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Problem 1 [12pts] For each of parts (a) through (c), indicate whether we would generally expect the performance of a flexible statistical learning method to be better or worse than an inflexible method. Justify your answer.

(a) The sample size n is extremely large, and the number of predictors p is small. **Answer:** Models flexibility is its ability to adapt, evolve and learn from input data. In the above case where sample size is large, a flexible statistical method would perform better than an inflexible one because it can capture the true underlying relationship between the data and predictors. An inflexible model might be too restrictive to accurately fit the data.

(b) The number of predictors p is extremely large, and the number of observations n is small. **Answer:** In this case the inflexible statistical method will perform better since it can restrict the complexity and prevent overfitting that the flexible methods are prone to.

(c) The relationship between the predictors and response is highly non-linear. **Answer:** Flexible statistical learning methods can capture non-linear relationships in data without making assumptions about the data's underlying distribution. While inflexible model might lead to prediction errors. So in this case flexible statistical methods will perform better.

Problem 2

a) [4pts] Use Figure 1a to predict $medv$ given $lstat=25$ with $K = 1$ and $K = 5$. **$lstat=25$ $k=1$ nearest neighbour is (24.39,8.3) Answer: $medv=8.3$ $k=5$ Answer: $medv=12.1$**

(b) [4pts] Repeat (a) for $lstat=27$. **$lstat=27$ $k=1$ nearest neighbour is (26.82,13.4) Answer: $medv=13.4$ $k=5$ nearest neighbours are (24.39,8.3), (25.68,9.7), (29.68,8.1), (26.82,13.4), (26.4,17.2) Answer: $medv=11.34$**

(c) [4pts] Use Figure 1b to predict $medv_cat$ given $lstat=25$ with $K = 1$ and $K = 5$. **$lstat=25$ $k=1$ nearest neighbour is (24.39,0) Answer: $medv=0$ $k=5$ nearest neighbour is (24.39,0), (25.68,0), (23.6,1.4), (24.16,2), (26.4,2) frequency of 0:2, 1:1, 2:2 taking the least median with highest frequency Answer: $medv=0$**

(d) [4pts] Repeat (c) for $lstat=27$. **$lstat=27$ $k=1$ nearest neighbour is (26.82,1) Answer: $medv=1$ $k=5$ nearest neighbours are (24.39,0), (25.68,0), (29.68,0), (26.82,1), (26.4,2) frequency of 0:3, 1:1, 2:1 Answer: $medv=0$**

(e) [4pts] If we increase K in KNN, is the model more flexible or less flexible? Explain why. **Answer: Let's run through the case where initially k is small, the decision boundary is highly flexible, that is the model reacts to even small variations in the data. But it can closely follow the training data, which can lead to overfitting. As we increase k the model takes into account more neighbors when**

classifying a new data point. This leads to a smoother decision boundary, as the prediction for any point now depends on a larger set of neighbors. But the model becomes less sensitive to noise or individual outliers. Increasing k reduces variance (making the model more stable and less prone to overfitting), but it increases bias (the model may become too simple and unable to capture the complexity of the data). So, higher k results in a less flexible model.

(f) [6pts] How do the square of bias, variance, training MSE, test MSE, and irreducible error change with K for KNN regression? Explain why. **Square of bias:** When k is small the model closely follows the training data, leading to low bias. However, as k increases, the predictions are based on more neighbors, making the model's decision boundary smoother and less fitted to specific patterns in the data. This leads to an increased bias as the model becomes less flexible and may not capture the underlying patterns in the data as well.

Variance: It is inversely proportional to the value of k . A small k makes the model very flexible, highly sensitive to variations in the training data, and prone to overfitting (high variance). As k increases, the predictions are based on more points, leading to more stable and smoother estimates. The model becomes less sensitive to changes in individual training points, reducing variance.

Training MSE: For small k , the model is overfitting and tends to closely match the training data, leading to a low training MSE. As k increases, the model fits the training data less accurately, so the training MSE increases.

Test MSE: With very small k , the model is prone to overfitting, resulting in high test MSE because it is capturing noise in the data (high variance). As k increases, the model generalizes better, reducing overfitting, and test MSE decreases. However, after a certain point, increasing k too much leads to underfitting (the model becomes too simple), and the test MSE starts increasing again due to high bias. This creates a U-shaped curve for test MSE.

Irreducible Error: This remains constant. It represents the noise inherent in the data that cannot be modeled or reduced by any model, including KNN. It's due to random variability or factors not captured by the available features, so it does not change with k .

