Multi-Output Regression Using SVM:

This problem is a multi-input and multi-output regression issue that we would like to solve by SVM algorithm. This is a regression problem since it involves four numerical continuous output variables which we want to predict as target values. The task here is to design and train an SVM to minimize the error between actual and predicted output values. We have 53 input-output data pairs, 6 features, and 4 outputs. The steps I did from beginning to end will be explained in the following.

Import required libraries and Load data from local drive and load dataset

```
[ ] # Standard imports
    import numpy as np
    import matplotlib.pyplot as plt
    from scipy import stats
    import pandas as pd
    %matplotlib inline

    # Use seaborn plotting defaults
    import seaborn as sns; sns.set()
```

```
#Load data from local drive
from google.colab import files
uploaded = files.upload()
```

Choose Files Plasma_Dataset.csv

- **Plasma_Dataset.csv**(application/vnd.ms-excel) - 2500 bytes, last modified: 2/23/2022 - 100% done

```
Saving Plasma_Dataset.csv to Plasma_Dataset.csv
```

```
[ ] #Load data set
    df = pd.read_csv('Plasma_Dataset.csv')
```

```
[ ] df.head()
```

	run	pressure	rf_power	electrode_gap	cci_flow	he_flow	o2_flow	etch_rate	etch_uniformity	oxide_selectivity	photoresist_selectivity
0	1	300	300	1.8	100	200	20	3491	14.2	6.48	2.01
1	2	200	400	1.8	100	50	10	3884	3.9	5.98	1.91
2	3	200	400	1.2	150	200	20	4931	24.8	5.39	1.85
3	4	300	400	1.8	150	200	20	4726	6.6	5.97	2.11
4	5	200	400	1.2	150	50	10	5089	12.4	5.61	2.16

1. **Exploratory data analysis**

   Now, I will explore the data to gain insights about the data.

```
[ ] # view dimensions of dataset
    df.shape
```

```
(53, 11)
```

```
df.describe()
```

	run	pressure	rf_power	electrode_gap	cci_flow	he_flow	o2_flow	etch_rate	etch_uniformity	oxide_selectivity	photoresist_selectivity
count	53.000000	53.000000	53.000000	53.000000	53.000000	53.000000	53.000000	53.000000	53.000000	53.000000	53.000000
mean	27.000000	250.000000	350.000000	1.518868	124.962264	124.056604	15.000000	4204.283019	11.635849	6.988302	2.226981
std	15.443445	45.641159	45.641159	0.285588	22.871684	62.203579	4.574175	689.441535	10.648241	2.186921	0.541315
min	1.000000	131.000000	231.000000	0.800000	64.000000	0.000000	3.000000	2704.000000	0.500000	2.650000	1.320000
25%	14.000000	200.000000	300.000000	1.200000	100.000000	50.000000	10.000000	3684.000000	3.900000	5.840000	1.970000
50%	27.000000	250.000000	350.000000	1.500000	125.000000	125.000000	15.000000	4390.000000	8.300000	6.410000	2.100000
75%	40.000000	300.000000	400.000000	1.800000	150.000000	200.000000	20.000000	4703.000000	15.100000	7.720000	2.310000
max	53.000000	369.000000	469.000000	2.200000	184.000000	200.000000	27.000000	5515.000000	55.200000	15.150000	4.170000

2. **view summary of dataset**

```
# view summary of dataset

df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 53 entries, 0 to 52
Data columns (total 11 columns):
 #   Column                   Non-Null Count  Dtype
---  ------                   --------------  -----
 0   run                      53 non-null     int64
 1   pressure                 53 non-null     int64
 2   rf_power                 53 non-null     int64
 3   electrode_gap            53 non-null     float64
 4   cci_flow                 53 non-null     int64
 5   he_flow                  53 non-null     int64
 6   o2_flow                  53 non-null     int64
 7   etch_rate                53 non-null     int64
 8   etch_uniformity          53 non-null     float64
 9   oxide_selectivity        53 non-null     float64
 10  photoresist_selectivity  53 non-null     float64
dtypes: float64(4), int64(7)
memory usage: 4.7 KB
```

We can see that there are no missing values in the dataset and all the variables are numerical variables.

