SMBO

January 29, 2019

1 SMBO for Neural Networks

1.1 Sebastian Pineda Arango M.N.: 246098

1.2 Hildesheim Universität

In [44]:
```
import tensorflow as tf
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

%matplotlib inline

#importing the data
data_train = pd.read_csv("train.csv")
data_test = pd.read_csv("test.csv")
```

In [45]:
```
data_train.head()
```

Out[45]:
```
          X  sigmoidOfX
0 -0.973277    0.274228
1 -0.498346    0.377929
2  0.881254    0.707082
3  0.966152    0.724352
4 -0.276218    0.431381
```

In [46]:
```
data_test.head()
```

Out[46]:
```
          X  sigmoidOfX
0  0.341577    0.584574
1  0.891632    0.709227
2  0.946714    0.720454
3  0.450208    0.610689
4 -0.345155    0.414558
```

In [47]:
```
#diving data in features and labels
X_train = np.array(data_train['X']).reshape(-1,1)
y_train = np.array(data_train['sigmoidOfX']).reshape(-1,1)
```

```
X_test = np.array(data_test['X']).reshape(-1,1)
y_test = np.array(data_test['sigmoidOfX']).reshape(-1,1)
```

In [48]:
```
#creating the network: one hidden layer with two neurons
n_input=1
n_hidden1 = 2
n_output = 1

X = tf.placeholder(tf.float32, shape=(None, 1))
y = tf.placeholder(tf.float32, shape=(None, 1))
learning_rate = tf.placeholder(tf.float32)

weights = {
    'W' : tf.Variable(tf.truncated_normal([n_input, n_hidden1], seed=1)),
    'out' : tf.Variable(tf.truncated_normal([n_hidden1, n_output], seed=1))
}

biases = {
    'b' : tf.Variable(tf.constant(0.1, shape=[n_hidden1] )),
    'b_out' : tf.Variable(tf.constant(0.1, shape = [n_output]))
}

layer = tf.add(tf.matmul(X, weights['W']), biases['b'])
output = tf.add(tf.matmul(layer, weights['out']), biases['b_out'])

l2_loss = tf.reduce_mean(tf.square(output-y),0)
train_step = tf.train.GradientDescentOptimizer(learning_rate).minimize(l2_loss)
```

In [49]:
```
#importing the gaussian process module from scikit-learn
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import (RBF)

#creating the surrogate model
kernel = RBF(length_scale=1.0, length_scale_bounds=(1e-1, 10.0))
gp = GaussianProcessRegressor(kernel=kernel)
```

In [50]:
```
#creating function to train and test the newtork
def train_and_test(X_train, y_train, lr, train_step):

    '''This function trains and tests the above-defined network '''

    n_train_samples = X_train.shape[0]

    with tf.Session() as sess:
        #initializing
        init = tf.global_variables_initializer()
        sess.run(init)
```

```
            #initializing index variables
            idx = list(range(n_train_samples))
            loss_list = list()

            #running the graph for training
            for i in range(2000):

                #picking a random sample
                idx = np.random.randint(n_train_samples)
                X_train_sample = X_train[idx,].reshape(-1, 1)
                y_train_sample = y_train[idx,].reshape(-1,1)

                #updating parameters
                sess.run(train_step, feed_dict={X: X_train_sample, y:y_train_sample, lear

                #calculating the loss
                loss = sess.run(l2_loss, feed_dict={X: X_train, y:y_train, learning_rate:l

                #appending the loss to list
                loss_list.append(loss)

            loss_test = sess.run(l2_loss, feed_dict={X: X_test, y:y_test})

        return loss_test, loss_list
```

```
In [51]: def acquisition(beta, mu, std):

             '''This acquisition function to evaluate the hyperparameter given the surrogate mo

             return (-mu+beta*std)

         #this is the search space for the hyperparameter to optimize
         lr_range = np.logspace(-5,0) #values generated in log scale
         beta = 2

         #initial points
         lr_list = [0.1, 0.00001]
         lr_loss = []

         for lr in lr_list:

             print("Trying ",lr)
             loss, loss_list = train_and_test(X_train, y_train, lr, train_step)
             lr_loss.append(loss[0])
             print("Loss:", loss[0])

         #Sequential model based optimization
         for i in range(10):
```