Problem 3

Part a

Number of observations(p): The sample size is specified in the function as 100, therefore $n=100$.

Number of features(p): As mentioned in the question different powers of x are different features, since in this equation there are 3 x variables with different powers number of features is 3($p=3$).

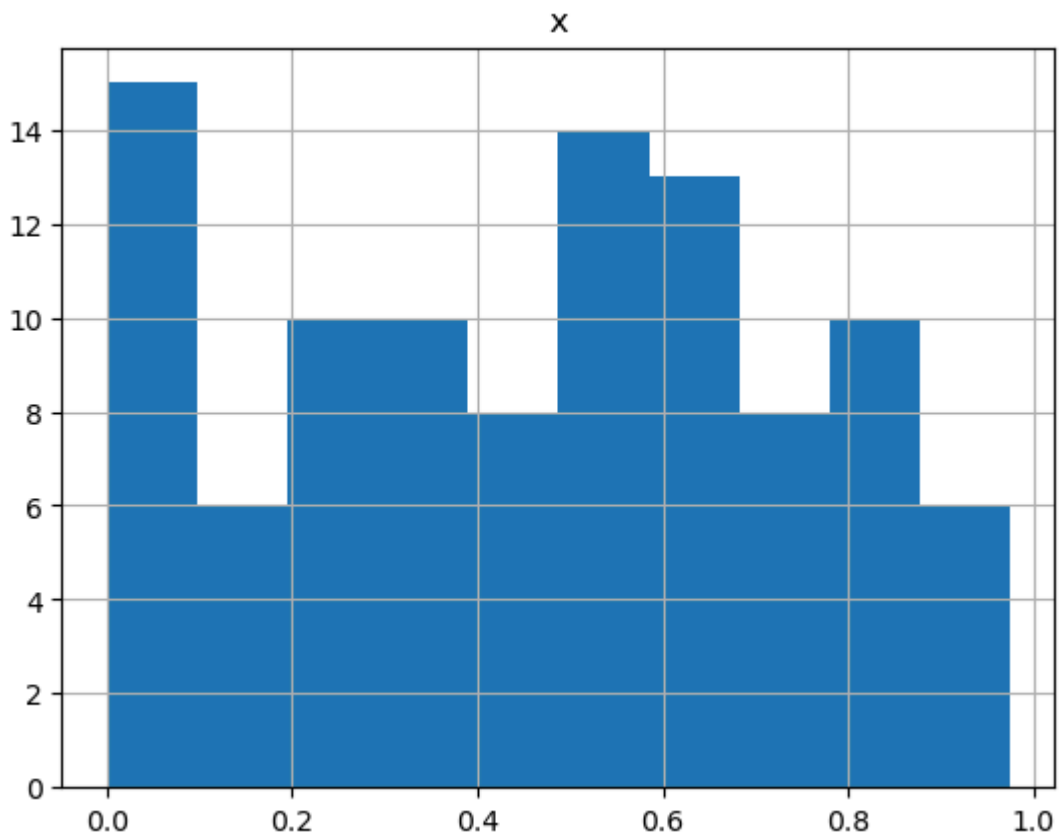
Model used in this question to generate the data is $y=x^5 - 2 * x^4 + x^3$

