Diamonds.csv - MLPRegressor Hyperparameter Optimization:

FEDERAL UNIVERSITY OF RIO DE JANEIRO - EEL817 Neural Networks - 2020.4

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Loading Libraries and Dataset

In [1]:

```
%%time
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from math import log, sqrt
from pandas_profiling import ProfileReport
```

```
Wall time: 1.52 s
```

In [2]:

```
arqPath = "diamonds.csv"
data = pd.read_csv(arqPath, index_col = 0)
```

Exploratory Data Analysis

In [3]:

```
%%time
#profile = ProfileReport(data)
#profile.to_file("profile.html")
```

```
Wall time: 0 ns
```

In [4]:

```
#color = ['J', 'I', 'H', 'G', 'F', 'E', 'D']
#cut = ['Fair', 'Good', 'Very Good', 'Premium', 'Ideal']
#clarity = ['I1', 'SI2', 'SI1', 'VS2', 'VS1', 'VVS2', 'VVS1', 'IF']

colorsDict = {'J':1, 'I':2, 'H':3, 'G':4, 'F':5, 'E':6, 'D':7}
cutDict =  {'Fair':1, 'Good':2, 'Very Good':3, 'Premium':4, 'Ideal':5}
clarityDict = {'I1':1, 'SI2':2, 'SI1':3, 'VS2':4, 'VS1':5, 'VVS2':6, 'VVS1':7, 'IF':

color = [colorsDict[i] for i in data['color']]
cut = [cutDict[i] for i in data['cut']]
clarity = [clarityDict[i] for i in data['clarity']]

data['cut'] = cut
data['color'] = color
data['clarity'] = clarity
```

In [5]:

```
# New variable 'volume'
data['volume'] = data['x'] * data['y'] * data['z']
```

In [6]:

```
# Excluding outliers:

data = data[(data[['x','y','z']] != 0).all(axis=1)]
data = data[(data[['y']] < 20).all(axis=1)]
data = data[(data[['z']] < 20).all(axis=1)]
```

In [7]:
```
# Linearizing price:
data['price'] = data['price'].map(log)
```

In [8]:
```
%%time
data.describe()
```

```
Wall time: 40 ms
```

Out[8]:

	carat	cut	color	clarity	depth	table	
count	53917.000000	53917.000000	53917.000000	53917.000000	53917.000000	53917.000000	53917.0(
mean	0.797687	3.904223	4.405939	4.051505	61.749565	57.456939	7.7{
std	0.473777	1.116593	1.701281	1.647017	1.432318	2.234069	1.0'
min	0.200000	1.000000	1.000000	1.000000	43.000000	43.000000	5.7{
25%	0.400000	3.000000	3.000000	3.000000	61.000000	56.000000	6.8!
50%	0.700000	4.000000	4.000000	4.000000	61.800000	57.000000	7.7{
75%	1.040000	5.000000	6.000000	5.000000	62.500000	59.000000	8.5
max	5.010000	5.000000	7.000000	8.000000	79.000000	95.000000	9.8

In [9]:
```
%%time
# Normalization
AVG = data.mean()
STD = data.std()
dataNorm = (data-AVG)/STD

dataNorm.describe()
```

```
Wall time: 67 ms
```

Out[9]:

	carat	cut	color	clarity	depth	table
count	5.391700e+04	5.391700e+04	5.391700e+04	5.391700e+04	5.391700e+04	5.391700e+04
mean	4.196863e-14	-8.434211e-17	1.233503e-16	2.129638e-16	5.523612e-13	-2.290837e-14
std	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00
min	-1.261536e+00	-2.600968e+00	-2.001984e+00	-1.852747e+00	-1.309036e+01	-6.471125e+00
25%	-8.393963e-01	-8.098054e-01	-8.263999e-01	-6.384302e-01	-5.233230e-01	-6.521461e-01
50%	-2.061870e-01	8.577595e-02	-2.386077e-01	-3.127175e-02	3.521209e-02	-2.045324e-01
75%	5.114503e-01	9.813573e-01	9.369769e-01	5.758867e-01	5.239303e-01	6.906952e-01
max	8.890921e+00	9.813573e-01	1.524769e+00	2.397362e+00	1.204372e+01	1.680479e+01

In [10]:
```
%%time
#pairplot = sns.pairplot(dataNorm)
```

```
Wall time: 0 ns
```

In [11]:
```
dataNorm
```

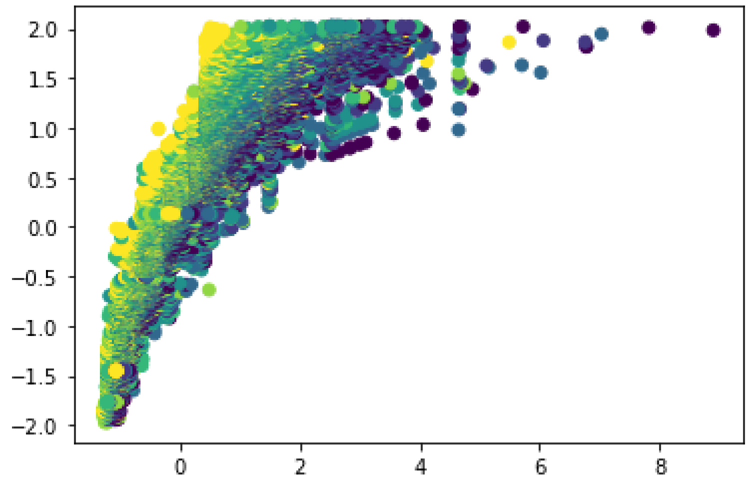
Out[11]:

	carat	cut	color	clarity	depth	table	price	x	
1	-1.198215	0.981357	0.936977	-1.245589	-0.174239	-1.099760	-1.970809	-1.591569	-1.577{

	carat	cut	color	clarity	depth	table	price	x	
2	-1.240429	0.085776	0.936977	-0.638430	-1.361126	1.585923	-1.970809	-1.645169	-1.7038
3	-1.198215	-1.705387	0.936977	0.575887	-3.385815	3.376378	-1.967790	-1.502235	-1.4968
4	-1.071573	0.085776	-1.414192	-0.031272	0.454113	0.243081	-1.946912	-1.368235	-1.3528
5	-1.029359	-1.705387	-2.001984	-1.245589	1.082465	0.243081	-1.943966	-1.243168	-1.2449
...	...	...	...	...	...	...	...	...	...
53936	-0.163973	0.981357	1.524769	-0.638430	-0.662957	-0.204532	0.133586	0.016433	0.0239
53937	-0.163973	-1.705387	1.524769	-0.638430	0.942832	-1.099760	0.133586	-0.037167	0.0149
53938	-0.206187	-0.809805	1.524769	-0.638430	0.733381	1.138309	0.133586	-0.063967	-0.0480
53939	0.131525	0.085776	-0.826400	-1.245589	-0.523323	0.243081	0.133586	0.373766	0.3478
53940	-0.100652	0.981357	1.524769	-1.245589	0.314480	-1.099760	0.133586	0.087899	0.1228

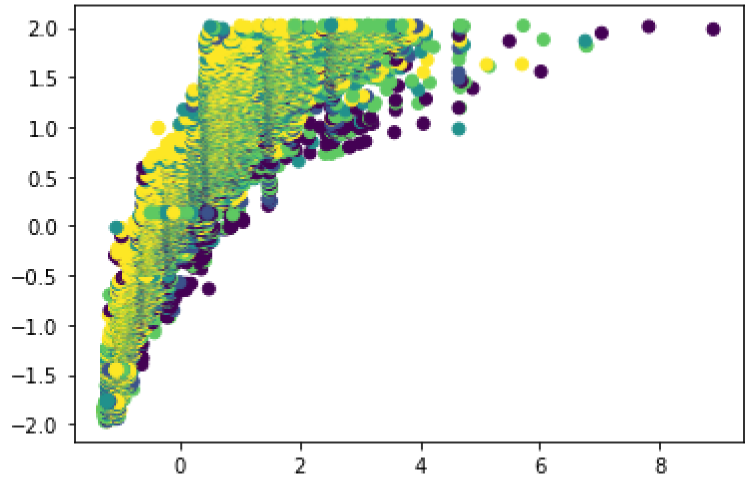
53917 rows × 11 columns

In [12]:
```
%%time
color = dataNorm['color']
plt.scatter(dataNorm['carat'], dataNorm['price'], c=color, cmap='viridis')
plt.show()
```

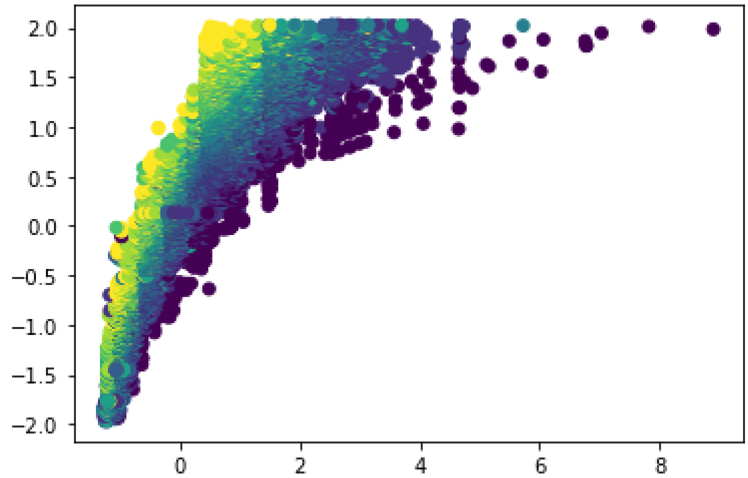



```
Wall time: 994 ms
```

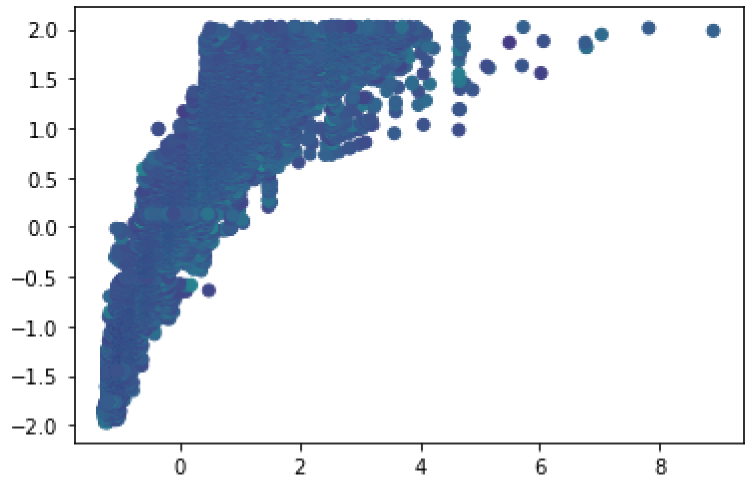
In [13]:
```
cut = dataNorm['cut']
plt.scatter(dataNorm['carat'], dataNorm['price'], c=cut, cmap='viridis')
plt.show()
```