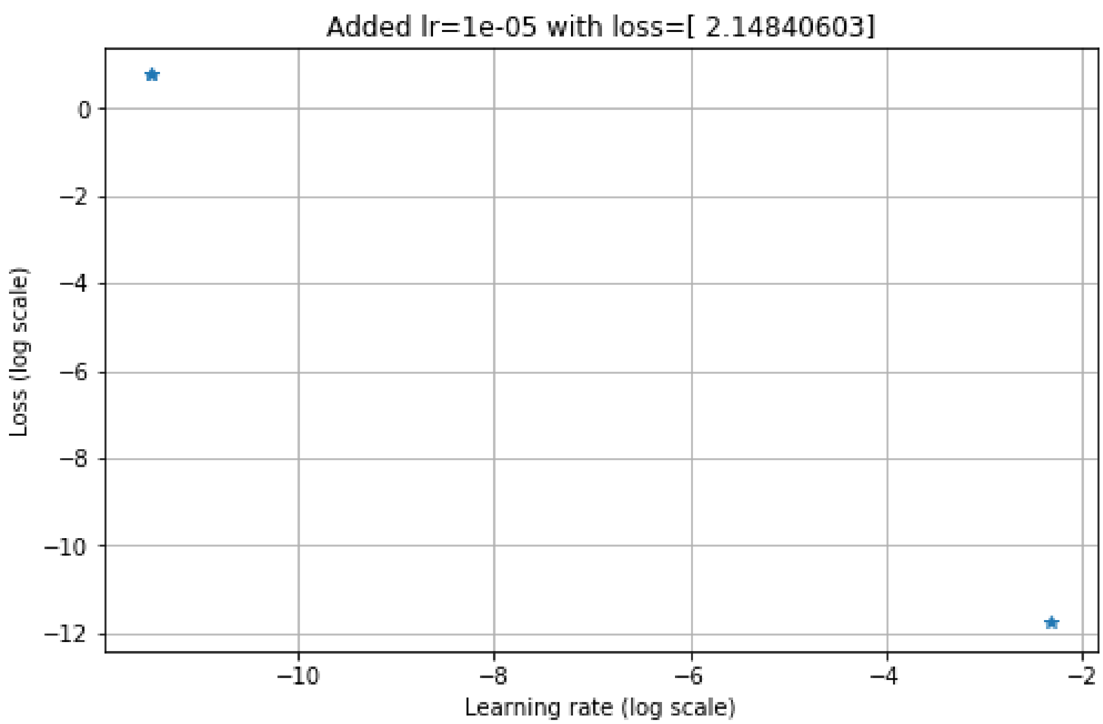
```python
            print("Iteration",i)

            x_1 = np.array(lr_list).reshape(-1,1)
            y_1 = np.array(lr_loss).reshape(-1,1)

            gp.fit(x_1,y_1)

            print("Making the prediction")
            mu, std = gp.predict(lr_range.reshape(-1,1), return_std=True)

            #adqusition evaluation of the hyperparameter
            a_lr = [acquisition(2, mu_i, std_i)[0] for mu_i, std_i in zip(mu,std)]
            new_lr = lr_range[np.argmin(a_lr)]
            loss, loss_list = train_and_test(X_train, y_train, new_lr, train_step)

            if(np.isnan(loss[0])):
                loss=1
                lr_loss.append(loss)
                lr_list.append(new_lr)
            else:
                lr_loss.append(loss[0])
                lr_list.append(new_lr)

            x_axis = np.log(lr_list)
            y_axis = np.log(lr_loss)
            fig, ax = plt.subplots(figsize=(8, 5))
            ax.plot( x_axis, y_axis , '*')
            ax.grid()
            ax.set_title("Added lr="+str(new_lr)+" with loss="+str(loss))
            ax.set_xlabel("Learning rate (log scale)")
            ax.set_ylabel("Loss (log scale)")
```