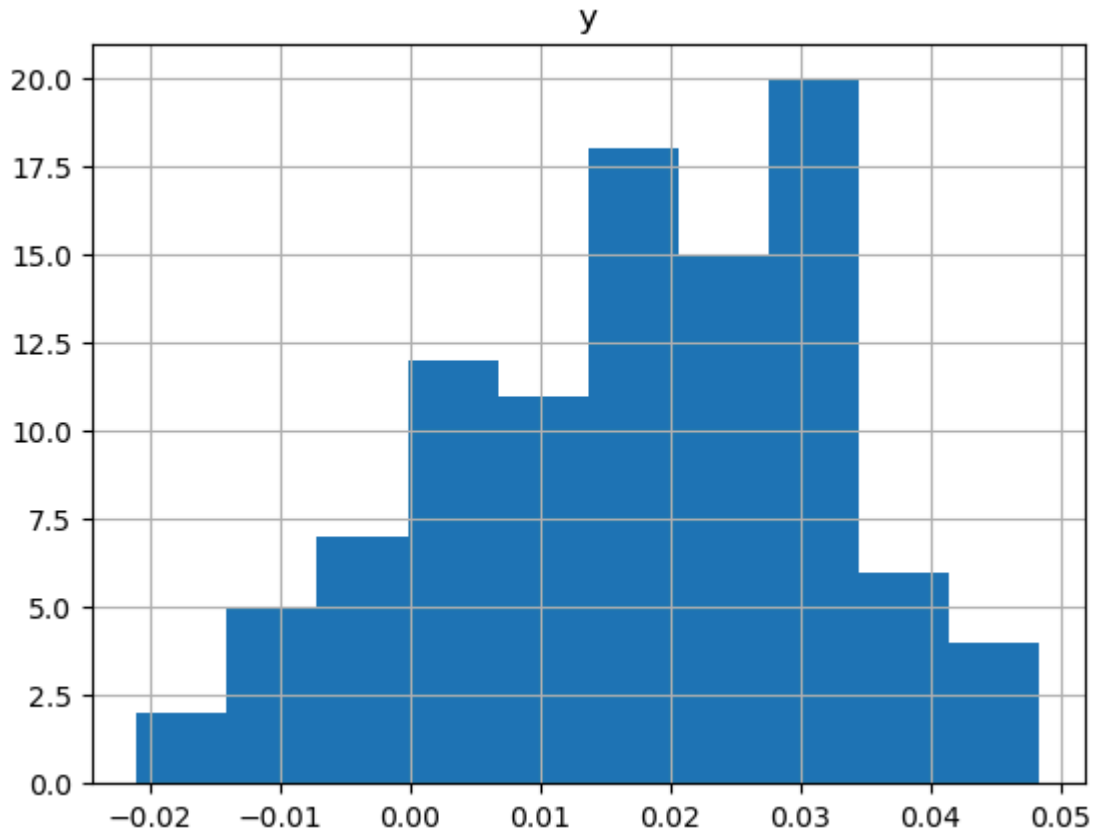
```
In [10]: import numpy as np
import pandas as pd
```

```
In [12]: def f(x):
return x ** 5 - 2 * x ** 4 + x ** 3 #true function
def get_sim_data(f, sample_size, std):
x = np.random.uniform(0, 1, sample_size)
y = f(x) + np.random.normal(0, std, sample_size)
df = pd.DataFrame({'x': x, 'y': y})
return df
df = get_sim_data(f, 100, 0.01)
#print(get_sim_data(f))
```

```
In [14]: df.hist('x') #uniformly distributed
df.hist('y') #normally distributed
```

```
Out[14]: array([[<Axes: title={'center': 'y'}>]], dtype=object)
```





```
In [16]: from sklearn.preprocessing import PolynomialFeatures
         from sklearn.linear_model import LinearRegression
```

```
In [18]: df.head(5)
```

```
Out[18]:
```

	x	y
0	0.683214	0.033149
1	0.004226	-0.014879
2	0.342745	0.014779
3	0.251840	0.014984
4	0.669353	0.022133

```
In [20]: df.shape
```

```
Out[20]: (100, 2)
```

Part b and c

```
In [24]: X = df['x'].values.reshape(-1, 1)
         Y = df['y'].values
         for i in range(16):
             poly=PolynomialFeatures(degree=i)
             degree_x=poly.fit_transform(X)#training set
             model=LinearRegression()
             model.fit(degree_x,Y)
             x0=0.18
```

```
x0_fit=poly.transform([[x0]])#test set
print(model.predict(x0_fit))
```

```
[0.01767839]
[0.01243638]
[0.0123963]
[0.00684651]
[0.00699582]
[0.00799499]
[0.00800465]
[0.00603613]
[0.00620828]
[0.00619444]
[0.00586755]
[0.00530537]
[0.00411163]
[0.00416807]
[0.00413081]
[0.00211689]
```

Part d

```
In [30]: # iterating for 250 times
predictions_per_degree = {j: [] for j in range(16)} #for part e
for i in range(250):
    def f(x):
        return x ** 5 - 2 * x ** 4 + x ** 3
    def get_sim_data(f, sample_size, std):
        x = np.random.uniform(0, 1, sample_size)
        y = f(x) + np.random.normal(0, std, sample_size)
        df = pd.DataFrame({'x': x, 'y': y})
        return df
    df = get_sim_data(f, 100, 0.01)
    X = df['x'].values.reshape(-1, 1)
    Y = df['y'].values
    for j in range(16):
        poly=PolynomialFeatures(degree=j)
        degree_x=poly.fit_transform(X)#training set
        model=LinearRegression()
        model.fit(degree_x,Y)
        y_pred=model.predict(poly.transform([[0.18]]))
        predictions_per_degree[j].append(y_pred)
```

