Hyperparameter Optimization with Hyperopt-Into & Implementation

Hyperparameter Optimization is the process of identifying the best combination of hyperparameters for a machine learning model to satisfy an objective function, which is usually defined as "minimizing" the objective function for consistency.

1. Objective Function: accepts a combination of hyperparameters as input and returns the mimized error/loss.
2. Search Space: Function Arguments
3. Optimization Algorithm: Like random search and Tree of Parzen Estimators(TPE) etc.

In [1]:

```
pip install hyperopt
```

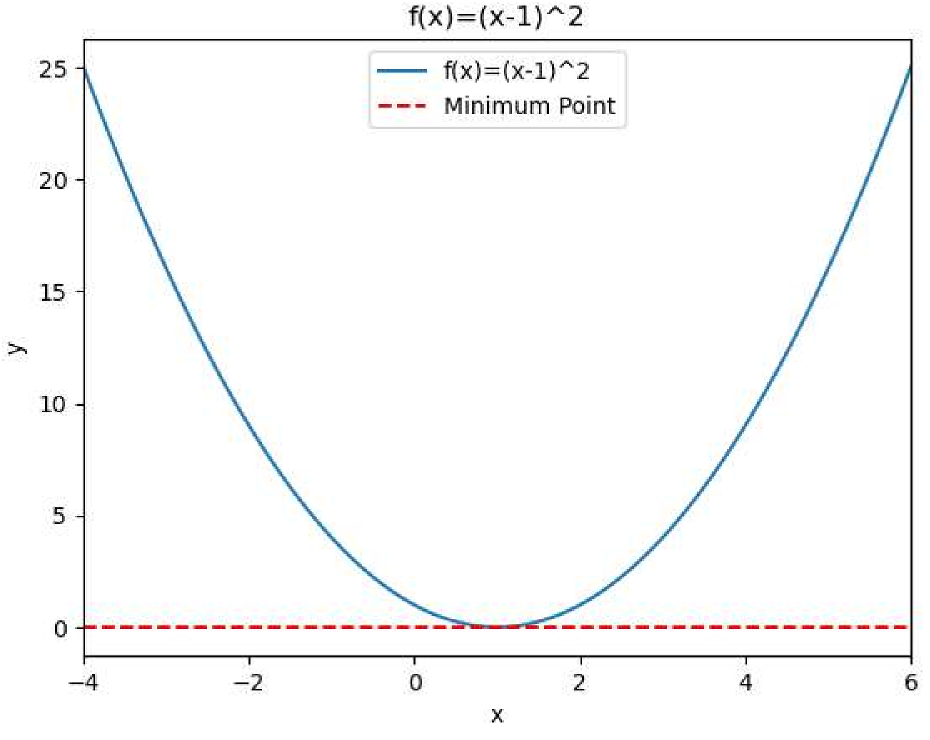
```
Collecting hyperoptNote: you may need to restart the kernel to use updated packa
ges.

  Downloading hyperopt-0.2.7-py2.py3-none-any.whl (1.6 MB)
     ---------------------------------------- 1.6/1.6 MB 301.4 kB/s eta 0:00:00
Requirement already satisfied: numpy in c:\users\kiran\anaconda3\lib\site-packag
es (from hyperopt) (1.23.5)
Requirement already satisfied: scipy in c:\users\kiran\anaconda3\lib\site-packag
es (from hyperopt) (1.9.1)
Requirement already satisfied: six in c:\users\kiran\anaconda3\lib\site-packages
(from hyperopt) (1.16.0)
Requirement already satisfied: networkx>=2.2 in c:\users\kiran\anaconda3\lib\sit
e-packages (from hyperopt) (2.8.4)
Requirement already satisfied: future in c:\users\kiran\anaconda3\lib\site-packa
ges (from hyperopt) (0.18.2)
Requirement already satisfied: tqdm in c:\users\kiran\anaconda3\lib\site-package
s (from hyperopt) (4.64.1)
Requirement already satisfied: cloudpickle in c:\users\kiran\anaconda3\lib\site-
packages (from hyperopt) (2.0.0)
Collecting py4j (from hyperopt)
  Downloading py4j-0.10.9.7-py2.py3-none-any.whl (200 kB)
     ------------------------------------ 200.5/200.5 kB 406.5 kB/s eta 0:00:00
Requirement already satisfied: colorama in c:\users\kiran\anaconda3\lib\site-pac
kages (from tqdm->hyperopt) (0.4.5)
Installing collected packages: py4j, hyperopt
Successfully installed hyperopt-0.2.7 py4j-0.10.9.7
```