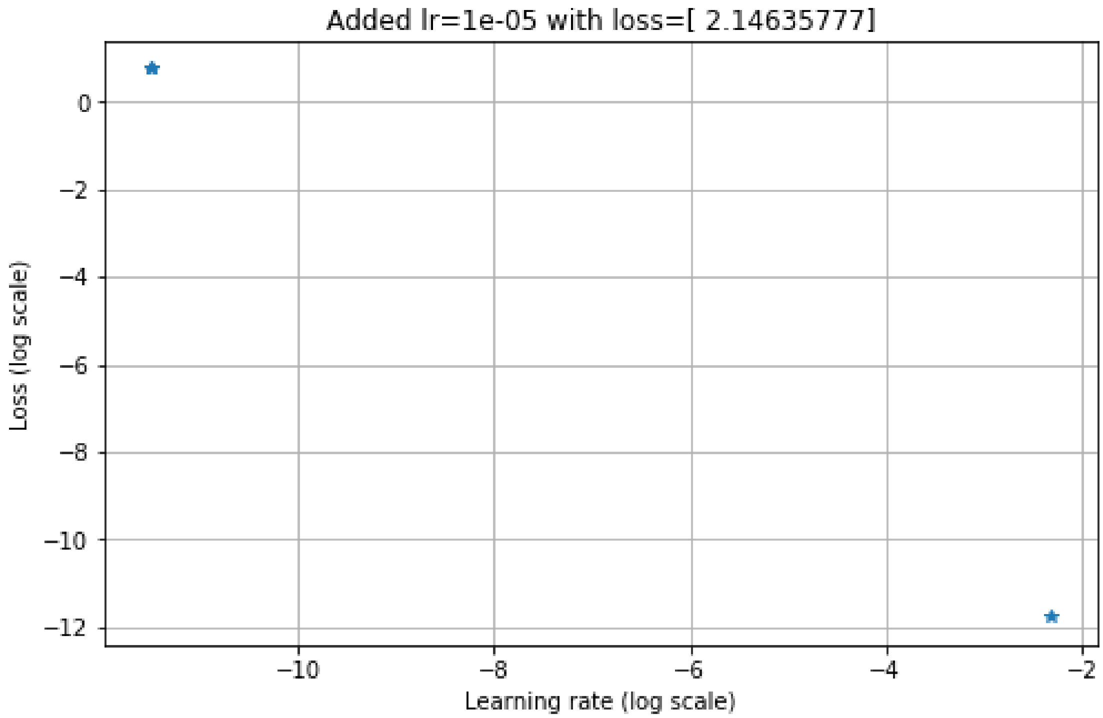
```
Trying  0.1
Loss: 7.62895e-06
Trying  1e-05
Loss: 2.15049
Iteration 0
Making the prediction
Iteration 1
Making the prediction
```

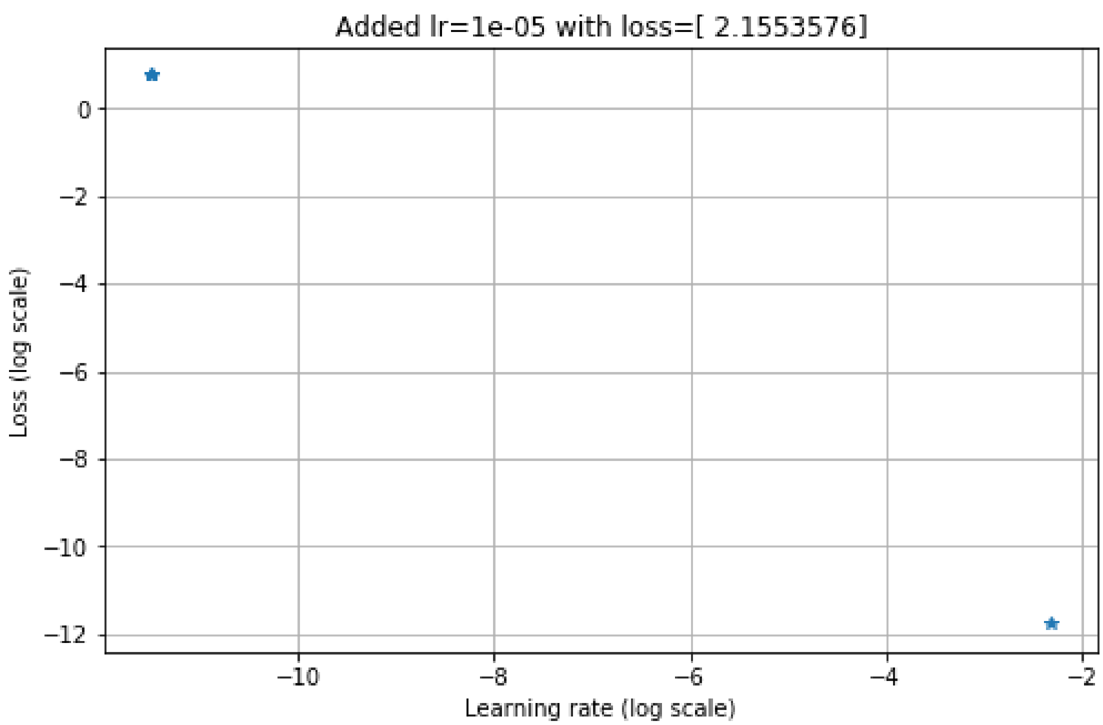
```
C:\Users\User\Anaconda3\lib\site-packages\sklearn\gaussian_process\gpr.py:335: UserWarning: Pre
  warnings.warn("Predicted variances smaller than 0. "
```

