02 - Linear Regression Modelling

October 23, 2022

1 Predicting Cement Compressive Strength Using Linear Regression Model

With the data explored, and familiarized from the previous notebook, we are now ready to conduct build a model to predict the compressive strenght of a cement.

1.1 Pre-processing

As we have discovered from the previous notebook, the features of our dataset were highly skewed. In this section, we will conduct several data pre-processing to our dataset so that we can enable our model to learn effectively and efficiently.

[ ]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

plt.style.use(['science', 'notebook'])
```

[ ]:
```
DATASET_URI = "https://archive.ics.uci.edu/ml/machine-learning-databases/
↪concrete/compressive/Concrete_Data.xls"

dataset = pd.read_excel(DATASET_URI)

# Replace the Headers for Readability
attributes = [
  "Cement", "Blast Furnace Slag", "Fly Ash", "Water", "Superplasticizer",
  "Coarse Aggregate", "Fine Aggregate", "Age", "Concrete Compressive Strength"
]

dataset.columns = attributes
```

1.1.1 Creating Training, Validation, and Test Set

Before we proceed to any pre-processing and modelling, let's split our dataset into three parts. 1. Training Set - To be used during training. 2. Validation Set - To be used during cross validation after training with the purpose of detecting bias/variance from training. 3. Test Set - To be used for evaluating our model.

```
[ ]: from sklearn.model_selection import train_test_split

X = dataset.iloc[:,0:-1]
y = dataset.iloc[:, -1]

# Split the dataset into 80% training set, and 20% cross validation + test set.
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2)

# Split the cross validation + test set from previous split and split them␣
 ↪equally
X_val, X_test, y_val, y_test = train_test_split(X_test, y_test, test_size=0.5)
```

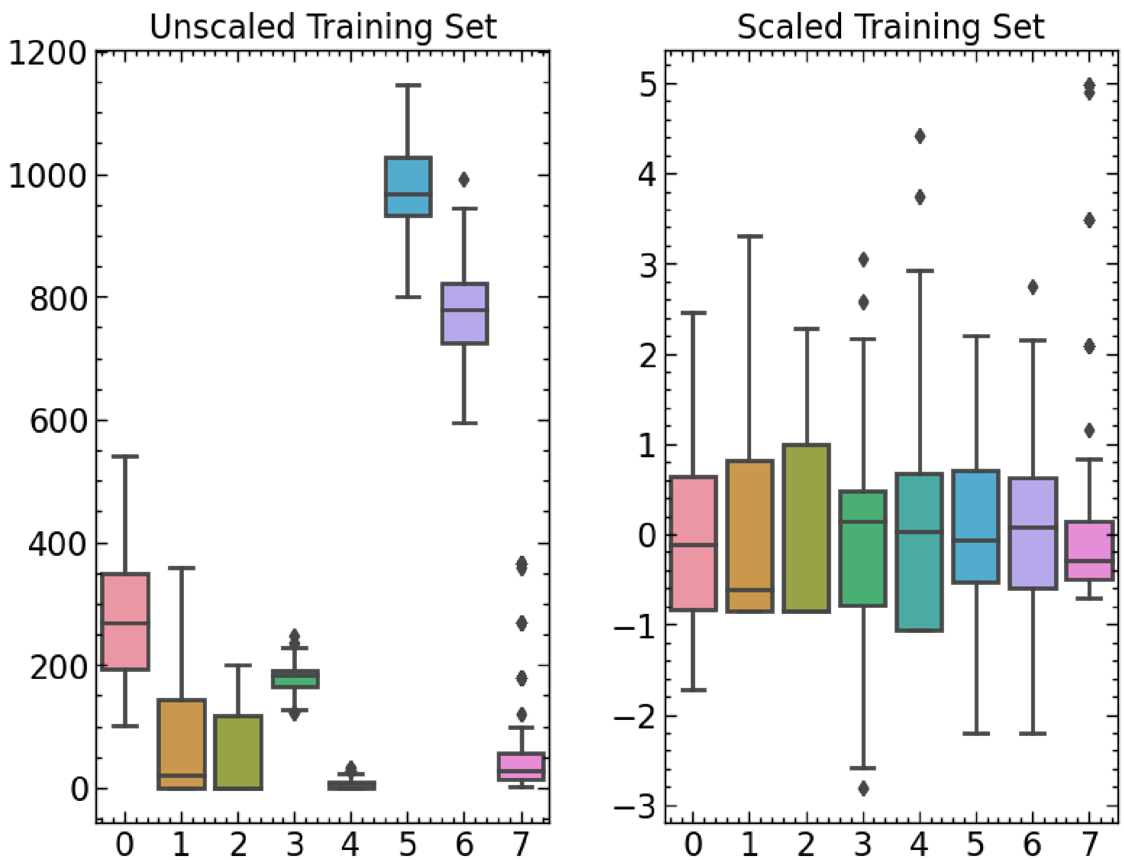
1.1.2 Scaling the Features

Now, lets scale our features, we will train the standard scaler from the training set and use this scaler to validation, and test set.

```
[ ]: from sklearn.preprocessing import StandardScaler
# Instanciate the Standard Scaler
std_scaler = StandardScaler()

# Train the scaler on the training set only
std_scaler.fit(X_train.values)

# Transform each splits into a standard scale
scaled_X_train = std_scaler.transform(X_train.values)
scaled_X_val = std_scaler.transform(X_val.values)
scaled_X_test = std_scaler.transform(X_test.values)
```

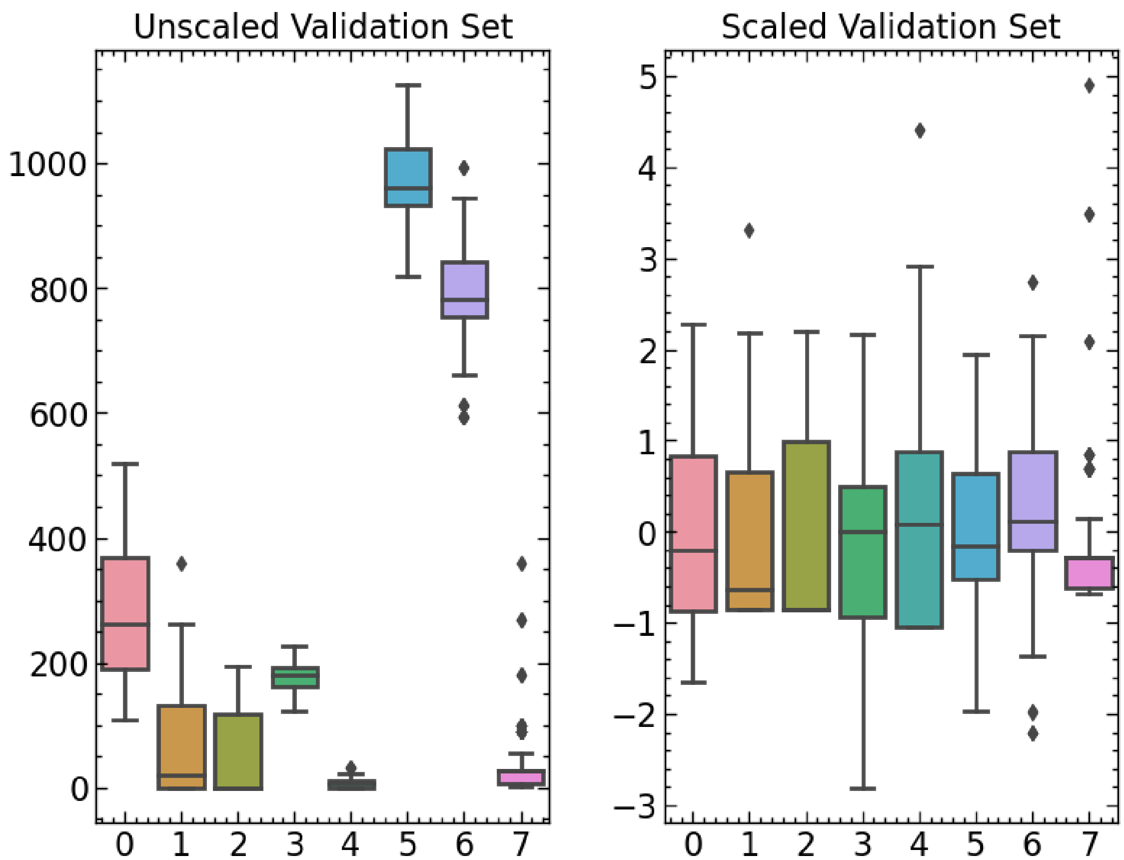
```
[ ]: figure, axes = plt.subplots(1,2)
figure.tight_layout()

sns.boxplot(X_train.to_numpy(), ax=axes[0]).set(title="Unscaled Training Set")
sns.boxplot(scaled_X_train, ax=axes[1]).set(title="Scaled Training Set")
```

```
[ ]: [Text(0.5, 1.0, 'Scaled Training Set')]
```



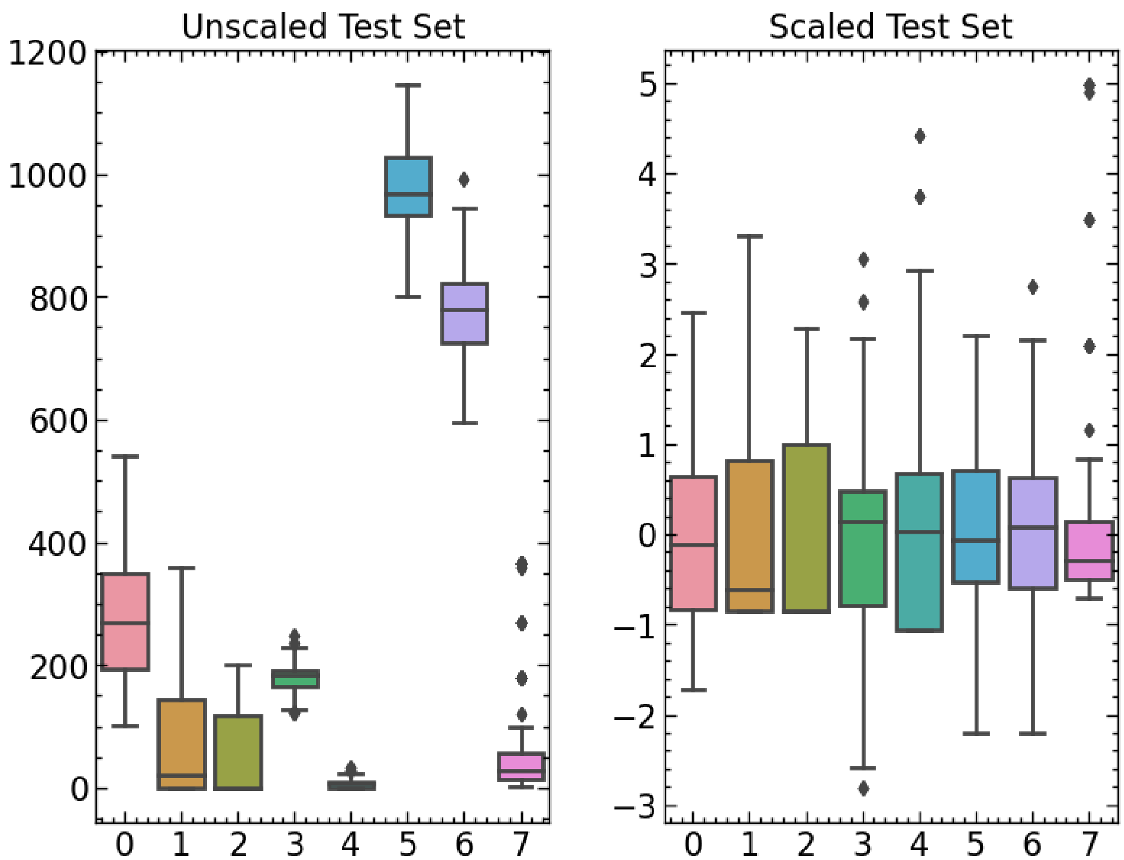
[ ]:
```
figure, axes = plt.subplots(1, 2)
figure.tight_layout()

sns.boxplot(X_val.to_numpy(), ax=axes[0]).set(title="Unscaled Validation Set")
sns.boxplot(scaled_X_val, ax=axes[1]).set(title="Scaled Validation Set")
```

[ ]:
```
[Text(0.5, 1.0, 'Scaled Validation Set')]
```



[ ]:
```
figure, axes = plt.subplots(1, 2)
figure.tight_layout()

sns.boxplot(X_train.to_numpy(), ax=axes[0]).set(title="Unscaled Test Set")
sns.boxplot(scaled_X_train, ax=axes[1]).set(title="Scaled Test Set")
```

[ ]:
```
[Text(0.5, 1.0, 'Scaled Test Set')]
```



The Dataset Is Now Ready With scaled features, our dataset is not very skewed and is now ready for modelling.

1.2 OLS Regression: Linear Regression

Now lets start conducting linear regression, we will begin with the most simple Linear regression, then we will try using different degrees of polynomial features, and finally we will apply regularization to minimize overfitting.

[ ]:
```
from sklearn.linear_model import LinearRegression

# Fit the model to our training set
linear_regression = LinearRegression()
linear_regression.fit(scaled_X_train, y_train.values)

# Predict compressive strength from each split
y_train_pred = linear_regression.predict(scaled_X_train)
y_val_pred = linear_regression.predict(scaled_X_val)
y_test_pred = linear_regression.predict(scaled_X_test)
```

[ ]:
```
from sklearn.metrics import mean_absolute_error, mean_squared_error

split_pairs = [
  (y_train, y_train_pred),
  (y_val, y_val_pred),
  (y_test, y_test_pred)
]

MAE  = []
MSE  = []
RMSE = []

for pair in split_pairs:
  MAE.append(mean_absolute_error(pair[0], pair[1]))
  MSE.append(mean_squared_error(pair[0], pair[1]))
  RMSE.append(mean_squared_error(pair[0], pair[1], squared=False))

linear_regression_errors = pd.DataFrame({
  "Error Type": ["Training Error", "Validation Error", "Testing Error"],
  "MAE (in Mega-Pascals)": MAE,
  "MSE(in Mega-Pascals)^2": MSE,
  "RMSE (in Mega-Pascals)": RMSE
})
linear_regression_errors
```

[ ]:
```
         Error Type  MAE (in Mega-Pascals)  MSE(in Mega-Pascals)^2  \
0    Training Error               8.037219              104.701221
1  Validation Error               8.155582               96.271840
2     Testing Error               9.782676              141.304387

   RMSE (in Mega-Pascals)
0               10.232361
1                9.811821
2               11.887152
```

1.2.1 Results

Our training, validation and test errors were almost near at each other. This might be an indicator that our model is not overfitting. However, our loss is still large. On the next section, we will try to use polynomial features and see if we can improve our linear model.

1.3 OLS Regression: Linear Regression with Polynomial Features

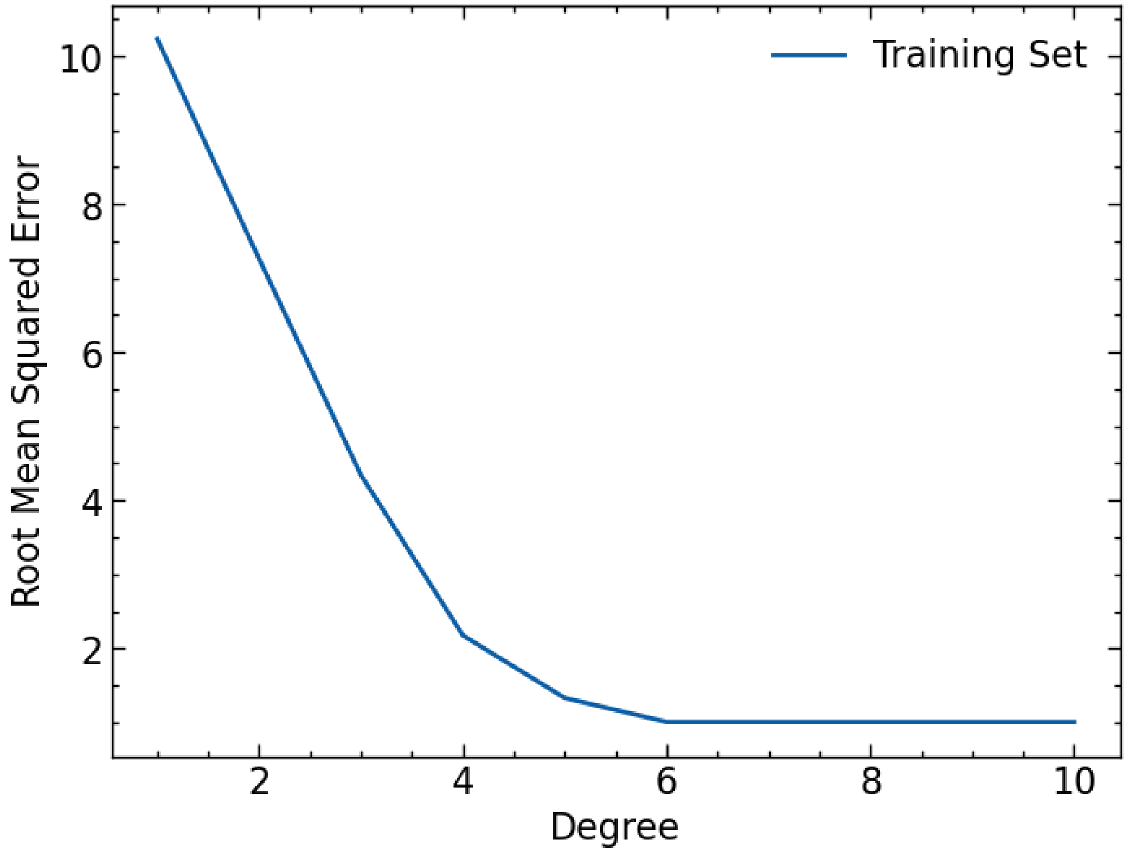
Now, let's improve our model by adding polynomial features, we will evaluate which polynomial degree will minimize the loss and overfitting.

[ ]:
```
from sklearn.preprocessing import PolynomialFeatures
```

```
MAE_train = []
MSE_train = []
RMSE_train = []

MAE_val = []
MSE_val = []
RMSE_val = []

MAE_test = []
MSE_test = []
RMSE_test = []

degrees = range(1, 11)

for degree in degrees:
  poly_features = PolynomialFeatures(degree=degree)
  linear_regression = LinearRegression()

  # Create polynomial features for each input splits
  scaled_X_train_poly = poly_features.fit_transform(scaled_X_train)
  scaled_X_val_poly = poly_features.fit_transform(scaled_X_val)
  scaled_X_test_poly = poly_features.fit_transform(scaled_X_test)

  # Fit the training data with polynomial features
  linear_regression.fit(scaled_X_train_poly, y_train)

  # Predict compressive strength from each split
  y_train_pred = linear_regression.predict(scaled_X_train_poly)
  y_val_pred = linear_regression.predict(scaled_X_val_poly)
  y_test_pred = linear_regression.predict(scaled_X_test_poly)

  MAE_train.append(mean_absolute_error(y_train, y_train_pred))
  MSE_train.append(mean_squared_error(y_train, y_train_pred))
  RMSE_train.append(mean_squared_error(y_train, y_train_pred, squared=False))

  MAE_val.append(mean_absolute_error(y_val, y_val_pred))
  MSE_val.append(mean_squared_error(y_val, y_val_pred))
  RMSE_val.append(mean_squared_error(y_val, y_val_pred, squared=False))

  MAE_test.append(mean_absolute_error(y_test, y_test_pred))
  MSE_test.append(mean_squared_error(y_test, y_test_pred))
  RMSE_test.append(mean_squared_error(y_test, y_test_pred, squared=False))
```

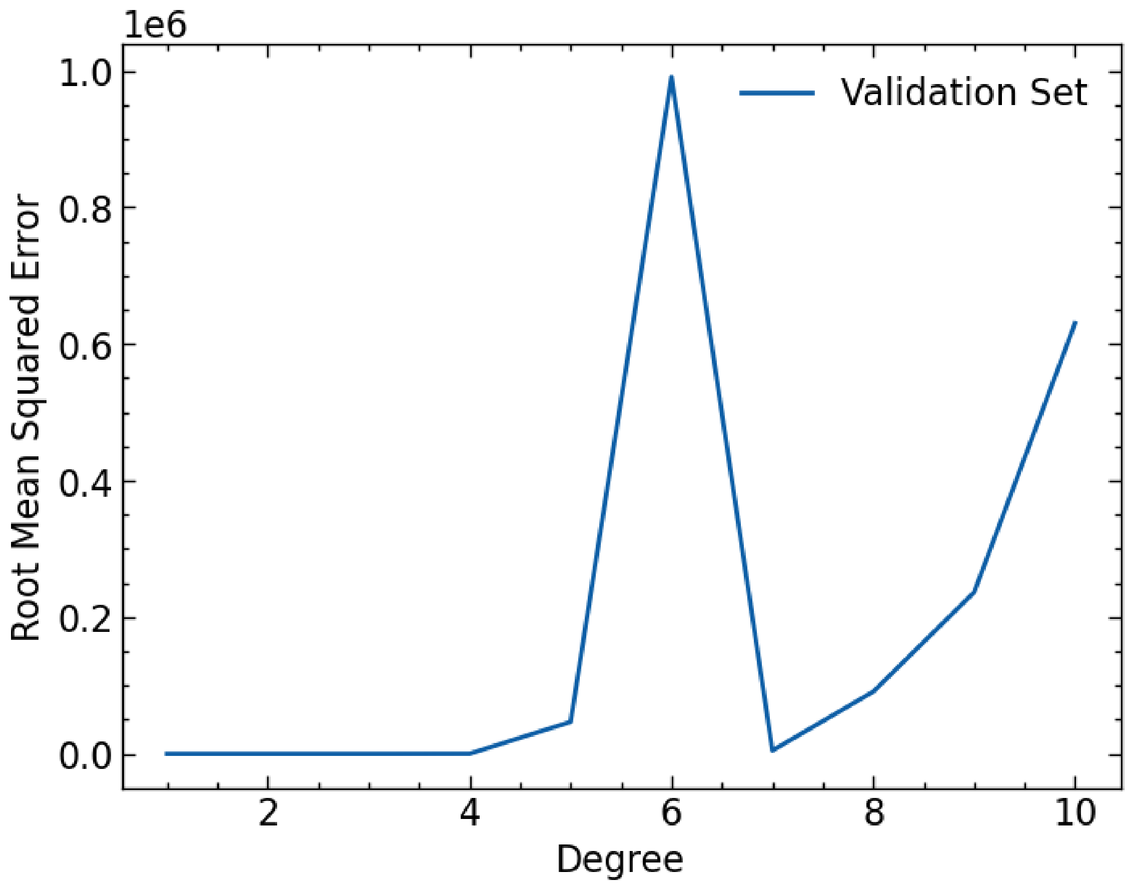
[ ]:
```
plt.plot(degrees, RMSE_train, label="Training Set")
plt.xlabel("Degree")
plt.ylabel("Root Mean Squared Error")
plt.legend()
```

[ ]: <matplotlib.legend.Legend at 0x2646b0ee6b0>



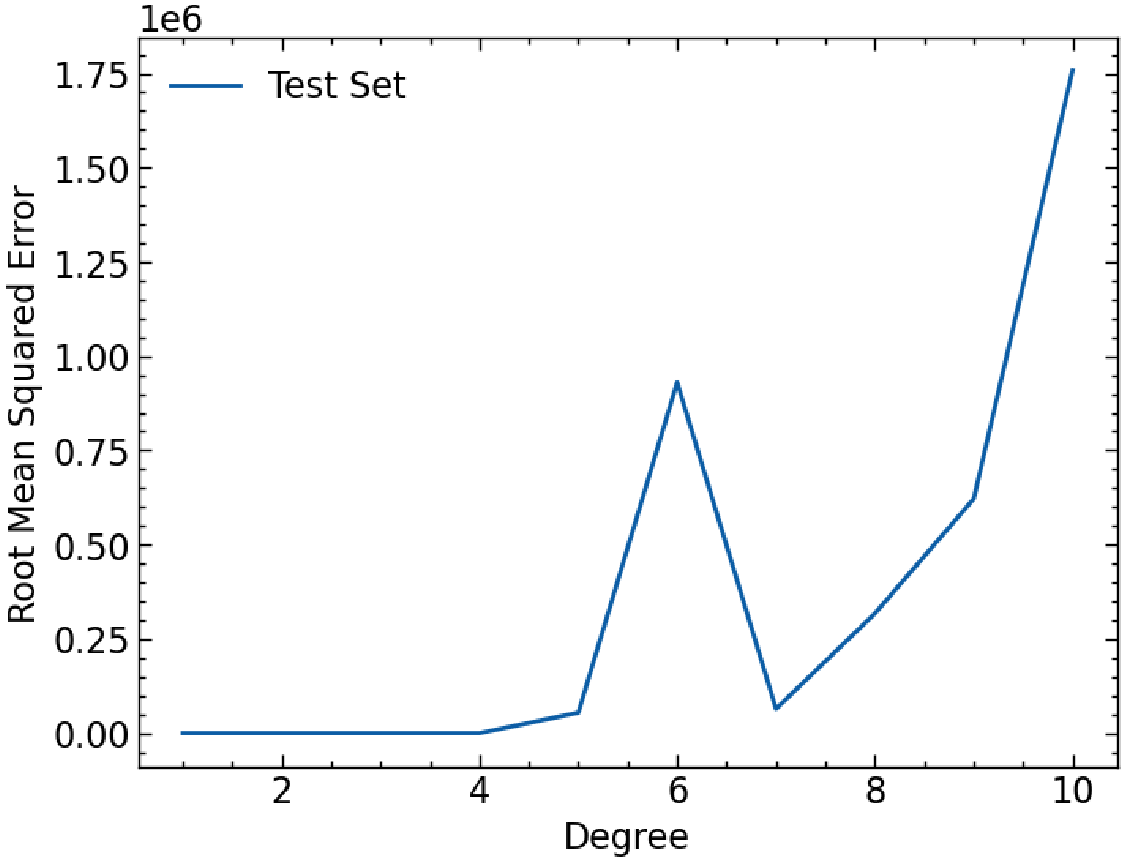
[ ]:
```python
plt.plot(degrees, RMSE_val, label="Validation Set")
plt.xlabel("Degree")
plt.ylabel("Root Mean Squared Error")
plt.legend()
```

[ ]: <matplotlib.legend.Legend at 0x2646b119360>




```
[ ]: plt.plot(degrees, RMSE_test, label="Test Set")
     plt.xlabel("Degree")
     plt.ylabel("Root Mean Squared Error")
     plt.legend()
```

```
[ ]: <matplotlib.legend.Legend at 0x2640474a620>
```



1.4 Selected Degree

The following code snippet below will display the degrees which returns a minimum RMSE per dataset split.

[ ]:
```
min_degree_train = np.argmin(RMSE_train) + 1
min_degree_val = np.argmin(RMSE_val) + 1
min_degree_test = np.argmin(RMSE_test) + 1

print(f"Degree with Minimum Training RMSE: {min_degree_train}")
print(f"Degree with Minimum Validation RMSE: {min_degree_val}")
print(f"Degree with Minimum Testing RMSE: {min_degree_test}")
```

```
Degree with Minimum Training RMSE: 7
Degree with Minimum Validation RMSE: 2
Degree with Minimum Testing RMSE: 3
```

Based on the results, we can attain minimum training error when we use 8th degree polynomial features, however we will be encountering overfitting as the RMSE on the validation and testing set were significantly higher especially at 4th degree. Thus we will be using the 3rd degree polynomial features.

[ ]:
```python
poly_features = PolynomialFeatures(degree=3)
linear_regression = LinearRegression()

# Create polynomial features for each input splits
scaled_X_train_poly = poly_features.fit_transform(scaled_X_train)
scaled_X_val_poly = poly_features.fit_transform(scaled_X_val)
scaled_X_test_poly = poly_features.fit_transform(scaled_X_test)

# Fit the training data with polynomial features
linear_regression.fit(scaled_X_train_poly, y_train)

# Predict compressive strength from each split
y_train_pred = linear_regression.predict(scaled_X_train_poly)
y_val_pred = linear_regression.predict(scaled_X_val_poly)
y_test_pred = linear_regression.predict(scaled_X_test_poly)

split_pairs = [
    (y_train, y_train_pred),
    (y_val, y_val_pred),
    (y_test, y_test_pred)
]

MAE = []
MSE = []
RMSE = []

for pair in split_pairs:
  MAE.append(mean_absolute_error(pair[0], pair[1]))
  MSE.append(mean_squared_error(pair[0], pair[1]))
  RMSE.append(mean_squared_error(pair[0], pair[1], squared=False))

linear_regression_with_poly_features_errors = pd.DataFrame({
    "Error Type": ["Training Error", "Validation Error", "Testing Error"],
    "MAE (in Mega-Pascals)": MAE,
    "MSE(in Mega-Pascals)^2": MSE,
    "RMSE (in Mega-Pascals)": RMSE
})
linear_regression_with_poly_features_errors
```

[ ]:
```
         Error Type  MAE (in Mega-Pascals)  MSE(in Mega-Pascals)^2  \
0    Training Error               3.333588               18.842223
1  Validation Error               5.301488               95.677762
2     Testing Error               5.036891               48.413525

   RMSE (in Mega-Pascals)
0                4.340763
1                9.781501
```

```
2                    6.957983
```

1.5 Comparing Results

Now, lets compare our new-found model with the previous one.

```
[ ]: change_MAE = linear_regression_with_poly_features_errors["MAE (in␣
      ↪Mega-Pascals)"] / linear_regression_errors["MAE (in Mega-Pascals)"] - 1
     change_MSE = linear_regression_with_poly_features_errors["MSE(in␣
      ↪Mega-Pascals)^2"] / linear_regression_errors["MSE(in Mega-Pascals)^2"] - 1
     change_RMSE = linear_regression_with_poly_features_errors["RMSE (in␣
      ↪Mega-Pascals)"] / linear_regression_errors["RMSE (in Mega-Pascals)"] - 1
```

```
[ ]: changes = pd.DataFrame({
       "Split": ["Training Set", "Validation Set", "Testing Set"],
       "MAE(% Change)": change_MAE,
       "MSE(% Change)": change_MSE,
       "RMSE(% Change)": change_RMSE,
     })
     changes
```

[ ]:

	Split	MAE(% Change)	MSE(% Change)	RMSE(% Change)
0	Training Set	-0.585231	-0.820038	-0.575781
1	Validation Set	-0.349956	-0.006171	-0.003090
2	Testing Set	-0.485121	-0.657381	-0.414664

1.6 Improvements

Overall, using 3rd degree polynomial features on linear regression greatly improves the error on training set by 58.49%, 21.85% on validation set, and 42.52% on test set.

can we still improve these prediction errors? in the next section, we will be trying to apply regularization techniques to further improve our model.