Part e

```
In [33]: bias_squared = {}
y_true = f(0.18)
for j in range(16):
    average = np.mean(predictions_per_degree[j])
    bias = average - y_true
    bias_squared[j] = bias ** 2
    print(f"Degree {j}: Bias Squared = {bias_squared[j]}")
```

```

Degree 0: Bias Squared = 0.00016340939284580186
Degree 1: Bias Squared = 7.114051374559911e-05
Degree 2: Bias Squared = 2.8683778681132882e-05
Degree 3: Bias Squared = 4.3240568498671105e-06
Degree 4: Bias Squared = 9.291226839446423e-07
Degree 5: Bias Squared = 1.4323114578246049e-08
Degree 6: Bias Squared = 1.8565648299011434e-08
Degree 7: Bias Squared = 4.425165338366436e-09
Degree 8: Bias Squared = 2.0299597089602324e-09
Degree 9: Bias Squared = 2.351206141546605e-09
Degree 10: Bias Squared = 1.1081813894659267e-09
Degree 11: Bias Squared = 2.3594601441624568e-08
Degree 12: Bias Squared = 3.8679247529445e-08
Degree 13: Bias Squared = 7.30168256541323e-08
Degree 14: Bias Squared = 7.458350625064033e-08
Degree 15: Bias Squared = 7.924088230195677e-08

```

Part f

```

In [36]: variance = {}
         for j in range(16):
             avg = np.mean(predictions_per_degree[j])
             variance[j] = np.mean((predictions_per_degree[j] - avg) ** 2)
             print(f"Degree {j}: Variance = {variance[j]}")

```

```

Degree 0: Variance = 2.5354433379671205e-06
Degree 1: Variance = 4.240572692102544e-06
Degree 2: Variance = 3.5497188527788246e-06
Degree 3: Variance = 3.1081128190596366e-06
Degree 4: Variance = 4.579659407803415e-06
Degree 5: Variance = 5.7102862135557875e-06
Degree 6: Variance = 5.836802853843687e-06
Degree 7: Variance = 7.896756351334372e-06
Degree 8: Variance = 9.052928298209146e-06
Degree 9: Variance = 9.411404498448661e-06
Degree 10: Variance = 9.529829833015183e-06
Degree 11: Variance = 1.1318754412689825e-05
Degree 12: Variance = 1.337533786987028e-05
Degree 13: Variance = 1.401296199282676e-05
Degree 14: Variance = 1.5659124894239428e-05
Degree 15: Variance = 1.796367822770741e-05