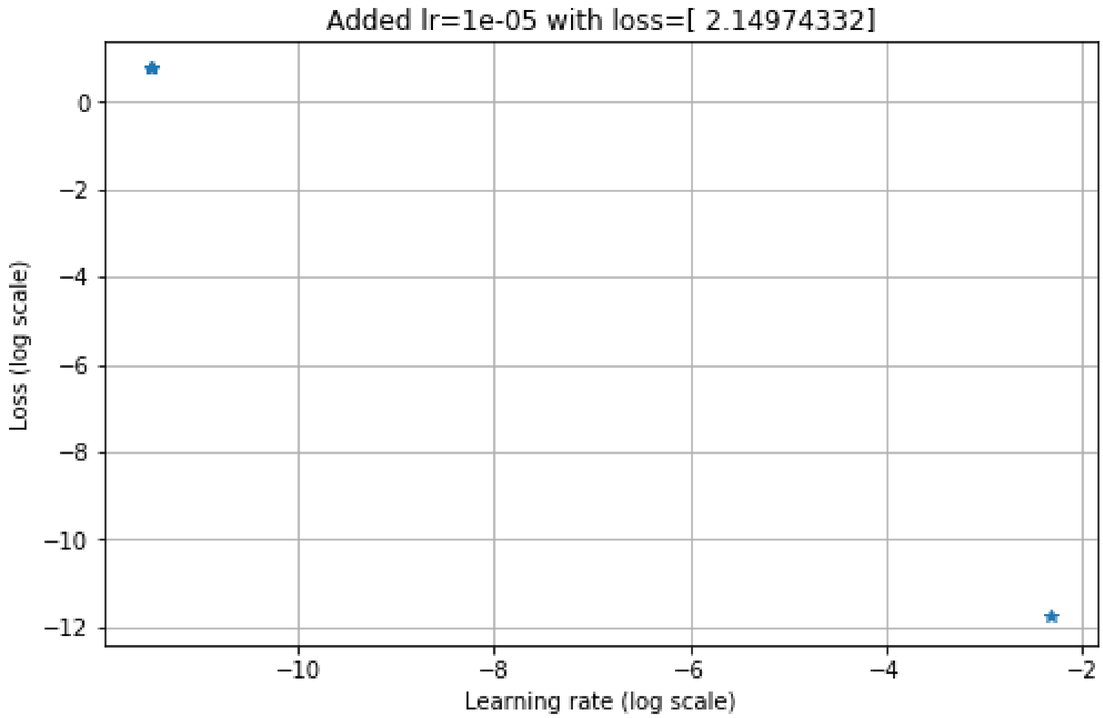
```
Iteration 2
```

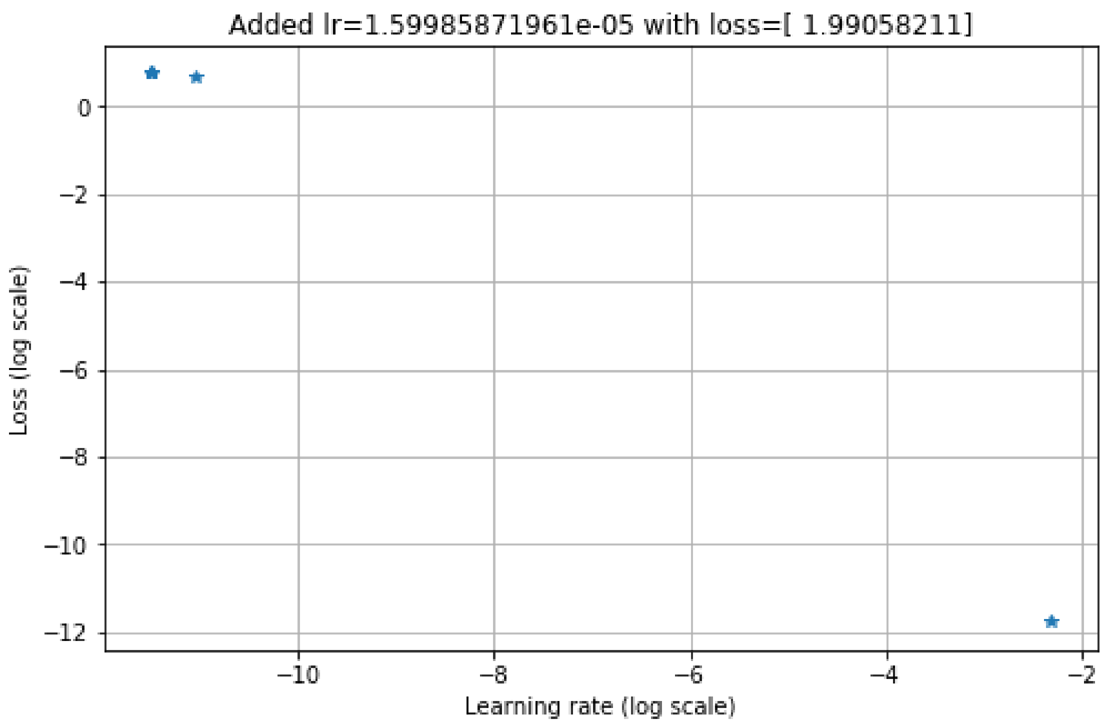
```
Making the prediction
Iteration 3
Making the prediction
Iteration 4
Making the prediction
Iteration 5
Making the prediction
Iteration 6
Making the prediction
Iteration 7
Making the prediction
Iteration 8
Making the prediction
Iteration 9
Making the prediction
```

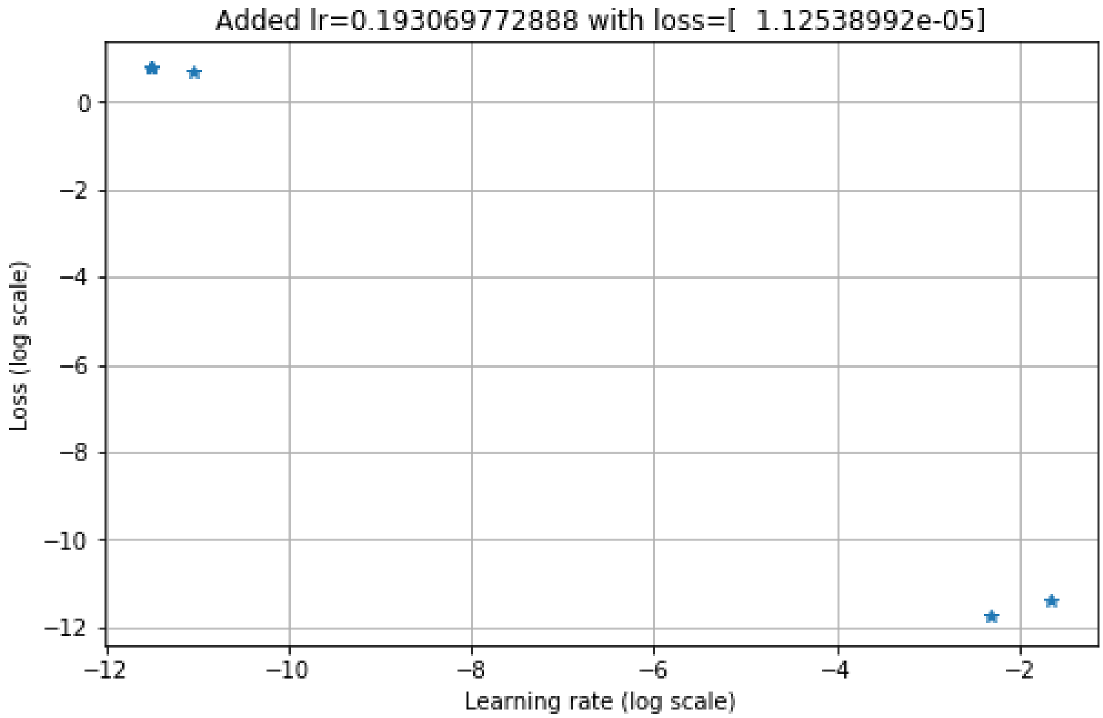


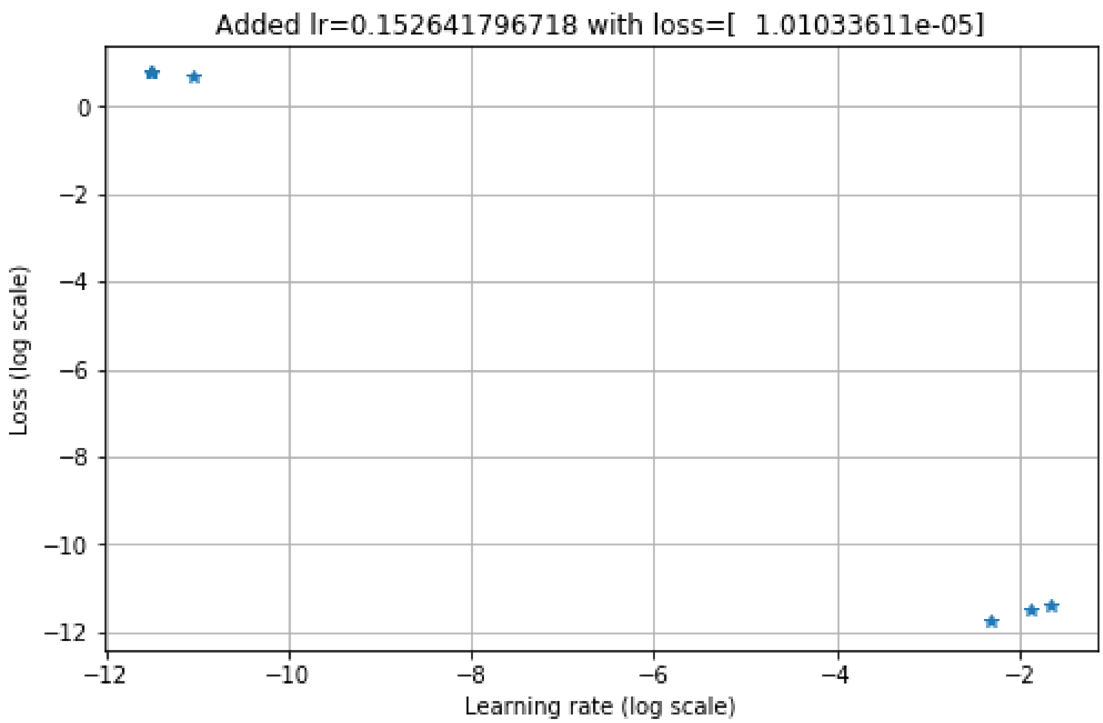

Added lr=1e-05 with loss=[2.14635777]
0
−2
−4
−6
−8
−10
−12
Loss (log scale)
−10
−8
−6
−4
−2