3. Drop 'run' column:

```
df.drop(['run'], axis = 1, inplace = True)
df.head()
```

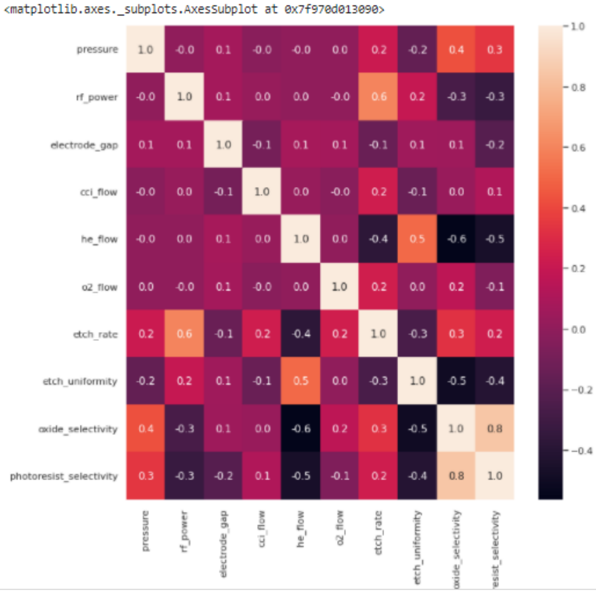
	pressure	rf_power	electrode_gap	cci_flow	he_flow	o2_flow	etch_rate	etch_uniformity	oxide_selectivity	photoresist_selectivity
0	300	300	1.8	100	200	20	3491	14.2	6.48	2.01
1	200	400	1.8	100	50	10	3884	3.9	5.98	1.91
2	200	400	1.2	150	200	20	4931	24.8	5.39	1.85
3	300	400	1.8	150	200	20	4726	6.6	5.97	2.11
4	200	400	1.2	150	50	10	5089	12.4	5.61	2.16

We can see that there are no missing values in the dataset and all the variables are numerical variables.

We can also plot a heat map to understand how each feature correlates to the other (Do they go hand in hand or are they inversely proportional)

```
import seaborn as sn
f= plt.subplots(figsize=(10,10))
sn.heatmap(df.corr(),annot=True,fmt='.1f',color='green')  #We can use a simple seaborn method to draw the heatmaps
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7f970d013090>
```



As we see in the above heatmap, most of the features are high related with one of the output targets which is etch_rate. Two of the targets, oxide_selectivity and photoresist_selectrivity are highly correlated. For pressure as a preditor variable, the most correlations are 0.4 and 0.3 with two of the targets,oxide_selectivity and photoresist_selectrivity, respectively. rf_power has the most correlation of 0.6 with etch_rate. he_flow has three most high correlation of -0.6, -0.5, 0.5, and -0.4 with oxide_selectivity, photoresist_selectrivity, etch_uniformity, and etch_rate, respectively. Tere are also highly correlations between target variables. I cannot say if these high correlations between predictors and targets are good for our study or not.

4. **Declare feature vector and target variable**

```
#Split data into training and test sets
#Train dataset:
df2 = df.copy()
df2_x = df.sample(frac=0.8, random_state=0)
df2_y = df2_x[['etch_rate','etch_uniformity','oxide_selectivity','photoresist_selectivity']]
df2_x.drop(['etch_rate','etch_uniformity','oxide_selectivity','photoresist_selectivity'], axis = 1, inplace = True)
print(df2_x.shape, df2_y.shape)
```

```
(42, 6) (42, 4)
```

```
#Test dataset:
df2_x_test = df.drop(df2_x.index)
df2_y_test = df2_x_test[['etch_rate','etch_uniformity','oxide_selectivity','photoresist_selectivity']]
df2_x_test.drop(['etch_rate','etch_uniformity','oxide_selectivity','photoresist_selectivity'], axis = 1, inplace = True)
print(df2_x_test.shape, df2_y_test.shape)
```

```
(11, 6) (11, 4)
```