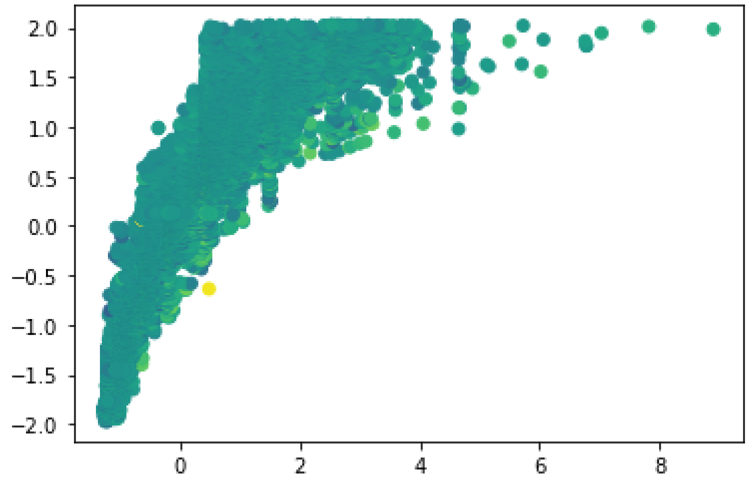
In [14]:
```
clarity = dataNorm['clarity']
plt.scatter(dataNorm['carat'], dataNorm['price'], c=clarity, cmap='viridis')
plt.show()
```



In [15]:
```
table = dataNorm['table']
plt.scatter(dataNorm['carat'], dataNorm['price'], c=table, cmap='viridis')
plt.show()
```



In [16]:
```
depth = dataNorm['depth']
plt.scatter(dataNorm['carat'], dataNorm['price'], c=depth, cmap='viridis')
plt.show()
```



In [17]:
```
%%time
# Shuffle
dataNorm = dataNorm.sample(frac=1).reset_index(drop=True)
```

```
Wall time: 6 ms
```

In [18]:
```
# x and y
y = dataNorm['price']

# Dropping 'x', 'y' and 'z'
x = dataNorm.drop(['price', 'x', 'y', 'z', 'volume'], axis=1)
```

In [19]:
```
x
```

Out[19]:

	carat	cut	color	clarity	depth	table
0	-0.311722	0.981357	1.524769	1.183045	-0.732774	-0.204532
1	-1.071573	-0.809805	-0.238608	1.183045	-0.593140	-0.204532
2	2.558827	-0.809805	0.349185	-1.245589	-1.012041	1.138309
3	1.461264	0.085776	-0.826400	-0.638430	0.105029	-0.204532
4	0.638092	0.981357	-2.001984	-0.638430	-0.174239	-1.099760
...	...	...	...	...	...	...
53912	0.891376	-0.809805	0.349185	-0.638430	1.222099	-0.652146
53913	0.469236	0.085776	0.349185	-1.245589	-0.174239	0.243081
53914	-0.565006	0.981357	0.349185	1.183045	0.105029	-0.652146
53915	0.532557	0.981357	-0.238608	0.575887	0.174846	-0.652146
53916	0.828055	0.981357	1.524769	-1.245589	-0.942224	-1.099760

53917 rows × 6 columns

In [20]:
```
y
```

Out[20]:
```
0        0.565939
1       -1.471548
2        1.910681
3        1.412975
4        0.592104
           ...
53912    0.783160
53913    0.625437
```

```
53914   -0.106950
53915    1.060827
53916    0.815008
Name: price, Length: 53917, dtype: float64
```

In [ ]:

Validation Curve Plot:

In [21]:

```
def plot_grid_search_validation_curve(grid, param_to_vary,
                                      title='Validation Curve', ylim=None,
                                      xlim=None, log=None):
    """Plots train and cross-validation scores from a GridSearchCV instance's
    best params while varying one of those params."""

    df_cv_results = pd.DataFrame(grid.cv_results_)
    #train_scores_mean = df_cv_results['mean_train_score']
    valid_scores_mean = df_cv_results['mean_test_score']
    #train_scores_std = df_cv_results['std_train_score']
    valid_scores_std = df_cv_results['std_test_score']

    param_cols = [c for c in df_cv_results.columns if c[:6] == 'param_']
    param_ranges = [grid.param_grid[p[6:]] for p in param_cols]
    param_ranges_lengths = [len(pr) for pr in param_ranges]

    #train_scores_mean = np.array(train_scores_mean).reshape(*param_ranges_lengths)
    valid_scores_mean = np.array(valid_scores_mean).reshape(*param_ranges_lengths)
   # train_scores_std = np.array(train_scores_std).reshape(*param_ranges_lengths)
    valid_scores_std = np.array(valid_scores_std).reshape(*param_ranges_lengths)

    param_to_vary_idx = param_cols.index('param_{}'.format(param_to_vary))

    slices = []
    for idx, param in enumerate(grid.best_params_):
        if (idx == param_to_vary_idx):
            slices.append(slice(None))
            continue
        best_param_val = grid.best_params_[param]
        idx_of_best_param = 0
        if isinstance(param_ranges[idx], np.ndarray):
            idx_of_best_param = param_ranges[idx].tolist().index(best_param_val)
        else:
            idx_of_best_param = param_ranges[idx].index(best_param_val)
        slices.append(idx_of_best_param)

   # train_scores_mean = train_scores_mean[tuple(slices)]
    valid_scores_mean = valid_scores_mean[tuple(slices)]
   # train_scores_std = train_scores_std[tuple(slices)]
    valid_scores_std = valid_scores_std[tuple(slices)]

    plt.clf()

    plt.title(title)
    plt.xlabel(param_to_vary)
    plt.ylabel('Score')

    if (ylim is None):
        plt.ylim(0.0, 1.1)
    else:
        plt.ylim(*ylim)

    if (not (xlim is None)):
        plt.xlim(*xlim)

    lw = 2
```

```
    plot_fn = plt.plot
    if log:
        plot_fn = plt.semilogx

    param_range = param_ranges[param_to_vary_idx]
    if (not isinstance(param_range[0], numbers.Number)):
        param_range = [str(x) for x in param_range]
    plot_fn(param_range, train_scores_mean, label='Training score', color='r',
            lw=lw)
    plt.fill_between(param_range, train_scores_mean - train_scores_std,
                     train_scores_mean + train_scores_std, alpha=0.1,
                     color='r', lw=lw)
    plot_fn(param_range, valid_scores_mean, label='Cross-validation score',
            color='b', lw=lw)
    plt.fill_between(param_range, valid_scores_mean - valid_scores_std,
                     valid_scores_mean + valid_scores_std, alpha=0.1,
                     color='b', lw=lw)

    plt.legend(loc='lower right')

    plt.show()
```

Grid Searches:

In [22]:
```
%%time
from sklearn.neural_network import MLPRegressor
from sklearn.model_selection import GridSearchCV
```

```
Wall time: 34 ms
```

In [23]:
```
%%time
mlp = MLPRegressor(hidden_layer_sizes=(100,100), activation='tanh', tol=1e-6, max_it
mlp
```

```
Wall time: 0 ns
```

Out[23]:
```
MLPRegressor(activation='tanh', alpha=0.001, batch_size='auto', beta_1=0.9,
             beta_2=0.999, early_stopping=False, epsilon=1e-08,
             hidden_layer_sizes=(100, 100), learning_rate='constant',
             learning_rate_init=0.001, max_fun=15000, max_iter=1000,
             momentum=0.9, n_iter_no_change=10, nesterovs_momentum=True,
             power_t=0.5, random_state=None, shuffle=True, solver='adam',
             tol=1e-06, validation_fraction=0.1, verbose=True,
             warm_start=False)
```

In [24]:
```
param_grid = [
    #{'solver': ['sgd', 'adam'], 'max_iter': [5000], 'tol': [1e-04], 'hidden_layer_s
    #{'learning_rate_init': [0.1, 0.01, 0.001, 0.0001, 0.00001]},
    #{'activation': ['tanh', 'relu', 'logistic']},
    #{'early_stopping': [True], 'validation_fraction': [0.01, 0.05, 0.1, 0.2, 0.3, 0
    #{'alpha': [0.0001, 0.001, 0.01, 0.1, 1, 0.00001, 0.000001, 10, 100]},
    #{'tol': [0.0001, 0.001, 0.01, 0.1, 0.00001, 0.000001, 0.0000001, 0.00000001]},
    ##{'hidden_layer_sizes':[(200,100)], 'tol':[1e-8]}
    #{'hidden_layer_sizes':[(1), (2), (4), (8), (16), (32), (64), (128), (256), (512
    #{'hidden_layer_sizes':[(1,1), (2,2), (4,4), (8,8), (16,16), (32,32), (64,64), (
    #{'hidden_layer_sizes':[(1,1), (2,2), (4,4), (8,8), (16,16), (32,32), (64,64), (
    #{'hidden_layer_sizes':[(1,1,1), (2,2,2), (4,4,4), (8,8,8), (16,16,16), (32,32,3
    #{'hidden_layer_sizes':[(1,1,1,1), (2,2,2,2), (4,4,4,4), (8,8,8,8), (16,16,16,16
]
```

In [25]:
```
grid = GridSearchCV(mlp, param_grid, cv=10, scoring='r2', n_jobs= 5, verbose=10)
```

In [26]:
```
%%time
#result = grid.fit(x,y)
```

```
Fitting 10 folds for each of 8 candidates, totalling 80 fits
[Parallel(n_jobs=5)]: Using backend LokyBackend with 5 concurrent workers.
[Parallel(n_jobs=5)]: Done   3 tasks      | elapsed:    9.8s
[Parallel(n_jobs=5)]: Done   8 tasks      | elapsed:   18.4s
[Parallel(n_jobs=5)]: Done  15 tasks      | elapsed:   29.2s
[Parallel(n_jobs=5)]: Done  22 tasks      | elapsed:   43.6s
[Parallel(n_jobs=5)]: Done  31 tasks      | elapsed:  1.2min
[Parallel(n_jobs=5)]: Done  40 tasks      | elapsed:  1.8min
[Parallel(n_jobs=5)]: Done  51 tasks      | elapsed:  2.6min
[Parallel(n_jobs=5)]: Done  62 tasks      | elapsed:  4.5min
[Parallel(n_jobs=5)]: Done  80 out of  80 | elapsed: 10.2min remaining:    0.0s
[Parallel(n_jobs=5)]: Done  80 out of  80 | elapsed: 10.2min finished
Iteration 1, loss = 0.02796823
Iteration 2, loss = 0.00887864
Iteration 3, loss = 0.00814863
Iteration 4, loss = 0.00801468
Iteration 5, loss = 0.00794595
Iteration 6, loss = 0.00787664
Iteration 7, loss = 0.00780412
Iteration 8, loss = 0.00774973
Iteration 9, loss = 0.00782104
Iteration 10, loss = 0.00762762
Iteration 11, loss = 0.00751741
Iteration 12, loss = 0.00763006
Iteration 13, loss = 0.00749978
Iteration 14, loss = 0.00732469
Iteration 15, loss = 0.00730890
Iteration 16, loss = 0.00721366
Iteration 17, loss = 0.00712447
Iteration 18, loss = 0.00707850
Iteration 19, loss = 0.00701594
Iteration 20, loss = 0.00700028
Iteration 21, loss = 0.00699904
Iteration 22, loss = 0.00690979
Iteration 23, loss = 0.00684218
Iteration 24, loss = 0.00679296
Iteration 25, loss = 0.00677561
Iteration 26, loss = 0.00680070
Iteration 27, loss = 0.00675232
Iteration 28, loss = 0.00673539
Iteration 29, loss = 0.00673135
Iteration 30, loss = 0.00667900
Iteration 31, loss = 0.00661037
Iteration 32, loss = 0.00659120
Iteration 33, loss = 0.00663044
Iteration 34, loss = 0.00647554
Iteration 35, loss = 0.00643785
Iteration 36, loss = 0.00645742
Iteration 37, loss = 0.00640050
Iteration 38, loss = 0.00636568
Iteration 39, loss = 0.00632987
Iteration 40, loss = 0.00634202
Iteration 41, loss = 0.00630555
Iteration 42, loss = 0.00620825
Iteration 43, loss = 0.00622172
Iteration 44, loss = 0.00620589
Iteration 45, loss = 0.00617194
Iteration 46, loss = 0.00613743
Iteration 47, loss = 0.00615057
Iteration 48, loss = 0.00610440
Iteration 49, loss = 0.00616281
Iteration 50, loss = 0.00607311
Iteration 51, loss = 0.00605508
Iteration 52, loss = 0.00603549
Iteration 53, loss = 0.00606776
Iteration 54, loss = 0.00599565
Iteration 55, loss = 0.00602574
Iteration 56, loss = 0.00597321
Iteration 57, loss = 0.00598387
```

```
Iteration 58, loss = 0.00594202
Iteration 59, loss = 0.00597703
Iteration 60, loss = 0.00588052
Iteration 61, loss = 0.00589016
Iteration 62, loss = 0.00588880
Iteration 63, loss = 0.00585380
Iteration 64, loss = 0.00586142
Iteration 65, loss = 0.00581939
Iteration 66, loss = 0.00582178
Iteration 67, loss = 0.00579754
Iteration 68, loss = 0.00577831
Iteration 69, loss = 0.00577603
Iteration 70, loss = 0.00575024
Iteration 71, loss = 0.00575539
Iteration 72, loss = 0.00573236
Iteration 73, loss = 0.00574185
Iteration 74, loss = 0.00569739
Iteration 75, loss = 0.00571820
Iteration 76, loss = 0.00575525
Iteration 77, loss = 0.00568169
Iteration 78, loss = 0.00572078
Iteration 79, loss = 0.00571464
Iteration 80, loss = 0.00568403
Iteration 81, loss = 0.00567195
Iteration 82, loss = 0.00567973
Iteration 83, loss = 0.00568467
Iteration 84, loss = 0.00565841
Iteration 85, loss = 0.00565592
Iteration 86, loss = 0.00567691
Iteration 87, loss = 0.00567334
Iteration 88, loss = 0.00563611
Iteration 89, loss = 0.00565683
Iteration 90, loss = 0.00563655
Iteration 91, loss = 0.00560811
Iteration 92, loss = 0.00560325
Iteration 93, loss = 0.00562423
Iteration 94, loss = 0.00561894
Iteration 95, loss = 0.00563437
Iteration 96, loss = 0.00558732
Iteration 97, loss = 0.00558165
Iteration 98, loss = 0.00560759
Iteration 99, loss = 0.00563051
Iteration 100, loss = 0.00557092
Iteration 101, loss = 0.00558417
Iteration 102, loss = 0.00560441
Iteration 103, loss = 0.00554915
Iteration 104, loss = 0.00556867
Iteration 105, loss = 0.00555858
Iteration 106, loss = 0.00558600
Iteration 107, loss = 0.00560318
Iteration 108, loss = 0.00553703
Iteration 109, loss = 0.00557197
Iteration 110, loss = 0.00555791
Iteration 111, loss = 0.00556440
Iteration 112, loss = 0.00554605
Iteration 113, loss = 0.00556583
Iteration 114, loss = 0.00554330
Iteration 115, loss = 0.00555350
Iteration 116, loss = 0.00556473
Iteration 117, loss = 0.00557678
Iteration 118, loss = 0.00549981
Iteration 119, loss = 0.00550622
Iteration 120, loss = 0.00552177
Iteration 121, loss = 0.00550021
Iteration 122, loss = 0.00551032
Iteration 123, loss = 0.00550452
Iteration 124, loss = 0.00554452
Iteration 125, loss = 0.00553675
Iteration 126, loss = 0.00552756
```

```
Iteration 127, loss = 0.00550733
Iteration 128, loss = 0.00553137
Iteration 129, loss = 0.00553477
Training loss did not improve more than tol=0.000001 for 10 consecutive epochs. Stop
ping.
Wall time: 11min 17s
```

In [27]:
```
result
```

Out[27]:
```
GridSearchCV(cv=10, error_score=nan,
             estimator=MLPRegressor(activation='tanh', alpha=0.001,
                                    batch_size='auto', beta_1=0.9, beta_2=0.999,
                                    early_stopping=False, epsilon=1e-08,
                                    hidden_layer_sizes=(100, 100),
                                    learning_rate='constant',
                                    learning_rate_init=0.001, max_fun=15000,
                                    max_iter=1000, momentum=0.9,
                                    n_iter_no_change=10,
                                    nesterovs_momentum=True, power_t=0.5,
                                    random_state=None, shuffle=True,
                                    solver='adam', tol=1e-06,
                                    validation_fraction=0.1, verbose=True,
                                    warm_start=False),
             iid='deprecated', n_jobs=5,
             param_grid=[{'hidden_layer_sizes': [(1, 1), (2, 2), (4, 4), (8, 8),
                                                 (16, 16), (32, 32), (64, 64),
                                                 (128, 128)]}],
             pre_dispatch='2*n_jobs', refit=True, return_train_score=False,
             scoring='r2', verbose=10)
```

In [28]:
```
grid.best_score_
```

Out[28]:
```
0.9898138713705279
```

In [29]:
```
grid.cv_results_
```

Out[29]:
```
{'mean_fit_time': array([  8.77038949,   7.69478083,  13.31355844,  17.96480463,
         25.60243015,  35.6792484 ,  67.42280395, 115.78187792]),
 'std_fit_time': array([ 0.94103814,  1.93664225,  5.29458661,  7.13276775,  8.18466
006,
         9.96937075, 13.55419298, 13.31227046]),
 'mean_score_time': array([0.00170176, 0.00180047, 0.00200572, 0.00320077, 0.0050008
5,
        0.00831139, 0.01690159, 0.03270683]),
 'std_score_time': array([4.56606613e-04, 3.99792812e-04, 1.12982235e-05, 4.00006966
e-04,
        4.82171736e-07, 8.96296774e-04, 2.62323152e-03, 4.49669032e-03]),
 'param_hidden_layer_sizes': masked_array(data=[(1, 1), (2, 2), (4, 4), (8, 8), (16,
16), (32, 32),
                    (64, 64), (128, 128)],
              mask=[False, False, False, False, False, False, False, False],
        fill_value='?',
             dtype=object),
 'params': [{'hidden_layer_sizes': (1, 1)},
  {'hidden_layer_sizes': (2, 2)},
  {'hidden_layer_sizes': (4, 4)},
  {'hidden_layer_sizes': (8, 8)},
  {'hidden_layer_sizes': (16, 16)},
  {'hidden_layer_sizes': (32, 32)},
  {'hidden_layer_sizes': (64, 64)},
  {'hidden_layer_sizes': (128, 128)}],
 'split0_test_score': array([0.97136131, 0.98242144, 0.98665914, 0.9871169 , 0.98867
457,
        0.98812648, 0.98975033, 0.99019875]),
 'split1_test_score': array([0.9710548 , 0.98209754, 0.98572301, 0.98773187, 0.98817
265,
        0.98979382, 0.98967197, 0.99018863]),
 'split2_test_score': array([0.97168023, 0.98222195, 0.98527957, 0.98740954, 0.98903
```

```
302,
        0.98937058, 0.98834841, 0.98997253]),
 'split3_test_score': array([0.97007458, 0.98148028, 0.98483175, 0.98758522, 0.98807
647,
        0.9892934 , 0.99015211, 0.98923216]),
 'split4_test_score': array([0.96923918, 0.98090582, 0.98521358, 0.98619912, 0.98911
32 ,
        0.98924814, 0.98964627, 0.98994459]),
 'split5_test_score': array([0.97012364, 0.98207246, 0.98594347, 0.98649486, 0.98814
2  ,
        0.98891848, 0.98932877, 0.98975009]),
 'split6_test_score': array([0.97067085, 0.9811906 , 0.98572896, 0.98826618, 0.98881
356,
        0.98976555, 0.98975859, 0.99006897]),
 'split7_test_score': array([0.97026895, 0.9813953 , 0.98456597, 0.98727673, 0.98832
941,
        0.98945724, 0.98925413, 0.98978664]),
 'split8_test_score': array([0.97061952, 0.98193806, 0.98503945, 0.98720892, 0.98757
234,
        0.98851593, 0.98953999, 0.98937539]),
 'split9_test_score': array([0.97089245, 0.98187026, 0.98556829, 0.98696044, 0.98783
715,
        0.98825929, 0.98934773, 0.98962096]),
 'mean_test_score': array([0.97059855, 0.98175937, 0.98545532, 0.98722498, 0.9883764
4,
        0.98907489, 0.98947983, 0.98981387]),
 'std_test_score': array([0.00067147, 0.00046598, 0.00057348, 0.00056346, 0.0004878
5,
        0.00056629, 0.00045193, 0.00031122]),
 'rank_test_score': array([8, 7, 6, 5, 4, 3, 2, 1])}
```

In [30]:

```
results = pd.DataFrame(grid.cv_results_)
results
```

Out[30]:

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_hidden_layer_sizes	
0	8.770389	0.941038	0.001702	4.566066e-04	(1, 1)	{'hidden_la
1	7.694781	1.936642	0.001800	3.997928e-04	(2, 2)	{'hidden_la
2	13.313558	5.294587	0.002006	1.129822e-05	(4, 4)	{'hidden_la
3	17.964805	7.132768	0.003201	4.000070e-04	(8, 8)	{'hidden_la
4	25.602430	8.184660	0.005001	4.821717e-07	(16, 16)	{'hidden_la
5	35.679248	9.969371	0.008311	8.962968e-04	(32, 32)	{'hidden_la
6	67.422804	13.554193	0.016902	2.623232e-03	(64, 64)	{'hidden_la
7	115.781878	13.312270	0.032707	4.496690e-03	(128, 128)	{'hidden_la (

In [31]:

```
results
```

Out[31]:

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_hidden_layer_sizes	
0	8.770389	0.941038	0.001702	4.566066e-04	(1, 1)	{'hidden_la

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_hidden_layer_sizes	
1	7.694781	1.936642	0.001800	3.997928e-04	(2, 2)	{'hidden_la
2	13.313558	5.294587	0.002006	1.129822e-05	(4, 4)	{'hidden_la
3	17.964805	7.132768	0.003201	4.000070e-04	(8, 8)	{'hidden_la
4	25.602430	8.184660	0.005001	4.821717e-07	(16, 16)	{'hidden_la
5	35.679248	9.969371	0.008311	8.962968e-04	(32, 32)	{'hidden_la
6	67.422804	13.554193	0.016902	2.623232e-03	(64, 64)	{'hidden_la
7	115.781878	13.312270	0.032707	4.496690e-03	(128, 128)	{'hidden_la (

In [32]:
```
results_pickle = results.to_pickle("results_8_log")
```

In [ ]:

In [33]:
```
#plot_grid_search_validation_curve(grid, 'activation', log=True, ylim=(.8, 1.02))
```

In [ ]:

In [ ]:

In [ ]:

In [ ]:

Plotting Results:

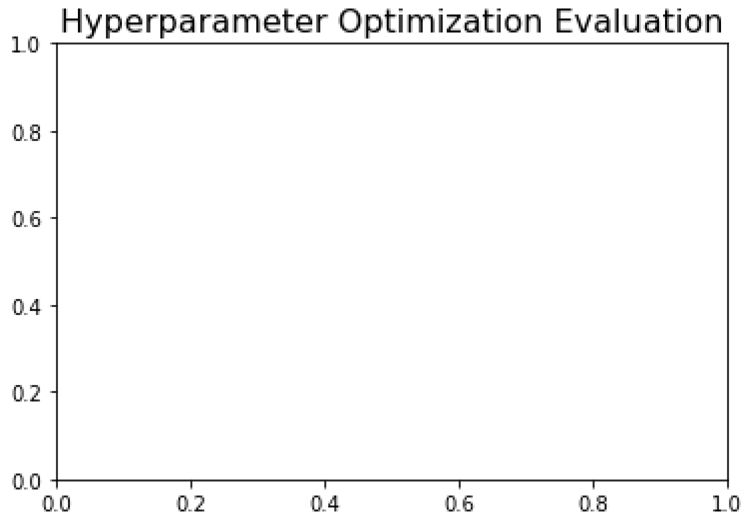
In [34]:
```
results = grid.cv_results_
```

In [35]:
```
plt.figure(figsize=(13, 13))
```

Out[35]:
```
<Figure size 936x936 with 0 Axes>
<Figure size 936x936 with 0 Axes>
```

In [36]:
```
plt.title("Hyperparameter Optimization Evaluation",
          fontsize=16)
```

Out[36]:
```
Text(0.5, 1.0, 'Hyperparameter Optimization Evaluation')
```



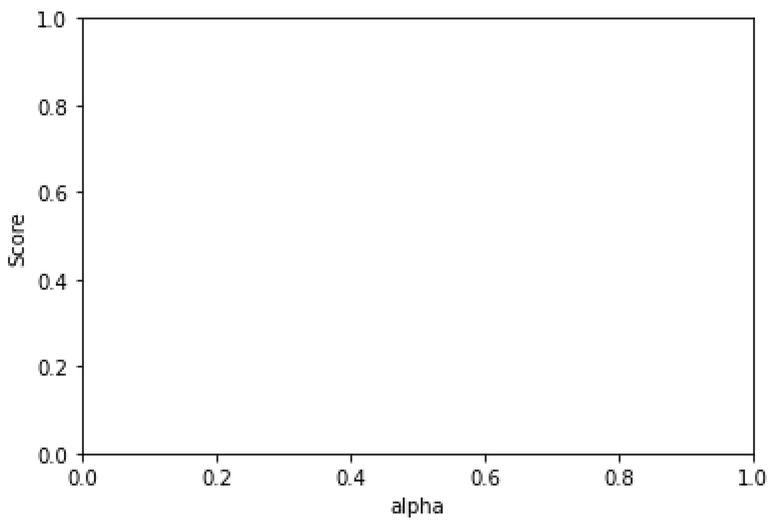
In [37]:
```
for param in param_grid:
    key = list(param.keys())[0]
    values = param[key]
    print(key)
    print(values)
```

```
hidden_layer_sizes
[(1, 1), (2, 2), (4, 4), (8, 8), (16, 16), (32, 32), (64, 64), (128, 128)]
```