```

Part g

```

In [39]: std=0.01
         irr_err=std**2

```

Part h

```

In [42]: mse=[]
         for i in range(16):
             mse_degree=bias_squared[i]+variance[i]+irr_err
             mse.append(mse_degree)
         print(mse)

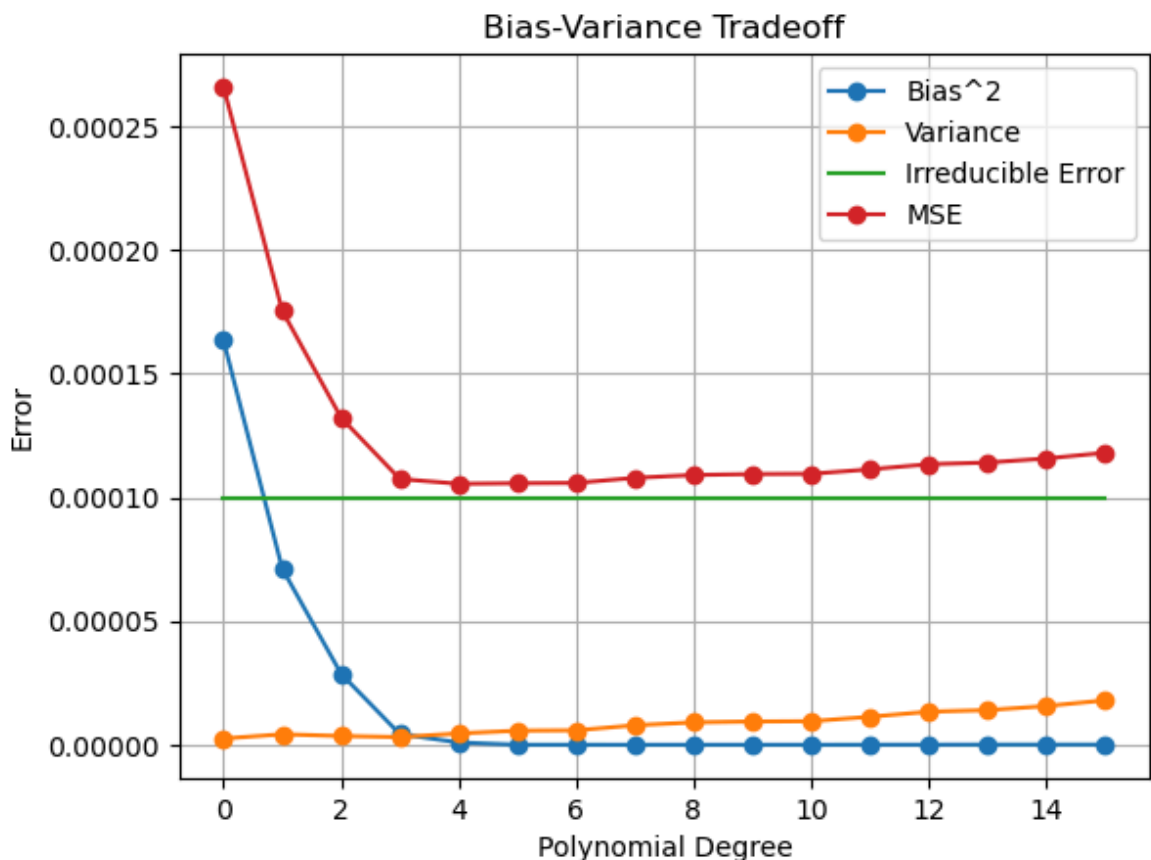
```

```
[0.000265944836183769, 0.00017538108643770168, 0.0001322334975339117, 0.00010743216966892675, 0.00010550878209174806, 0.00010572460932813404, 0.00010585536850214271, 0.00010790118151667274, 0.00010905495825791811, 0.00010941375570459022, 0.00010953093801440465, 0.00011134234901413146, 0.00011341401711739972, 0.0001140859788184809, 0.00011573370840049007, 0.00011804291911000937]
```

Part i

```
In [46]: import matplotlib.pyplot as plt
```

```
In [48]: degrees=range(16)
plt.plot(degrees,[bias_squared[i] for i in degrees], label='Bias^2', marker='o')
plt.plot(degrees, [variance[i] for i in degrees], label='Variance', marker='o')
plt.plot(degrees, [irr_err for _ in degrees], label='Irreducible Error')#
plt.plot(degrees, [mse[i] for i in degrees], label='MSE', marker='o')
plt.xlabel('Polynomial Degree')
plt.ylabel('Error')
plt.title('Bias-Variance Tradeoff')
plt.legend()
plt.grid(True)
plt.show()
```



Bias: As the polynomial degree increases, the bias squared tends to decrease. A low-degree polynomial (underfitting) cannot capture the complexity of the true function, leading to high bias.

Variance: The variance increases with the degree of the polynomial because higher-degree polynomials are more flexible and tend to fit the noise in the data (overfitting).
Irreducible Error: This is constant across all degrees, representing the inherent noise in the data.

MSE (Mean Squared Error): The MSE initially decreases as we reduce bias by increasing the degree of the polynomial. However, as the degree becomes too high, the variance dominates, causing the MSE to increase again. The optimal degree minimizes the MSE.

Bias-Variance Tradeoff: Lower-degree polynomials have higher bias and lower variance, while higher-degree polynomials have lower bias but higher variance. There is a tradeoff between bias and variance. The optimal model lies somewhere between too simple (high bias, low variance) and too complex (low bias, high variance). In this case, it looks like around degree 5 may provide the best tradeoff since it's closest to the true function and minimizes MSE.