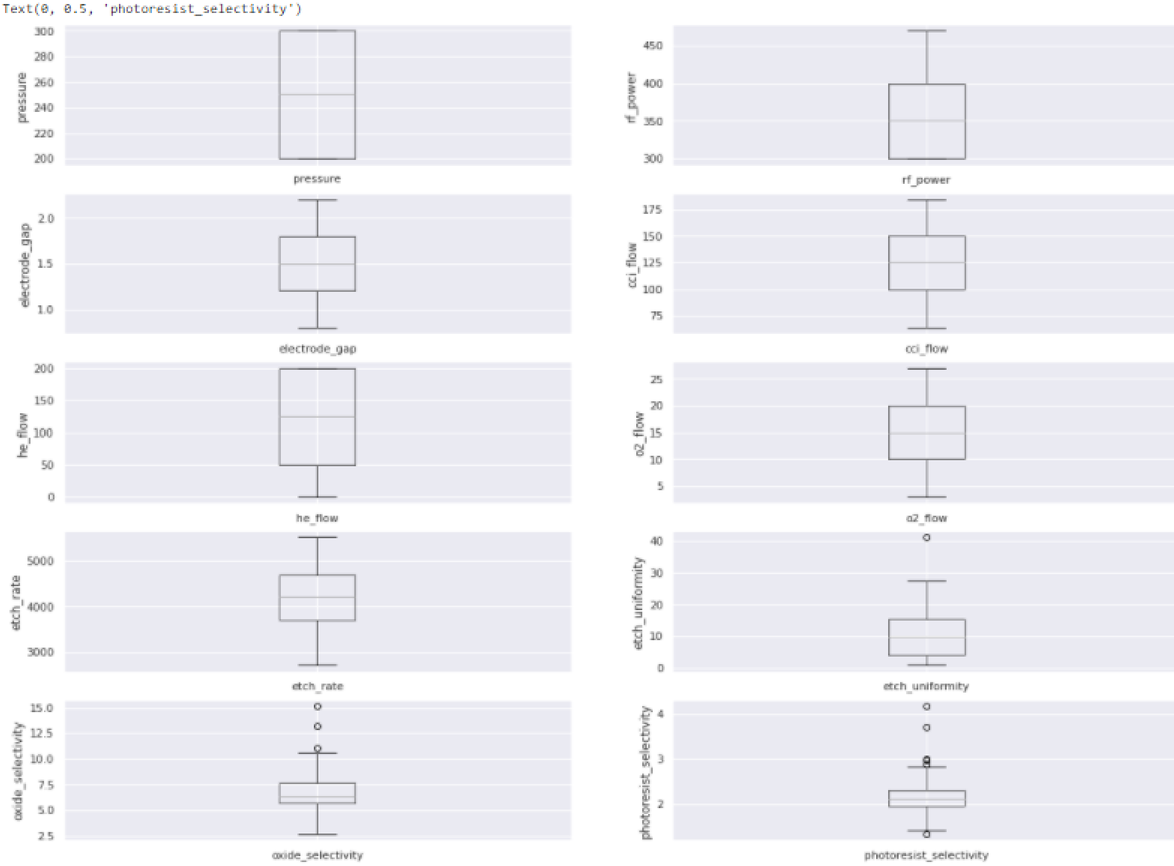
Summary of numerical variables
Train dataset has 42 numerical datapoints.
Train dataset has 11 numerical datapoints.
y variables are target variables.
There are no missing values in the dataset.