Simple Example

Quadratic function of f(x)=(x-1)2

In [3]:

```python
import numpy as np
import matplotlib.pyplot as plt

#Define the function
def f(x):
    return(x-1)**2

#Generate x values from -5 to 5
x=np.linspace(-4,6,100)

#Calculate corresponding y values
y=f(x)

#Find the minimum point
min_point=np.min(y)

#Create the plot
plt.plot(x,y,label='f(x)=(x-1)^2')
plt.xlabel('x')
plt.ylabel('y')
plt.title('f(x)=(x-1)^2')

#Set the x-axis limits
plt.xlim(-4,6)

#Add horizontal dashed line at the minimum point
plt.axhline(y=min_point,color='red',linestyle='dashed',label='Minimum Point')

#Add a legend
plt.legend()

#Display the plot
plt.show()

```



```
# As we can see, the minimum point happens where x=1.
```

```
Let`s implement this using Hyperopt and see how it works.
In order to do so, we will take the following steps:
1. import necessary libraries and packages
2. define the objective function and the search space
3. run the optimization process
4. print the results(i.e the optimized point that we expect to be x=1)
```

In [9]:

```python
#1. import necessary libraries and packages

from hyperopt import hp,fmin,tpe,Trials

#2. define the objective function and the search space

def objective_function(x):
    return (x-1)**2
search_space=hp.uniform('x',-2,2)

#3. run the optimization process

#Trails object to store the results

trials=Trials()

#run the optimization

best=fmin(fn=objective_function,space=search_space,algo=tpe.suggest,trials=trails,max_eval


#4. print the results(i.e the optimized point that we expect to be x=1)

print(best)

```

```
100%|██████████████████████████████████████████████████| 1
00/100 [00:00<?, ?trial/s, best loss=?]
{'x': 0.9873345471340685}
```

best returns the best combination of hyperparameters that the mode was

able to find and in this case it is almost equal to x=1, as we expected.

Hyperopt implementation

We will implement two separate examples as follows.

1. A classification with Support Vector Machine

2. A regression with Random Forest Regressor

1. Support Vector Machines and Iris Data Set with two parameter that we can optimize as follows: c: Regularization parameter, which trades off misclassification of

```
training examples against simplicity of the decision surface.
```

gamma: Kernel coefficient, which defines how much influence a single training exaple has.

```
The larger gamma is, the closer other examples must be to be affected.
```

In [11]:

```
from sklearn import datasets
from sklearn.svm import SVC
from sklearn.model_selection import cross_val_score

iris=datasets.load_iris()
X=iris.data
y=iris.target

```

Define objective function and search space

Objective function, which will train an SVM and returns the negetive of the cross-validation score that is what we want to minimize. Note that we are minimizing the negetive of cross-validation score to be consistent with the general goal of minimizing the objective function.

In [12]:

```
def objective_function(parameters):
    clf=SVC(**parameters)
    score=cross_val_score(clf,X,y,cv=5).mean()
    return -score
```

Next we will define the search space, which consists of the values that our parameters of c and gamma can take. Note that we will use Hyperopt`s hp.uniform(label,low,high), which returns a value uniformly between low and high.