Problem 4

Part a

```
In [54]: import numpy as np
import pandas as pd
```

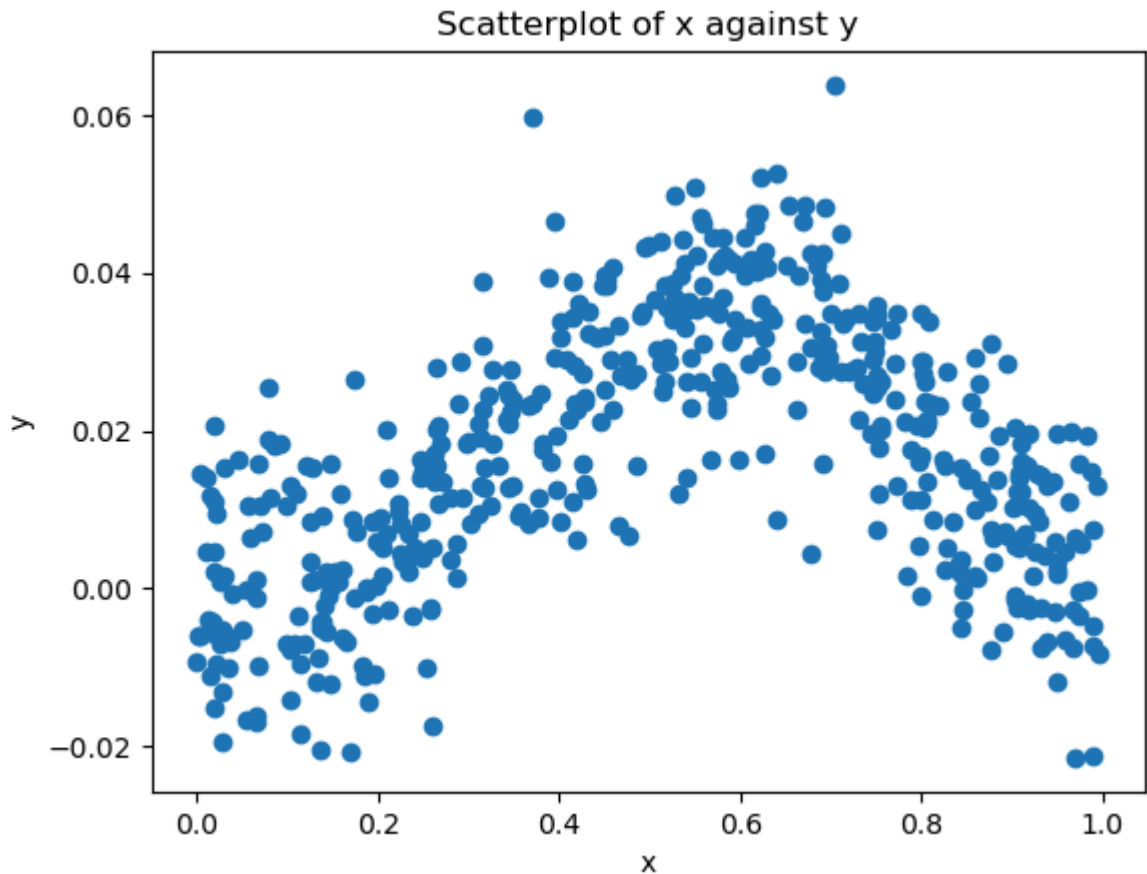
```
In [56]: def f(x):
return x ** 5 - 2 * x ** 4 + x ** 3
np.random.seed(1)
x = np.random.uniform(0, 1, size=500)
y = f(x) + np.random.normal(0, 0.01, size=500)
df = pd.DataFrame({'x': x, 'y': y})
df.head()
```

```
Out [56]:
```

	x	y
0	0.417022	0.023488
1	0.720324	0.027480
2	0.000114	-0.009339
3	0.302333	0.008121
4	0.146756	-0.011964

Part b

```
In [59]: import matplotlib.pyplot as plt
plt.scatter(x, y)
plt.title("Scatterplot of x against y")
plt.xlabel("x")
plt.ylabel("y")
plt.show()
```

The scatterplot has a parabolic pattern, which corresponds to the shape of the underlying function $f(x)$. The curve starts low at $x=0$, increases to a peak near $x=0.5$, and then declines again toward $x=1$. This is typical behavior for polynomials of degree 5

Part c

```
In [62]: from sklearn.model_selection import LeaveOneOut, cross_val_score
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error
```

```
In [69]: np.random.seed(123)
x = np.random.uniform(0, 1, size=500)
y = f(x) + np.random.normal(0, 0.01, size=500)
df = pd.DataFrame({'x': x, 'y': y})
#df.head()
errors1=[]
loo = LeaveOneOut()
degrees = np.arange(1, 8)
for degree in degrees:
    poly = PolynomialFeatures(degree)
    X_poly = poly.fit_transform(x.reshape(-1, 1))

    model = LinearRegression()

    neg_mse = cross_val_score(model, X_poly, y, cv=loo, scoring='neg_mse')
    mse = -np.mean(neg_mse) # Mean squared error
    errors1.append(mse)
# Print LOOCV errors for each model
```

```
for i, mse in enumerate(errors1):
    print(f"Degree {i+1} polynomial L00CV error: {mse}")
```

```
Degree 1 polynomial L00CV error: 0.00023872667496951678
Degree 2 polynomial L00CV error: 0.00012610526499073603
Degree 3 polynomial L00CV error: 0.00011087924643876155
Degree 4 polynomial L00CV error: 0.00010574321537933433
Degree 5 polynomial L00CV error: 0.00010460992336824871
Degree 6 polynomial L00CV error: 0.00010463444234900385
Degree 7 polynomial L00CV error: 0.0001050017444614648
```

Part d

```
In [83]: np.random.seed(12345)
x = np.random.uniform(0, 1, size=500)
y = f(x) + np.random.normal(0, 0.01, size=500)
df = pd.DataFrame({'x': x, 'y': y})
#df.head()
errors2=[]
loo = LeaveOneOut()
# Fit polynomial models from degree 1 to 7
degrees = np.arange(1, 8)
for degree in degrees:
    # Create polynomial features
    poly = PolynomialFeatures(degree)
    X_poly = poly.fit_transform(x.reshape(-1, 1))

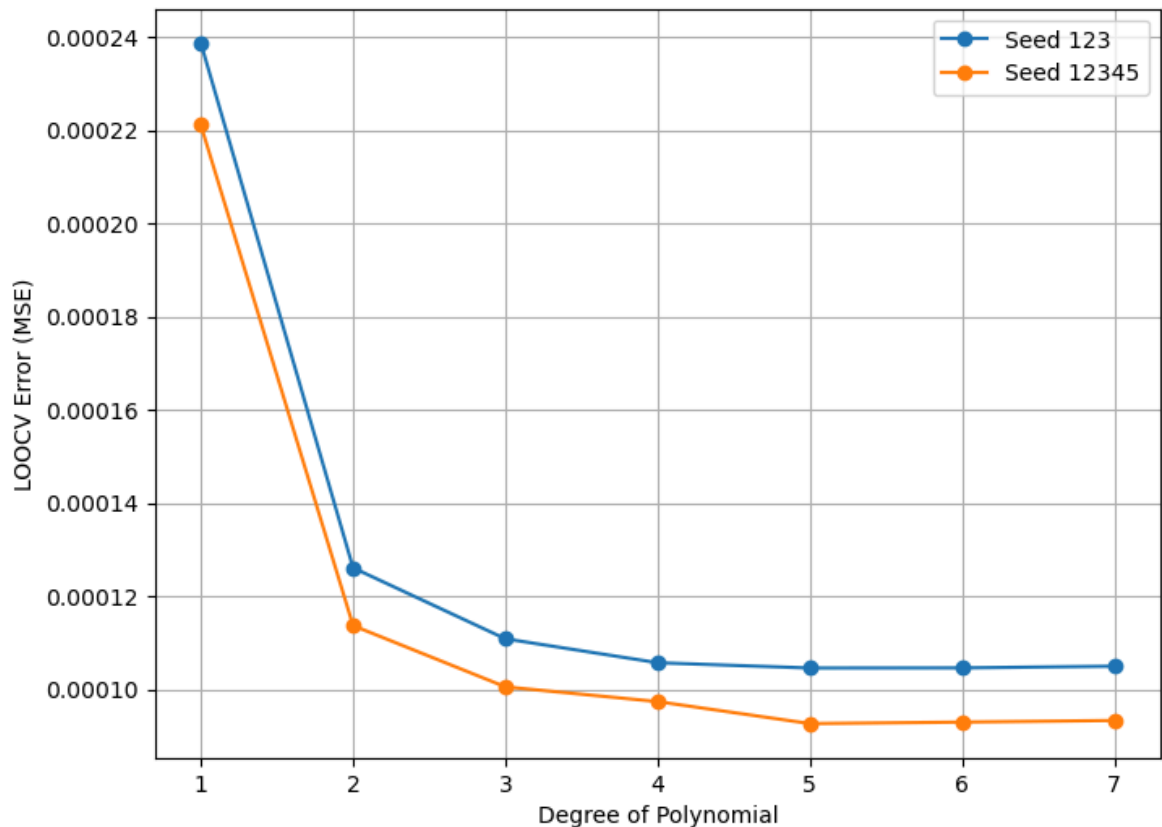
    # Fit the model using linear regression
    model = LinearRegression()

    # Perform L00CV
    neg_mse = cross_val_score(model, X_poly, y, cv=loo, scoring='neg_mean_squared_error')
    mse = -np.mean(neg_mse) # Mean squared error
    errors2.append(mse)

# Print L00CV errors for each model
for i, mse in enumerate(errors2):
    print(f"Degree {i+1} polynomial L00CV error: {mse}")
```

```
Degree 1 polynomial L00CV error: 0.00022114215496333624
Degree 2 polynomial L00CV error: 0.00011371176055646527
Degree 3 polynomial L00CV error: 0.00010057119012530982
Degree 4 polynomial L00CV error: 9.740695636902108e-05
Degree 5 polynomial L00CV error: 9.268909299573358e-05
Degree 6 polynomial L00CV error: 9.30073090859531e-05
Degree 7 polynomial L00CV error: 9.335757987940265e-05
```

```
In [85]: plt.figure(figsize=(8, 6))
plt.plot(degrees, errors1, marker='o', label='Seed 123')
plt.plot(degrees, errors2, marker='o', label='Seed 12345')
plt.xlabel('Degree of Polynomial')
plt.ylabel('L00CV Error (MSE)')
plt.legend()
plt.grid(True)
plt.show()
```