5. **Outliers:**

On closer inspection, we can suspect that all the continuous variables may contain outliers. I will draw boxplots to visualise outliers in the above variables.

```python
# draw boxplots to visualize outliers

plt.figure(figsize=(20,15))


plt.subplot(5, 2, 1)
fig = df2_x.boxplot(column='pressure')
fig.set_title('')
fig.set_ylabel('pressure')


plt.subplot(5, 2, 2)
fig = df2_x.boxplot(column='rf_power')
fig.set_title('')
fig.set_ylabel('rf_power')


plt.subplot(5, 2, 3)
fig = df2_x.boxplot(column='electrode_gap')
fig.set_title('')
fig.set_ylabel('electrode_gap')


plt.subplot(5, 2, 4)
fig = df2_x.boxplot(column='cci_flow')
fig.set_title('')
fig.set_ylabel('cci_flow')


plt.subplot(5, 2, 5)
fig = df2_x.boxplot(column='he_flow')
fig.set_title('')
fig.set_ylabel('he_flow')


plt.subplot(5, 2, 6)
fig = df2_x.boxplot(column='o2_flow')
fig.set_title('')
fig.set_ylabel('o2_flow')
```

```
Text(0, 0.5, 'photoresist_selectivity')
```

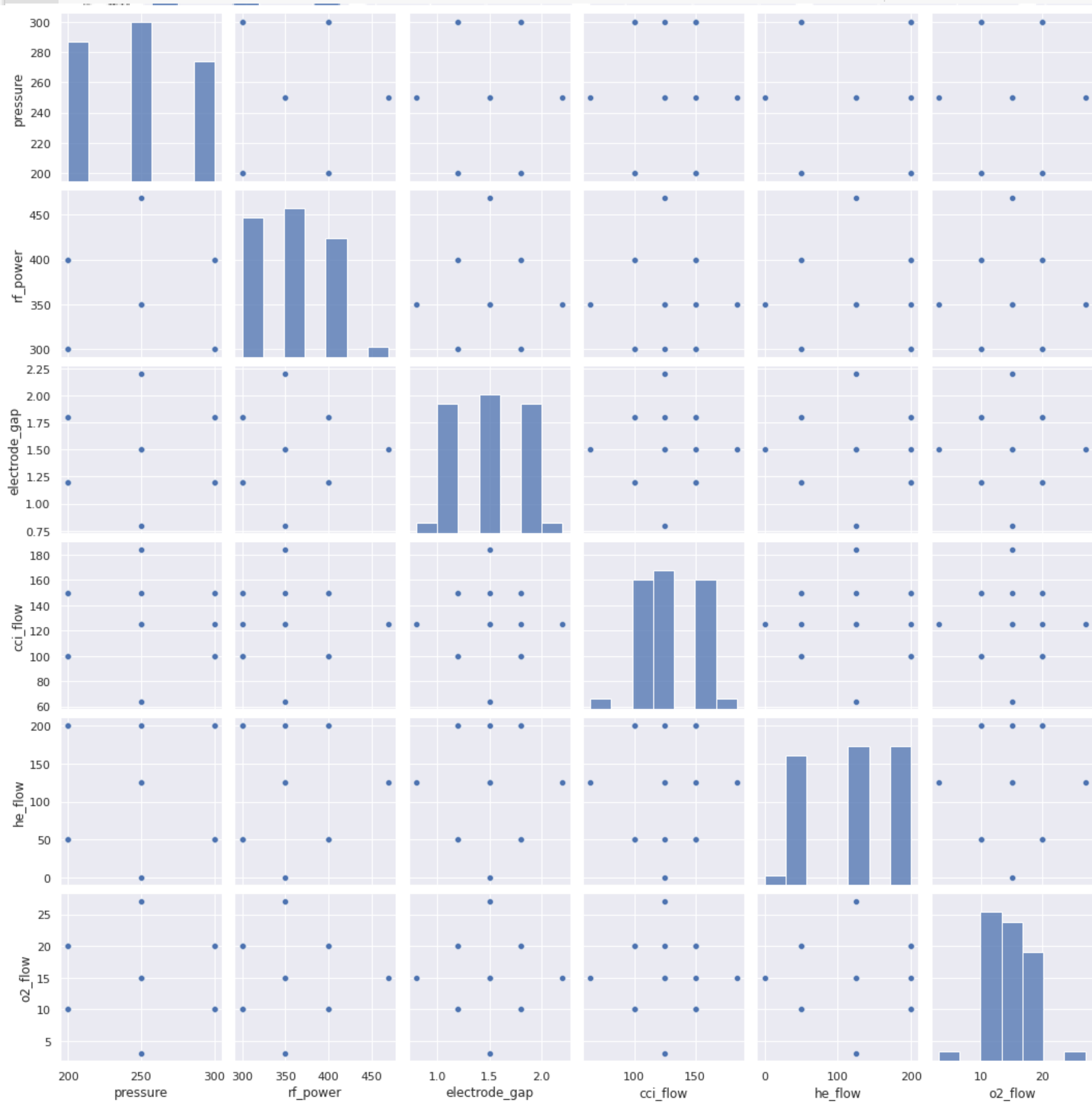


The above boxplots confirm that there are no outliers in train input variables but there are outliers in train output variables including etch_uniformity, oxide_selectivity, and photoresist_selectivity. Also, most of the variables have a skewed distribution not normal distribution. When we see skeweness, it means we need to do normalizatyion to bring all values of a column closer to each other by subtracting min value or mean value. Also, when different variables have different values, it means a column is more weighted compared to other. There, we need to do normalization, as well.

6. **Check the distribution of variables**

Now, I will plot the histograms to check distributions to find out if they are normal or skewed.

```
sns.pairplot(df2_x[['pressure', 'rf_power', 'electrode_gap', 'cci_flow', 'he_flow', 'o2_flow']])
```



We can see that this figure confirms the result that we got in previous section that most of the input variables are skewed.

7. **Feature Scaling**

A standardization is scaling features to lie between a given minimum and maximum value, often between zero and one, or so that the maximum absolute value of each feature is scaled to unit size. This can be achieved using MinMaxScaler or MaxAbsScaler, respectively. The motivation to use this scaling include robustness to very small standard deviations of features and preserving zero entries in sparse data.

```
[ ] cols = X_train.columns
```

```
[ ] from sklearn import preprocessing
    from sklearn.preprocessing import MinMaxScaler
```

```
[ ] scaler = preprocessing.MinMaxScaler()
    X_train = scaler.fit_transform(X_train) #fit means training the model which is done on training data, by using this line X_train will be an array not a dataframe
    X_train.dtype

    dtype('float64')
```

The same instance of the transformer can then be applied to some new test data unseen during the fit call: the same scaling and shifting operations will be applied to be consistent with the transformation performed on the train data:

```
X_test = scaler.transform(X_test) #The output is an array
X_test
X_test.dtype

dtype('float64')
```

```
[ ] X_train = pd.DataFrame(X_train, columns=[cols]) #Convert numpy array to dataframe, we do this since we want to add this dataframe to the other dataframe and make a new dataframe
```

8. Encoding target variables for implementing SVR:

One challenge of solving SVM for regression problem with int and float values for target variables (not predictor variables) is that SVM classifier cannot work with such values. So, we need to encode these values to convert them to only numeric values. Then, train SVM on it.

```
# Convert train target values to numeric using encoder
trainingScores = np.zeros((42,4)) #zero numpy array with shape of 42*4
encoded_y= np.zeros((42,4))
lab_enc = preprocessing.LabelEncoder()
for i in range(0,4):
  trainingScores[:,i] = np.array(df2_y.iloc[:,i])
  encoded_y[:,i] = lab_enc.fit_transform(trainingScores[:,i])
print(encoded_y)
```

```
[[29. 14. 26. 21.]
 [24.  6. 40. 31.]
 [39.  9. 23. 30.]
 [36.  2. 32. 25.]
 [ 5. 27.  4. 14.]
 [35. 34.  6.  5.]
 [ 3. 35.  0.  1.]
 [22. 25. 30. 11.]
 [ 2. 28.  9.  8.]
 [12.  5. 37. 29.]
 [38. 23. 10. 17.]
 [ 1. 24.  1.  1.]
 [ 9. 27. 14. 15.]
 [33.  4. 27. 20.]
 [32.  3. 20.  5.]
 [17. 30. 24. 16.]
 [21. 36. 15.  4.]
 [18. 18. 11.  6.]
 [10.  0. 25. 13.]
 [26. 32.  7. 10.]
 [41. 13. 21.  9.]
 [ 4. 31.  8. 12.]
 [34. 15. 31. 19.]
 [16. 12. 12. 22.]
 [ 0. 37.  2.  2.]
 [ 6. 11. 22. 21.]
 [11. 33. 18. 18.]
 [ 8. 22. 13. 10.]
 [27. 19. 29. 21.]
 [19. 29.  3.  3.]
 [28. 16. 33. 24.]
```

```
[ ] type(encoded_y)
```

```
numpy.ndarray
```

```
[ ] encoded_y.dtype # check the data type of an array
```

```
dtype('float64')
```

```
[ ] #Convert train target array to dataframe
    encoded_df = pd.DataFrame(encoded_y)
    type(encoded_df)
```

```
pandas.core.frame.DataFrame
```

```
# Convert test target values to numeric using encoder
trainingScores1 = np.zeros((11,4)) #zero numpy array with shape of 42*4
encoded_y_test= np.zeros((11,4))
lab_enc = preprocessing.LabelEncoder()
for i in range(0,4):
  trainingScores1[:,i] = np.array(df2_y_test.iloc[:,i])
  encoded_y_test[:,i] = lab_enc.fit_transform(trainingScores1[:,i])
print(encoded_y_test)
```

```
[[ 2.  8.  6.  2.]
 [ 7.  6.  2.  6.]
 [10.  0.  9.  9.]
 [ 0.  7.  1.  5.]
 [ 9.  9.  3.  0.]
 [ 5. 10.  0.  1.]
 [ 1.  2.  8. 10.]
 [ 8.  4. 10.  8.]
 [ 4.  3.  5.  3.]
 [ 6.  1.  7.  7.]
 [ 3.  5.  4.  4.]]
```

9. Run SVM with default hyperparameters

We have support vector classifiers. I will use two of them:'linear' and 'RBF' classifiers
The following is a default hyperparameter SVM.

```
# import SVC classifier
from sklearn import svm

# import metrics to compute accuracy
from sklearn.metrics import accuracy_score


#Simply fit the values of X and Y
for i in range(0,4):
  # instantiate classifier with default hyperparameters
  clf = svm.SVC()
  clf.fit(df2_x, encoded_df.iloc[:,i])


# make predictions on test set
  y_pred=clf.predict(df2_x_test)


# compute and print accuracy score
  print('Model accuracy score with default hyperparameters: {0:0.4f}'. format(accuracy_score(encoded_df1.iloc[:,i], y_pred)))
```

```
Model accuracy score with default hyperparameters: 0.0000
Model accuracy score with default hyperparameters: 0.0909
Model accuracy score with default hyperparameters: 0.0000
Model accuracy score with default hyperparameters: 0.0000
```

As we see, the accuracy scores with SVM default hyperparameters are extremely low. So, we need to tune hyperparameters.

10. ow determining parameters for the SVM model. The **GridSearchCV** utility from sklearn is perfect here.Run SVM with RBF kernel and C=100.0
    We have seen that there are outliers in our dataset. So, we should increase the value of C as higher C means fewer outliers. So, I will run SVM with kernel=rbf and C=100.0.

```
from sklearn.model_selection import cross_val_score, GridSearchCV
from sklearn.svm import SVR

gsc = GridSearchCV(
    estimator=SVR(kernel='rbf'),
    param_grid={
        'C': range(1, 100),
        'epsilon': (0.06, 0.08, 0.1),
    },
    cv=5
)
for i in range(0,i):
  grid_result = gsc.fit(df2_x, encoded_df.iloc[:,i])

print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
```

```
Best: 0.583974 using {'C': 99, 'epsilon': 0.07}
```

Plot the relation between the SVM parameters

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

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

ax.scatter([row['C'] for row in grid_result.cv_results_['params']],
           [row['epsilon'] for row in grid_result.cv_results_['params']],
           grid_result.cv_results_['mean_test_score'],
           c='b', marker='^')

ax.set_xlabel('C')
ax.set_ylabel('Epsilon')
ax.set_zlabel('Score')
```

```
Text(0.5, 0, 'Score')
```