In [38]:
```
parameter = 'alpha'
```

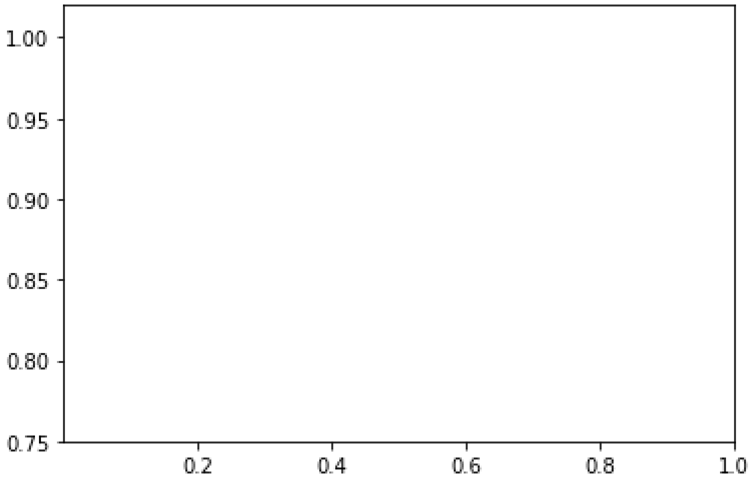
In [39]:
```
plt.xlabel(parameter)
plt.ylabel('Score')
```

Out[39]:
```
Text(0, 0.5, 'Score')
```



In [40]:
```
ax = plt.gca()
ax.set_xlim(0.001, 1)
ax.set_ylim(0.75, 1.02)
```

Out[40]:
```
(0.75, 1.02)
```



In [41]:
```
X_axis = np.array(results['param_min_samples_split'].data, dtype=float)
```

```
---------------------------------------------------------------------------
KeyError                                  Traceback (most recent call last)
<ipython-input-41-98581fcc4c37> in <module>
----> 1 X_axis = np.array(results['param_min_samples_split'].data, dtype=float)

KeyError: 'param_min_samples_split'
```

In [ ]:
```
for scorer, color in zip(sorted(scoring), ['g', 'k']):
    for sample, style in (('train', '--'), ('test', '-')):
        sample_score_mean = results['mean_%s_%s' % (sample, scorer)]
        sample_score_std = results['std_%s_%s' % (sample, scorer)]
        ax.fill_between(X_axis, sample_score_mean - sample_score_std,
                        sample_score_mean + sample_score_std,
                        alpha=0.1 if sample == 'test' else 0, color=color)
        ax.plot(X_axis, sample_score_mean, style, color=color,
                alpha=1 if sample == 'test' else 0.7,
                label="%s (%s)" % (scorer, sample))

    best_index = np.nonzero(results['rank_test_%s' % scorer] == 1)[0][0]
    best_score = results['mean_test_%s' % scorer][best_index]

    # Plot a dotted vertical line at the best score for that scorer marked by x
    ax.plot([X_axis[best_index], ] * 2, [0, best_score],
            linestyle='-.', color=color, marker='x', markeredgewidth=3, ms=8)

    # Annotate the best score for that scorer
    ax.annotate("%0.2f" % best_score,
                (X_axis[best_index], best_score + 0.005))
```

In [ ]:
```
plt.legend(loc="best")
plt.grid(False)
plt.show()
```

In [ ]:

In [ ]:
```
def plot_grid_search(cv_results, grid_param_1, grid_param_2, name_param_1, name_para
    # Get Test Scores Mean and std for each grid search
    scores_mean = cv_results['mean_test_score']
    scores_mean = np.array(scores_mean).reshape(len(grid_param_2),len(grid_param_1))

    scores_sd = cv_results['std_test_score']
    scores_sd = np.array(scores_sd).reshape(len(grid_param_2),len(grid_param_1))

    # Plot Grid search scores
    _, ax = plt.subplots(1,1)
```

```
    # Param1 is the X-axis, Param 2 is represented as a different curve (color line)
    for idx, val in enumerate(grid_param_2):
        ax.plot(grid_param_1, scores_mean[idx,:], '-o', label= name_param_2 + ': ' +

    ax.set_title("Grid Search Scores", fontsize=20, fontweight='bold')
    ax.set_xlabel(name_param_1, fontsize=16)
    ax.set_ylabel('CV Average Score', fontsize=16)
    ax.legend(loc="best", fontsize=15)
    ax.grid('on')

# Calling Method
plot_grid_search(grid.cv_results_, n_estimators, max_features, 'N Estimators', 'Max
```

In [ ]: