat,train_error_all,'b--',label='training')
pylab.plot(feat,cv_error_all,'r--',label='cross-validation')
pylab.legend(loc='upper right')
pylab.xlabel('Max Features to Consider for Split')
pylab.ylabel('MAE')
```

Out[13]:

```
<matplotlib.text.Text at 0x1129a5cf8>
```



In [ ]:

```
# Try on the test set and make kaggle output
loss_pred_test = rf.predict(test.iloc[:,1:])
#loss_pred_test = rf.predict(test_pca)

test_results_id = test['id']
test_results_loss = loss_pred_test

# Create results data frame
test_df = pd.DataFrame(data=test_results_id)
test_df.insert(1, 'loss', test_results_loss)

# Save output to csv format
test_df.to_csv('RF_results.csv',index = False)
```

Lasso Model

In [14]:

```
# Lasso Regression
lasso = Lasso(alpha=0.1);

pca_bool = True;

x_train = train_sub_pca
x_cv = cross_val_pca

if (pca_bool == True):
    lasso.fit(x_train,train_sub.iloc[:,0])
    loss_pred_train = lasso.predict(x_train)
    loss_pred_cv = lasso.predict(x_cv)
else:
    lasso.fit(train_sub.iloc[:,2:],train_sub.iloc[:,0])
    loss_pred_train = lasso.predict(train_sub.iloc[:,2:])
    loss_pred_cv = lasso.predict(cross_val.iloc[:,2:])

# predict the loss for training and cross validation
MAE_train = mean_absolute_error(train_sub.iloc[:,0],loss_pred_train)
print('MAE on training set = %f' % MAE_train)

MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)
print('MAE on cross validation set = %f' % MAE_cv)
```

```
MAE on training set = 1359.122693
MAE on cross validation set = 1364.807023
```

In [ ]:

```
# Try on the test set and make kaggle output
loss_pred_test = lasso.predict(test_pca)

test_results_id = test['id']
test_results_loss = loss_pred_test

# Create results data frame
test_df = pd.DataFrame(data=test_results_id)
test_df.insert(1, 'loss', test_results_loss)

# Save output to csv format
test_df.to_csv('LASSO_results.csv',index = False)
```

Support Vector Model

In [ ]:

```
# Support Vector Regression
svr = SVR(kernel='rbf', epsilon = 0.1);
#svr = SVR(kernel='poly', degree=2);
size = 100;
svr.fit(train_sub_pca[0:size,:],train_sub.iloc[0:size,0])

# predict the loss for training and cross validation
#loss_pred_train = rf.predict(train_sub.iloc[:,2:])
loss_pred_train = svr.predict(train_sub_pca)
MAE_train = mean_absolute_error(train_sub.iloc[:,0],loss_pred_train)
print('MAE on training set = %f' % MAE_train)

#loss_pred_cv = rf.predict(cross_val.iloc[:,2:])
loss_pred_cv = svr.predict(cross_val_pca)
MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)
print('MAE on cross validation set = %f' % MAE_cv)
```

Bayesian Model

In [ ]:

```
poly = PolynomialFeatures(degree=2,interaction_only=True)
x = poly.fit_transform(train_sub_pca)
x.shape
```

In [ ]:

```
# Bayesian regression w/ poly features
br = BayesianRidge();

x_poly = poly.transform(train_sub_pca)
cv_poly = poly.transform(cross_val_pca)

br.fit(x_poly,train_sub.iloc[:,0])

# predict the loss for training and cross validation
#loss_pred_train = br.predict(train_sub_pca)
loss_pred_train = br.predict(x_poly)
MAE_train = mean_absolute_error(train_sub.iloc[:,0],loss_pred_train)
print('MAE on training set = %f' % MAE_train)

#loss_pred_cv = br.predict(cross_val_pca)
loss_pred_cv = br.predict(cv_poly)
MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)
print('MAE on cross validation set = %f' % MAE_cv)
```

In [ ]:

```
# Try on the test set and make kaggle output
loss_pred_test = br.predict(poly.transform(test_pca))

test_results_id = test['id']
test_results_loss = loss_pred_test

# Create results data frame
test_df = pd.DataFrame(data=test_results_id)
test_df.insert(1, 'loss', test_results_loss)

# Save output to csv format
test_df.to_csv('Poly_Bayesian_results.csv',index = False)
```

Multi-layer Perceptron

In [15]:

```
# MLP Regressor
#nn = MLPRegressor(hidden_layer_sizes=(100, 100, 100, 100, 100, 100, 100, 100, 100
, 100), activation = 'relu',random_state = 13)
nn = MLPRegressor(hidden_layer_sizes=(30, 30, 30,), activation = 'relu',random_sta
te = 2)

start_time = time.time()
# train the model
nn.fit(train_sub.iloc[0:,2:],train_sub.iloc[0:,0])

elapsed_time = time.time() - start_time
print('Model trained in  %f seconds' % elapsed_time)

# predict the loss for training and cross validation
loss_pred_train = nn.predict(train_sub.iloc[:,2:])

MAE_train = mean_absolute_error(train_sub.iloc[:,0],loss_pred_train)
print('MAE on training set = %f' % MAE_train)

loss_pred_cv = nn.predict(cross_val.iloc[:,2:])


MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)
print('MAE on cross validation set = %f' % MAE_cv)
```

```
Model trained in  54.765320 seconds
MAE on training set = 1242.430098
MAE on cross validation set = 1257.990008
```

In [16]:

```
# Choose Activation Function
act = ['identity', 'logistic', 'tanh', 'relu']
train_error_all = []
cv_error_all = []
size = 1000;
for i in range(len(act)):
    nn = MLPRegressor(activation = act[i])
    nn.fit(train_sub.iloc[:size,2:],train_sub.iloc[:size,0])
    loss_pred_train = nn.predict(train_sub.iloc[:size,2:])
    MAE_train = mean_absolute_error(train_sub.iloc[:size,0],loss_pred_train)
    loss_pred_cv = nn.predict(cross_val.iloc[:,2:])
    MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)

    train_error_all = np.append(train_error_all,MAE_train)
    cv_error_all = np.append(cv_error_all,MAE_cv)

print(cv_error_all)
print(train_error_all)
```

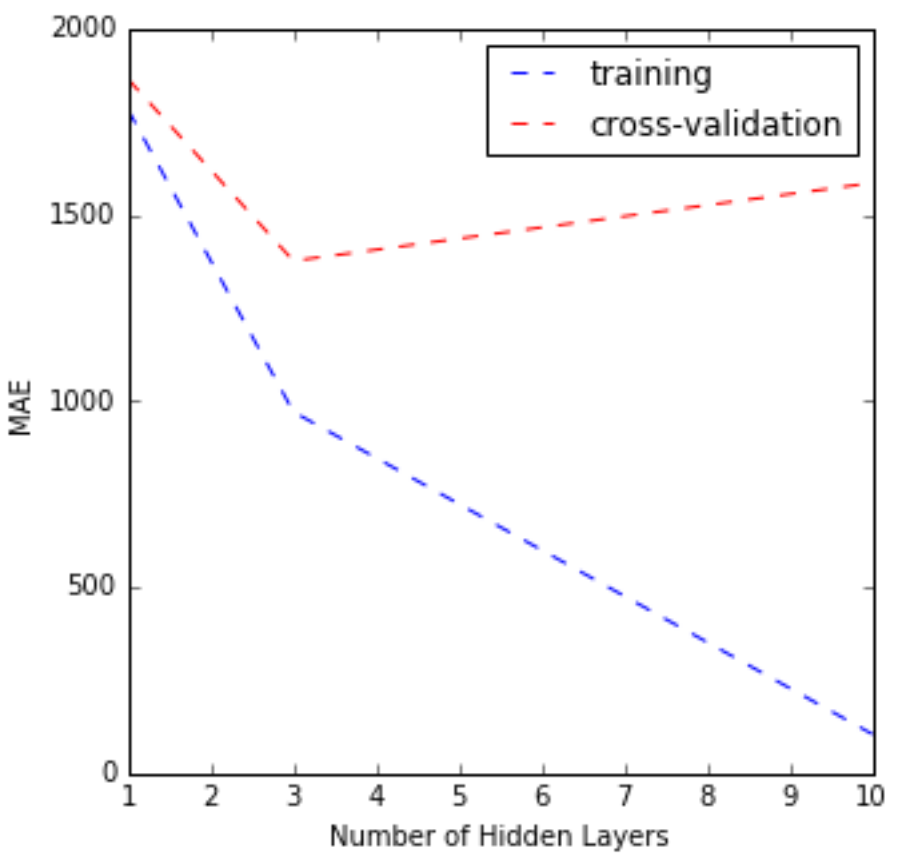
```
[ 1824.86250227  2940.84139112  2909.51261542  1868.47162348]
[ 1741.52089315  2802.98512511  2771.7013301   1786.74260806]
```

In [18]:

```
# Choose Number of Hidden Layers
num_layers = [1,3,10]

train_error_all = []
cv_error_all = []
size = 1000;
for i in range(len(num_layers)):
    if (i ==0):
        nn = MLPRegressor(activation = 'relu', hidden_layer_sizes=(100,))
    elif (i == 1):
        nn = MLPRegressor(activation = 'relu', hidden_layer_sizes=(100,100,100,))
    elif (i == 2):
        nn = MLPRegressor(activation = 'relu', hidden_layer_sizes=(100,100,100,100
,100,100,100,100,100,100,))
    nn.fit(train_sub.iloc[:size,2:],train_sub.iloc[:size,0])
    loss_pred_train = nn.predict(train_sub.iloc[:size,2:])
    MAE_train = mean_absolute_error(train_sub.iloc[:size,0],loss_pred_train)
    loss_pred_cv = nn.predict(cross_val.iloc[:,2:])
    MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)

    train_error_all = np.append(train_error_all,MAE_train)
    cv_error_all = np.append(cv_error_all,MAE_cv)

pylab.plot(num_layers,train_error_all,'b--',label='training')
pylab.plot(num_layers,cv_error_all,'r--',label='cross-validation')
pylab.legend(loc='upper right')
pylab.xlabel('Number of Hidden Layers')
pylab.ylabel('MAE')
```

Out[18]:

```
<matplotlib.text.Text at 0x122b77ac8>
```

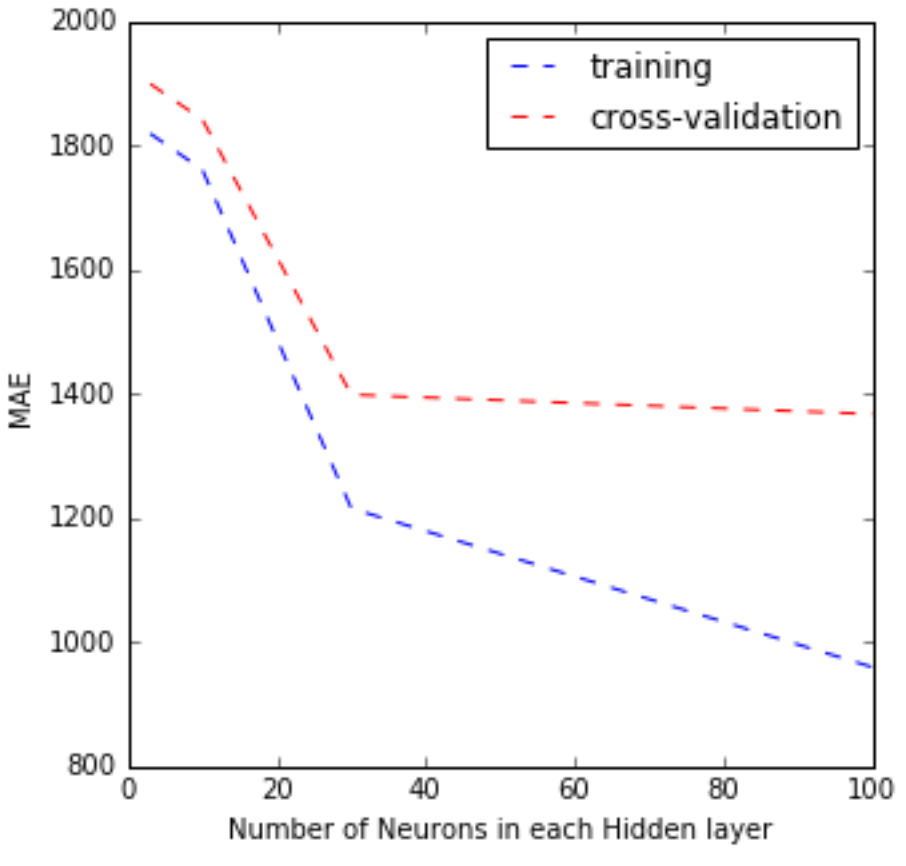


In [19]:

```
# Choose Hidden Layer Size
layer_size = [3,10,30,100]

train_error_all = []
cv_error_all = []
size = 1000;
for i in range(len(layer_size)):
    nn = MLPRegressor(activation = 'relu', hidden_layer_sizes=(layer_size[i],layer
_size[i],layer_size[i],))
    nn.fit(train_sub.iloc[:size,2:],train_sub.iloc[:size,0])
    loss_pred_train = nn.predict(train_sub.iloc[:size,2:])
    MAE_train = mean_absolute_error(train_sub.iloc[:size,0],loss_pred_train)
    loss_pred_cv = nn.predict(cross_val.iloc[:,2:])
    MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)

    train_error_all = np.append(train_error_all,MAE_train)
    cv_error_all = np.append(cv_error_all,MAE_cv)

pylab.plot(layer_size,train_error_all,'b--',label='training')
pylab.plot(layer_size,cv_error_all,'r--',label='cross-validation')
pylab.legend(loc='upper right')
pylab.xlabel('Number of Neurons in each Hidden layer')
pylab.ylabel('MAE')
```

Out[19]:

```
<matplotlib.text.Text at 0x117782ba8>
```



In [ ]:

```
# Try on the test set and make kaggle output
loss_pred_test = nn.predict(test.iloc[:,1:])
#loss_pred_test = rf.predict(test_pca)

test_results_id = test['id']
test_results_loss = loss_pred_test

# Create results data frame
test_df = pd.DataFrame(data=test_results_id)
test_df.insert(1, 'loss', test_results_loss)

# Save output to csv format
test_df.to_csv('NN_results.csv',index = False)
```

Combine MLP and RF

In [ ]:

```
# Combine RF and MLP
loss_pred_cv_rf = rf.predict(cross_val.iloc[:,2:])
loss_pred_cv_nn = nn.predict(cross_val.iloc[:,2:])
loss_pred_cv = (loss_pred_cv_rf + loss_pred_cv_nn)/2
#loss_pred_cv = rf.predict(cross_val_pca)
MAE_cv = mean_absolute_error(cross_val.iloc[:,0],loss_pred_cv)
print('MAE on cross validation set = %f' % MAE_cv)
```

In [ ]:

```
# Try on the test set and make kaggle output
loss_pred_test = (nn.predict(test.iloc[:,1:]) + rf.predict(test.iloc[:,1:]))/2
#loss_pred_test = rf.predict(test_pca)

test_results_id = test['id']
test_results_loss = loss_pred_test

# Create results data frame
test_df = pd.DataFrame(data=test_results_id)
test_df.insert(1, 'loss', test_results_loss)

# Save output to csv format
test_df.to_csv('NN_RF_combo_results.csv',index = False)
```