Learning rate (log scale)

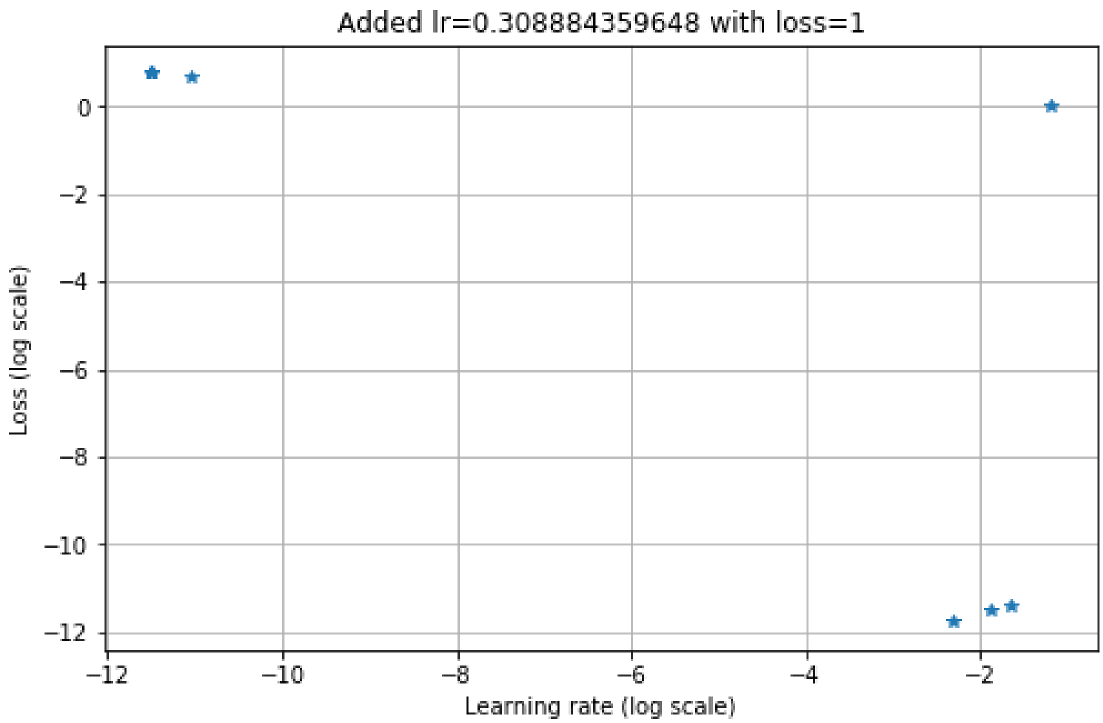

Added lr=1e-05 with loss=[2.1553576]
0
−2
−4
−6
−8
−10
−12
Loss (log scale)
−10
−8
−6
−4
−2
Learning rate (log scale)

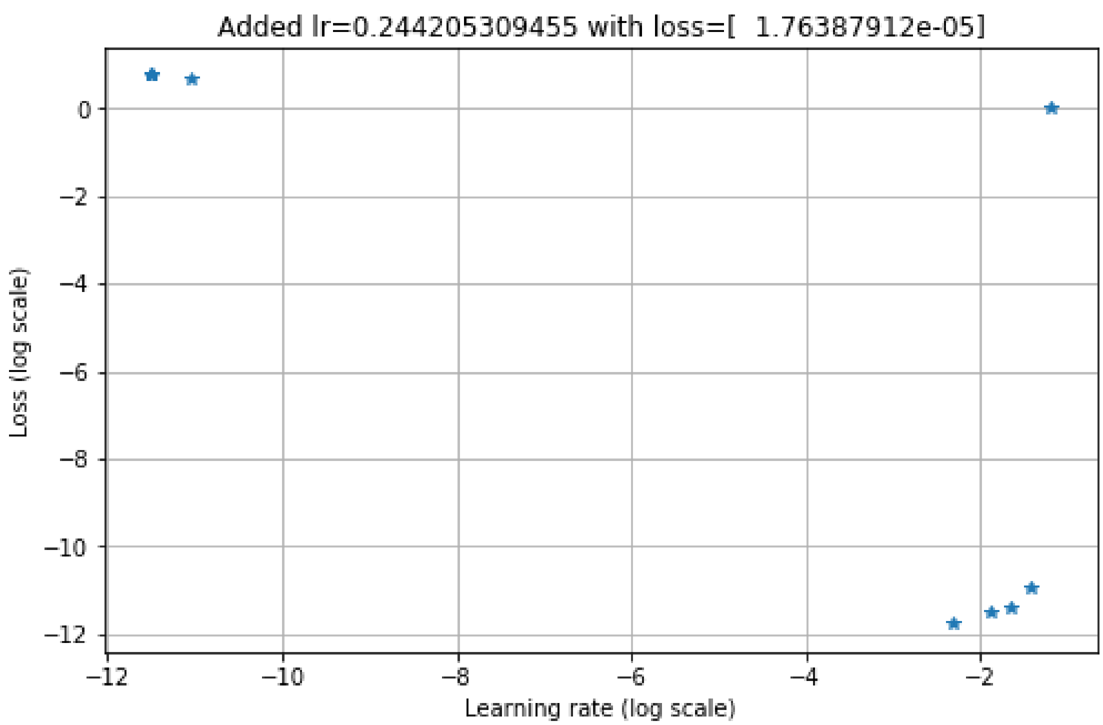

Added lr=1e-05 with loss=[2.14974332]
Loss (log scale)
Learning rate (log scale)

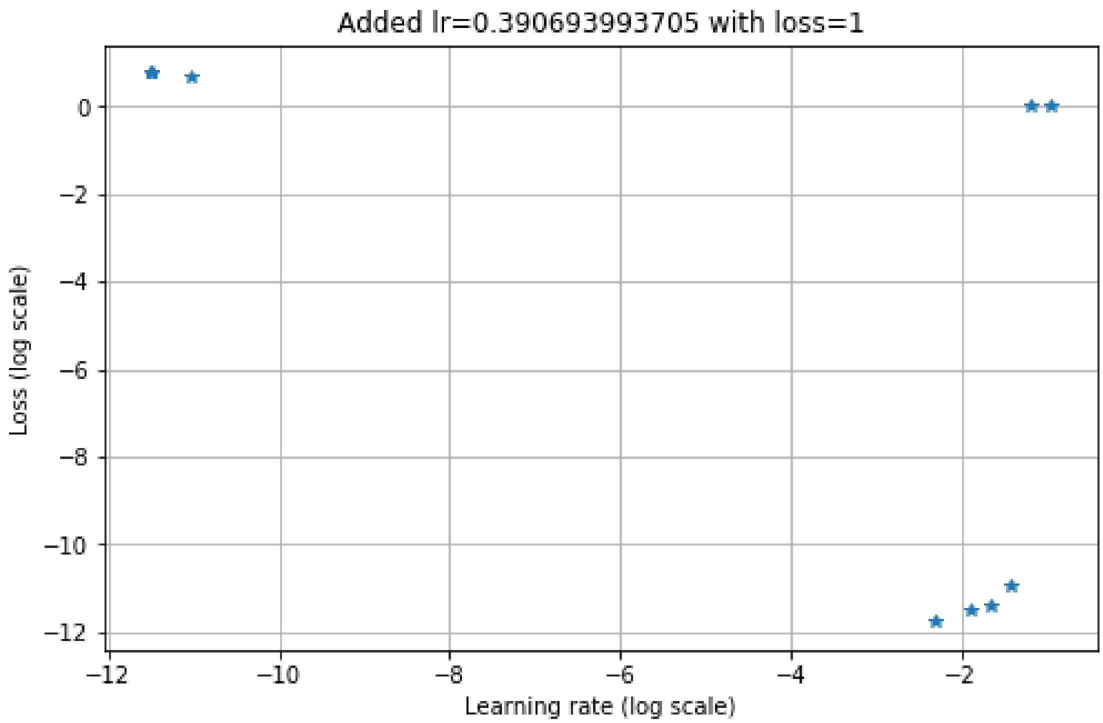

Added lr=1.59985871961e-05 with loss=[1.99058211]
Loss (log scale)
Learning rate (log scale)


Added lr=0.193069772888 with loss=[1.12538992e-05]
Loss (log scale)
0
−2
−4
−6
−8
−10
−12
−12
−10
−8
−6
−4
−2
Learning rate (log scale)


Added lr=0.152641796718 with loss=[1.01033611e-05]
Loss (log scale)
0
−2
−4
−6
−8
−10
−12
−12
−10
−8
−6
−4
−2
Learning rate (log scale)

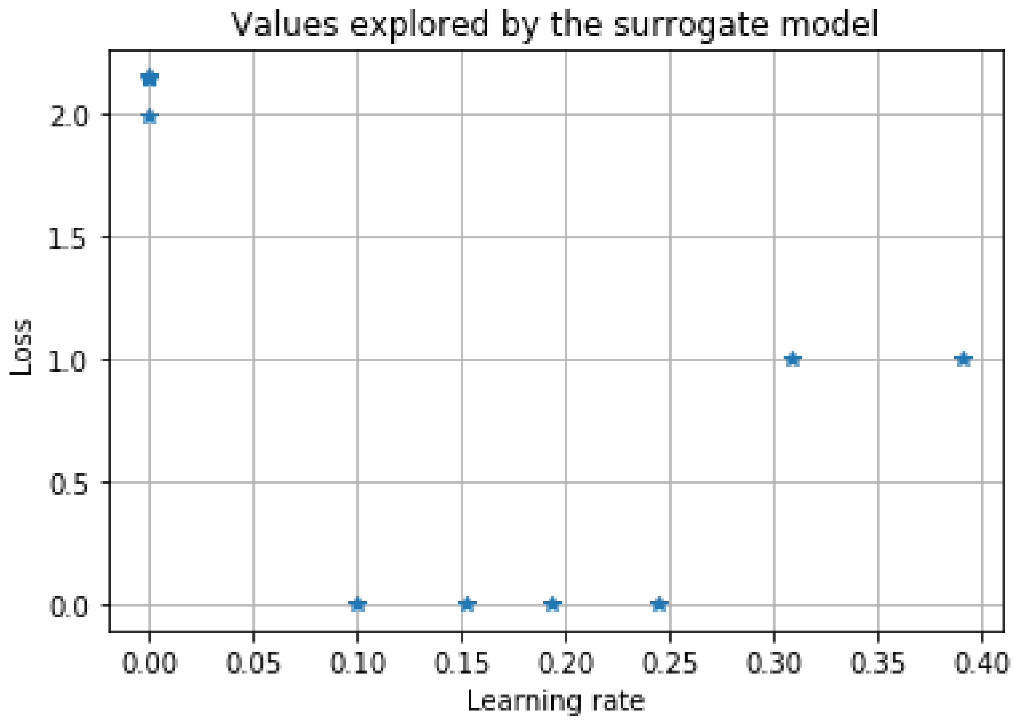

Added lr=0.308884359648 with loss=1
Loss (log scale)
0
−2
−4
−6
−8
−10
−12
Learning rate (log scale)
−12
−10
−8
−6
−4
−2


Added lr=0.244205309455 with loss=[1.76387912e-05]
Loss (log scale)
0
−2
−4
−6
−8
−10
−12
Learning rate (log scale)
−12
−10
−8
−6
−4
−2



In [52]:
```
#plotting the loss vs. hyperaparameters
plt.plot(lr_list, lr_loss, '*')
plt.grid()
plt.xlabel("Learning rate")
plt.ylabel("Loss")
plt.title("Values explored by the surrogate model")
```

Out[52]:
```
Text(0.5,1,'Values explored by the surrogate model')
```



In [53]:
```
best_lr= lr_list[np.argmin(lr_loss)]
print("Best learning rate:", best_lr)
```

```
Best learning rate: 0.1
```

In [54]:
```
#printing values learn by the surrogate model
pd.DataFrame({'Learning_rate': lr_list, 'Loss': lr_loss})
```

Out[54]:

	Learning_rate	Loss
0	0.100000	0.000008
1	0.000010	2.150491
2	0.000010	2.148406
3	0.000010	2.146358
4	0.000010	2.155358
5	0.000010	2.149743
6	0.000016	1.990582
7	0.193070	0.000011
8	0.152642	0.000010
9	0.308884	1.000000
10	0.244205	0.000018
11	0.390694	1.000000

In [55]:
```
#predicting over test samples
with tf.Session() as sess:
```

```
init = tf.global_variables_initializer()
sess.run(init)
y_pred = sess.run(output,  feed_dict={X: X_test, y:y_test})
```

In [56]:
```
#plotting predicted vs. expected values of test set
plt.plot(y_pred, y_test)
plt.grid()
plt.xlabel("Predicted")
plt.ylabel("Expected")
```

Out[56]:
```
Text(0,0.5,'Expected')
```