In [13]:

```
search_space={
    'C':hp.uniform('C',0.1,10),
    'gamma':hp.uniform('gamma',0.01,1)
}
```

Run Optimization

We will use a TPE algorithm and store the results in a trials object

In [14]:

```
trials=Trials()

best=fmin(fn=objective_function,space=search_space,algo=tpe.suggest, trials=trials,max_eva

```

```
100%|██████████████████████████████████████████████████| 100/100 [00:02<00:00, 45.94t
rial/s, best loss: -0.9866666666666667]
```

In [15]:

```python
# Visualize Optimization

print(best)
```

{'C': 6.323329285556576, 'gamma': 0.12538458670925196}

```
Now we have a combination of hyperparameters that minimize the optimization function using Hyperopt.

```

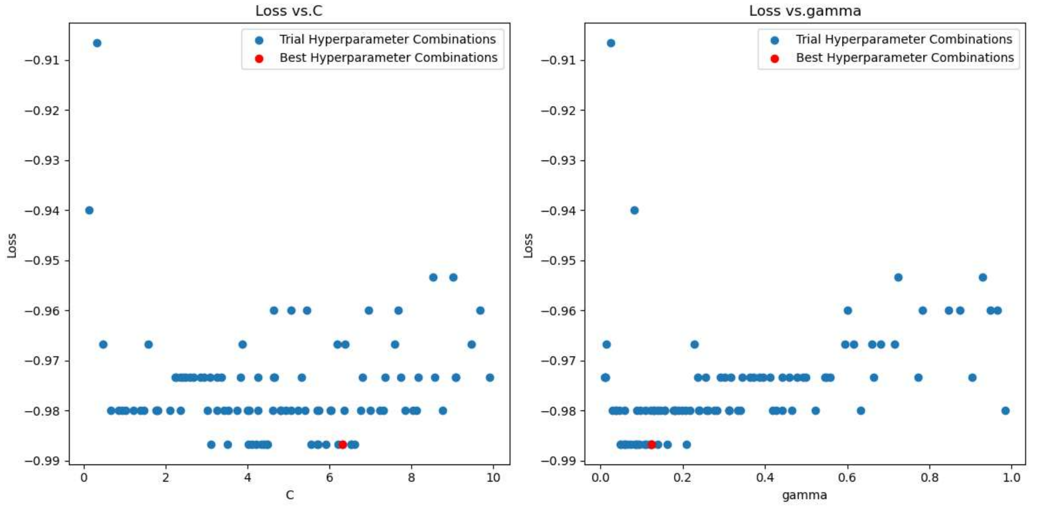
```
Let`s visually look at how the objective function values changes as the hyperparameters change.

We will start with defining a function named plot_obj_vs_hp() that accomplishes this visualization.
Make sure to look for the red dot-- that one indicates the best combination of hyperparameters, according to our
hyperparameter optimization!
```

In [23]:

```
import matplotlib.pyplot as plt

def plot_obj_vs_hp(trials,search_space,best):

    #Extract the results

    results=trials.trials

    #Create a list of hyperparameters

    hyperparameters=list(search_space.keys())

    #Create a new figure with 2 subpots side by side

    fig,axes= plt.subplots(1,2,figsize=(12, 6))

    #Loop through hyperparameters and generate plots

    for idx,hp in enumerate(hyperparameters):

        #Extract the values of a given hyperparameter

        hp_values=[res['misc']['vals'][f'{hp}'] for res in results]

        #Flatten the list of values

        hp_values=[item for sublist in hp_values for item in sublist]

        #Extract the corresponding objective function values

        objective_values=[res['result']['loss'] for res in results]

        #Create the scatter plot

        axes[idx].scatter(hp_values,objective_values,label='Trial Hyperparameter Combinati

        #Highlight the best hyperparameters

        axes[idx].scatter(best[hp],min(objective_values),color='red',label='Best Hyperpara
        axes[idx].set_xlabel(f'{hp}')
        axes[idx].set_ylabel('Loss')
        axes[idx].set_title(f'Loss vs.{hp}')
        axes[idx].legend(loc='upper right')

    plt.tight_layout()
    plt.show()
```

In [24]:

```
#Plot optimization vs hyperparameters in 2D
plot_obj_vs_hp(trials,search_space,best)
```



Note that since c and gamma are not really related to each other, we are showing them separately versus changes of the objective function.

Since we want the objective function to be minimized, then we`re looking for the furthest bottom side of the plots above and based on the results of the hyperparameter optimization, we know that waht we are looking for is where {'C':6.323329285556576, 'gamma':0.12538458670925196}, which results in an objective function loss of around -0.986 and is indicated by a red dot.

I was also curious to look at these plots in a three-dimensional manner so I created the function below to accomplish that.

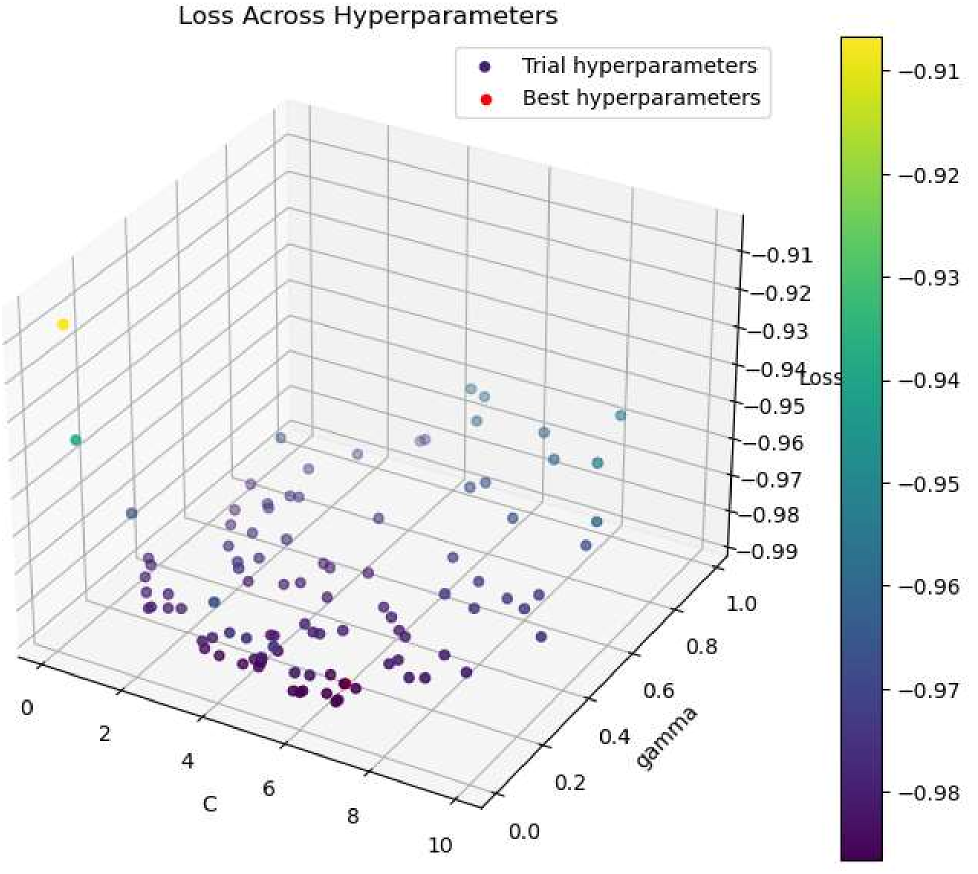
Let`s look at the plot

In [32]:

```
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt

# define 3D plot function

def plot_obj_vs_hp_3d(trials,search_space,best):

    #Extract the results

    results=trials.trials

    #Create a list of hyperparameters

    hyperparameters=list(search_space.keys())

    #Extract the values of hyperparameters

    hp_values_0=[res['misc']['vals'][f'{hyperparameters[0]}'] for res in results]
    hp_values_1=[res['misc']['vals'][f'{hyperparameters[1]}'] for res in results]

    #Flatten the lists of values

    hp_values_0=[item for sublist in hp_values_0 for item in sublist]
    hp_values_1=[item for sublist in hp_values_1 for item in sublist]

    #Extract the corresponding objective function values

    objective_values=[res['result']['loss'] for res in results]

    #Create a new figure

    fig=plt.figure(figsize=(10,7))

    #Add a 3D subplot

    ax=fig.add_subplot(111,projection='3d')

    #Create the scatter plot

    scatter=ax.scatter(hp_values_0,hp_values_1,objective_values,c=objective_values,cmap='v

    #Highlight the best hyperparameters

    ax.scatter(best[hyperparameters[0]],best[hyperparameters[1]],min(objective_values),col

    #Add labels using hyperparameters from search_space
    ax.set_xlabel(hyperparameters[0])
    ax.set_ylabel(hyperparameters[1])
    ax.set_zlabel('Loss')
    ax.set_title('Loss Across Hyperparameters')
    fig.colorbar(scatter)
    ax.legend(loc='upper right')

    plt.show()

```

In [33]:

```
#plot optimization vs. hyperparameters in 3D

plot_obj_vs_hp_3d(trials,search_space,best)
```



Admittedly, this is not very easy to read but let`s give it a shot. We are looking for the lowest loss, which is the darkest dots on the plot(and the red dot is almost hidden by one of the dark dots). Visually it aligns with the two-dimensional plots that we had generated before.

Random Forest and Diabetes Data Set

This example focuses on a regression model that attempts at measuring the progression of the disease, one year after baseline.

We will use a Random Forest Regressor model for this example and will optimize the objective function for two hyperparameters as follows:

1. `n_estimators:Number of tress in the random forest`
2. `max_depth:Maximum depth of trees in the random forest`

In [35]:

```
from sklearn import datasets
from sklearn.ensemble import RandomForestRegressor
from hyperopt import fmin,tpe,hp,Trials
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

#Load Diabetes dataset
diabetes=datasets.load_diabetes()

X=diabetes.data
y=diabetes.target

```

In [42]:

```
#Define objective function

def objective_function(parameters):

    #Initiate RandomForestRegressor

    regressor=RandomForestRegressor(**parameters)

    #Calculate the mean cross-validation score using 5 folds

    score=cross_val_score(regressor,X,y,cv=5).mean()

    return -score

#Define search Space

search_space={
        'n_estimators':hp.choice('n_estimators',range(10,300)),
        'max_depth':hp.choice('max_depth',range(1,30)),
    }
```

Run Optimization

In [43]:

```
#Trials object to store the results

trials=Trials()

#Run Optimization

best=fmin(fn=objective_function,space=search_space,algo=tpe.suggest,trials=trials,max_eval

```

```
100%|██████████████████████████████████████████████████| 100/100 [11:59<00:00,  7.19
s/trial, best loss: -0.4395051293022144]
```

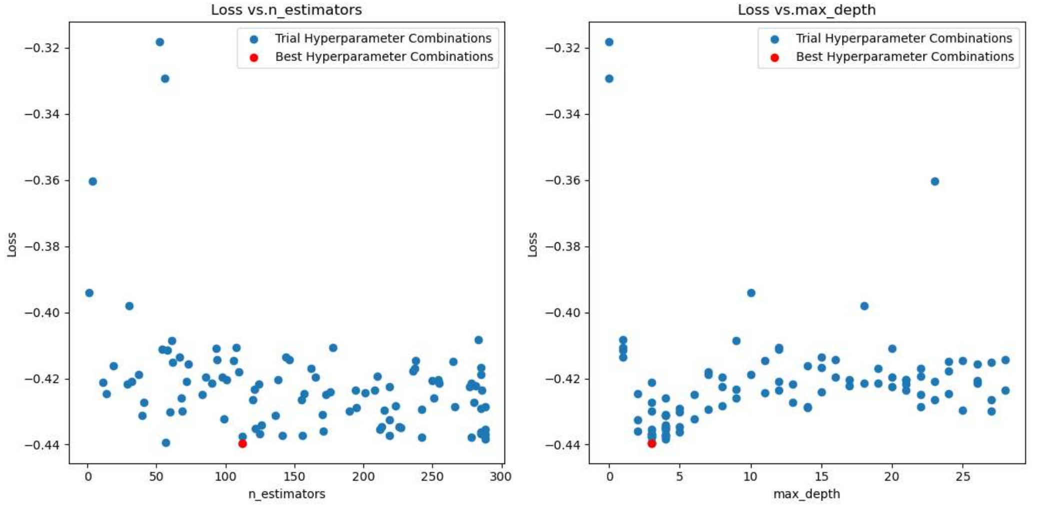
In [44]:

```
print(best)
```

```
{'max_depth': 3, 'n_estimators': 112}
```

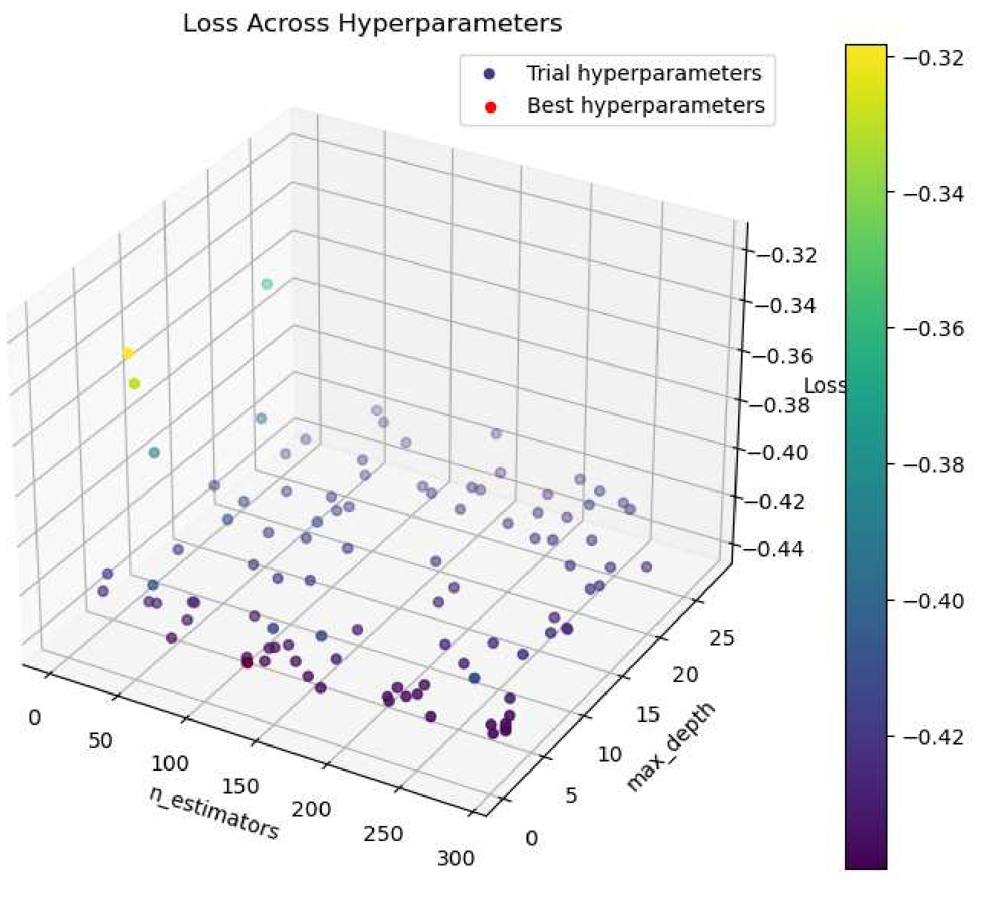
In [45]:

```
#plot optimization vs.hyperparameters in 2D

plot_obj_vs_hp(trials,search_space,best)
```



In [47]:

```
#plot optimization vs.hyperparameters in 3D
plot_obj_vs_hp_3d(trials,search_space,best)
```



In [ ]:

```
```