No, the results with seed 12345 differ from the results with seed 123 due to the randomness in generating the x values and the noise in y . Changing the seed affects the initial random generation of x and the random noise added to y . But the curve or the pattern of the graph remains somewhat the same. This is because the cross-validation itself doesn't involve randomness as LeaveOneOut (LOOCV) uses all data points except one for each validation step. However, the difference arises from the different datasets generated due to different seeds.

Part e

```
In [88]: min_error1 = np.argmin(errors1)
          print(f"Polynomial degree with the smallest error: {min_error1 + 1}")
          min_error2 = np.argmin(errors2)
          print(f"Polynomial degree with the smallest error: {min_error2 + 1}")
```

```
Polynomial degree with the smallest error: 5
Polynomial degree with the smallest error: 5
```

Yes, this is what I expected because lower-degree Polynomials may underfit the data because the true relationship between x and y appears to be nonlinear and somewhat complex. Higher-degree Polynomials may overfit the data, capturing the noise in addition to the true pattern. 5-degree polynomial gives a right balance between these two by giving the smallest LOOCV.

Part f

```
In [97]: import statsmodels.api as sm
          from sklearn.preprocessing import PolynomialFeatures
```

```
degree = 5
poly = PolynomialFeatures(degree)
X_poly = poly.fit_transform(x.reshape(-1, 1))
X_poly = sm.add_constant(X_poly)
# Fit the model using Ordinary Least Squares (OLS)
model = sm.OLS(y, X_poly)
results = model.fit()
print(results.summary())
```

OLS Regression Results

```

=====
=====
Dep. Variable:          y      R-squared:
0.615
Model:                  OLS    Adj. R-squared:
0.611
Method:                 Least Squares    F-statistic:          1
57.7
Date:                  Fri, 27 Sep 2024    Prob (F-statistic):      6.80e
-100
Time:                  20:51:29    Log-Likelihood:          16
18.0
No. Observations:      500    AIC:                      -3
224.
Df Residuals:          494    BIC:                      -3
199.
Df Model:               5
Covariance Type:       nonrobust
=====
=====

```

	coef	std err	t	P> t	[0.025	0.
975]						

const	-0.0053	0.002	-2.130	0.034	-0.010	-
0.000						
x1	0.1436	0.051	2.813	0.005	0.043	
0.244						
x2	-0.8814	0.321	-2.749	0.006	-1.511	-
0.252						
x3	3.1448	0.819	3.838	0.000	1.535	
4.754						
x4	-4.2798	0.909	-4.708	0.000	-6.066	-
2.494						
x5	1.8827	0.364	5.172	0.000	1.167	
2.598						

```

=====
=====
Omnibus:                1.498    Durbin-Watson:
2.076
Prob(Omnibus):          0.473    Jarque-Bera (JB):
1.536
Skew:                   0.131    Prob(JB):
0.464
Kurtosis:               2.932    Cond. No.                3.91
e+03
=====
=====

```

Notes:

[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

[2] The condition number is large, 3.91e+03. This might indicate that there are strong multicollinearity or other numerical problems.

A low p-value (typically less than 0.05) suggests that the coefficient is statistically significant, meaning there's strong evidence that the

corresponding term contributes meaningfully to explaining the variation in y. In this case the x_3, x_4, x_5 polynomial term are very significant while the constant, x_1 and x_2 terms are significant too.

In []: