

24-787: Machine Learning and Artificial Intelligence for Engineers

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Homework 2

Due: Feb 3 2024

Concept Questions:

Problem 1

- a) The design matrix X will have the size of 11 by 3.
The parameter vector w will have the size of 3 by 1.
The product of $X'X$ will have the size of 3 by 3.
- b) The design matrix X will have the size of 1000 by 3.
The parameter vector w will have the size of 3 by 1.
The product of $X'X$ will have the size of 3 by 3.
- c) Statement 2 “The model complexity is determined by the number of model parameters” is true.

Problem 2

3rd order polynomial will perfectly interpolate these points.

Problem 3

Formulation 2 ($x_{new} = x_{old} + \eta \cdot \frac{\partial obj}{\partial x}$) will lead me to the top of the mountain.

Problem 4

Switch to stochastic gradient descent and reduce the learning rate will help resolve the oscillation issue.

Problem 5

The formulation is equivalent to an LLS with L2 regularization.

Problem 1 (30 points)

Problem Description

In this problem you will implement polynomial linear least squares regression on two datasets, with and without regularization. Additionally, you will use gradient descent to optimize for the model parameters.

Fill out the notebook as instructed, making the requested plots and printing necessary values.

You are welcome to use any of the code provided in the lecture activities.

Summary of deliverables:

Results:

- Print fitted model parameters \mathbf{w} for the 4 models requested without regularization
- Print fitted model parameters \mathbf{w} for the 2 models requested *with* L_2 regularization
- Print fitted model parameters \mathbf{w} for the one model solved via gradient descent

Plots:

- 2 plots of each dataset along with the ground truth function
- 4 plots of the fitted function along with the respective data and ground truth function for LLS without regularization
- 2 plots of the fitted function along with the respective data and ground truth function for LLS with L_2 regularization
- 1 plot of the fitted function along with the respective data and ground truth function for LLS with L_2 regularization solved via gradient descent

Discussion:

- Discussion of challenges fitting complex models to small datasets
- Discussion of difference between the L_2 regularized model versus the standard model
- Discussion of whether gradient descent could get stuck in a local minimum
- Discussion of gradient descent results versus closed form results

Imports and Utility Functions:

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

def gt_function():
    xt = np.linspace(0,1,101)
    yt = np.sin(2 * np.pi * xt)
    return xt, yt
```

```
def plot_data(x,y,xt,yt,title = None):
    # Provide title as a string e.g. 'string'
    plt.plot(x,y,'bo',label = 'Data')
    plt.plot(xt,yt,'g-', label = 'Ground Truth')
    plt.xlabel('x')
    plt.ylabel('y')
    plt.grid()
    plt.legend()
    if title:
        plt.title(title)
    plt.show()

def plot_model(x,y,xt,yt,xr,yr,title = None):
    # Provide title as a string e.g. 'string'
    plt.plot(x,y,'bo',label = 'Data')
    plt.plot(xt,yt,'g-', label = 'Ground Truth')
    plt.plot(xr,yr,'r-', label = 'Fitted Function')
    plt.xlabel('x')
    plt.ylabel('y')
    plt.grid()
    plt.legend()
    if title:
        plt.title(title)
    plt.show()
```

Load and visualize the data

The data is contained in `d10.npy` and `d100.npy` and can be loaded with `np.load()`.

Store the data as:

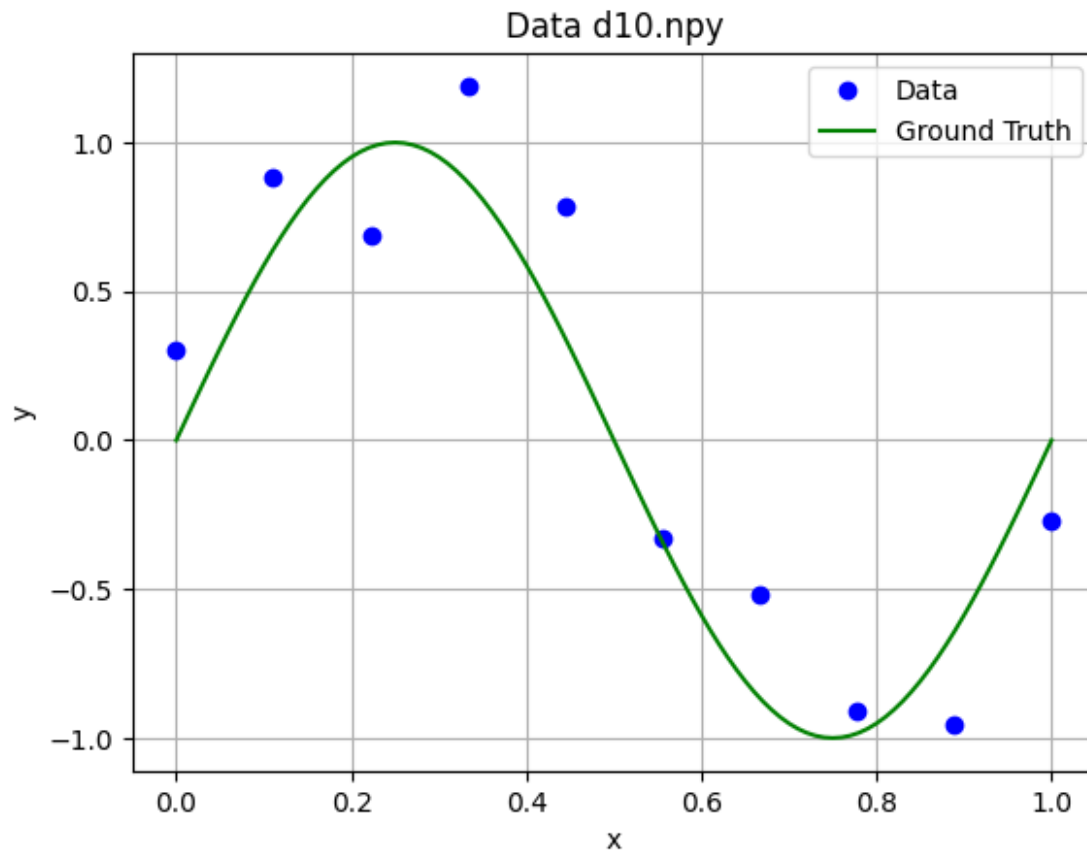
- `x10` and `x100` (the first column of the data)
- `y10` and `y100` (the second column of the data)

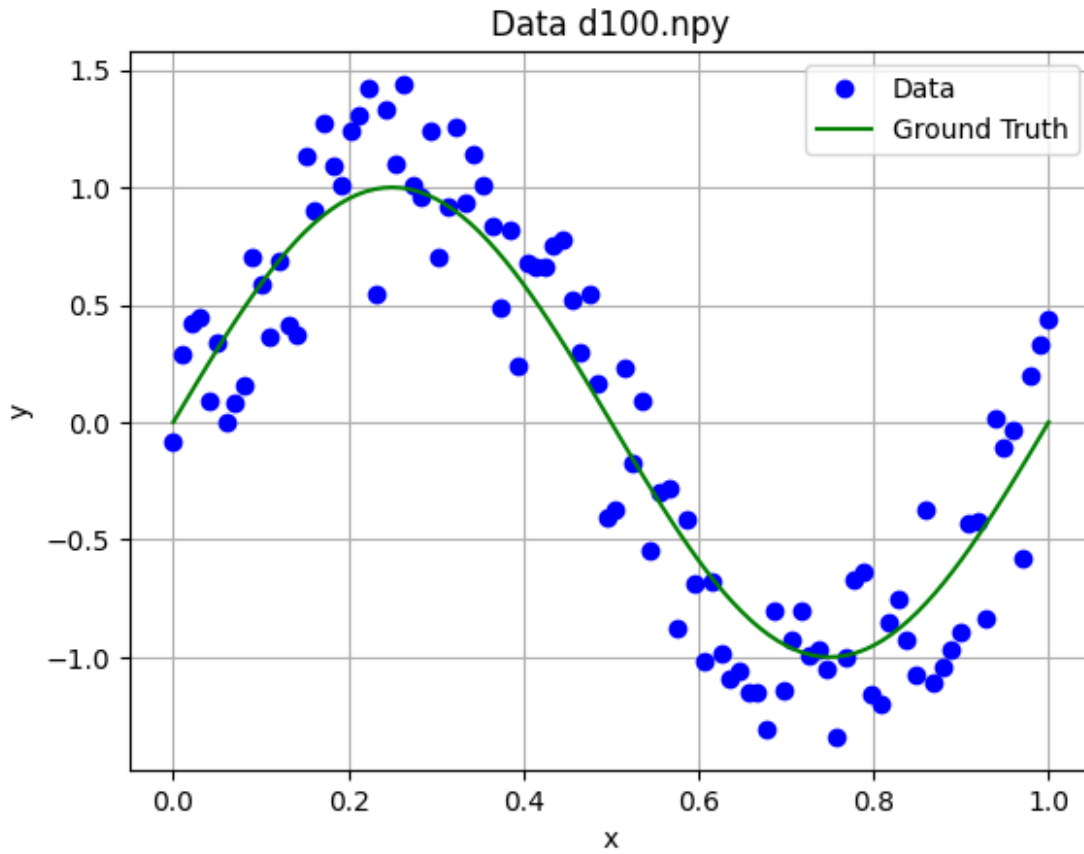
Generate the ground truth function $f(x) = \sin(2\pi x)$ using `xt, yt = gt_function()`.

Then visualize the each dataset with `plotxy(x,y,xt,yt,title)` with an appropriate title. You should generate two plots.

```
# YOUR CODE GOES HERE
# load the data
data_d10 = np.load('d10.npy')
data_d100 = np.load('d100.npy')
# store the loaded data into x and y
x10 = data_d10[:,0] # first column
y10 = data_d10[:,1] # second column
x100 = data_d100[:,0] # first column
y100 = data_d100[:,1] # second column
# ground truth fucntion
```

```
xt, yt = gt_function()  
# plot the data  
plot_data(x10,y10,xt,yt, 'Data d10.npy')  
plot_data(x100,y100,xt,yt, 'Data d100.npy')
```





Implement polynomial linear regression

Now you will implement polynomial linear least squares regression without regularization using the closed form solution from lecture to compute the model parameters. You will consider the following 4 cases:

1. Data: data10.txt, Model: 2nd order polynomial (highest power of x in your regression model = 2)
2. Data: data100.txt, Model: 2nd order polynomial (highest power of x in your regression model = 2)
3. Data: data10.txt, Model: 9th order polynomial (highest power of x in your regression model = 9)
4. Data: data100.txt, Model: 9th order polynomial (highest power of x in your regression model = 9)

For each model:

- Print the learned model parameters `w`
- Use the model parameters `w` to predict `yr` values over a range of `x` values given by `xr = np.linspace(0, 1, 101)`

- Plot the data, ground truth function, and regressed model using `plot_model(x,y,xt,yt,xr,yr,title)` with an appropriate title.

```
# YOUR CODE GOES HERE
# linear regression
def ploy_linear_regression(x,y,deg):
    X = np.vander(x, deg+1)
    w = np.linalg.inv(X.T @ X) @ X.T @ y.reshape(-1,1)

    # print model parameters (w)
    print('Model parameters [w]: \n', w)

    # plot the fitted function
    xr = np.linspace(0,1,101)
    XR = np.vander(xr, deg+1)
    yr = XR @ w
    plot_model(x,y,xt,yt,xr,yr, f'Fitted Function for data {data},
{deg}nd order polynomial')

    return w

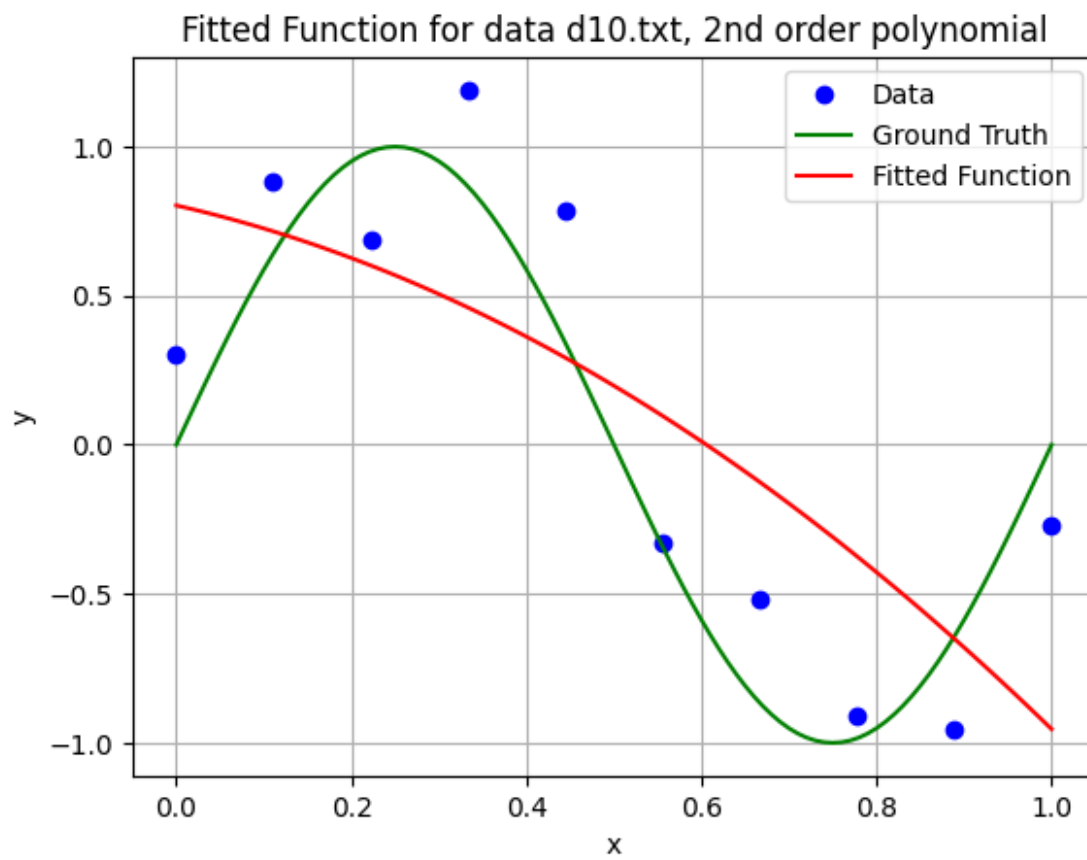
# [case 1] data10.txt, model: 2nd order polynomial
data = 'd10.txt'
deg = 2
w = ploy_linear_regression(x10,y10,deg)

# [case 2] data100.txt, model: 2th order polynomial
data = 'd100.txt'
deg = 2
w = ploy_linear_regression(x100,y100,deg)

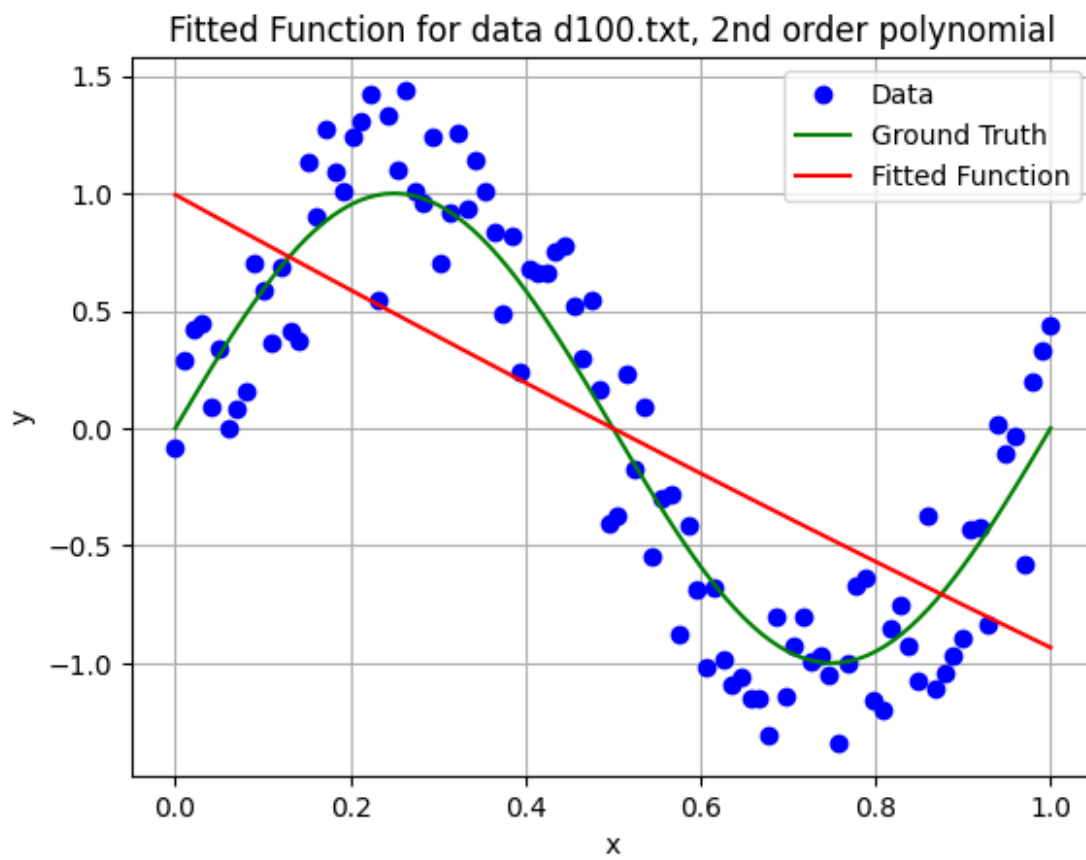
# [case 3] data10.txt, model: 9nd order polynomial
data = 'd10.txt'
deg = 9
w = ploy_linear_regression(x10,y10,deg)

# [case 4] data100.txt, model: 9th order polynomial
data = 'd100.txt'
deg = 9
w = ploy_linear_regression(x100,y100,deg)

Model parameters [w]:
[[-1.09384447]
 [-0.66283292]
 [ 0.80276877]]
```

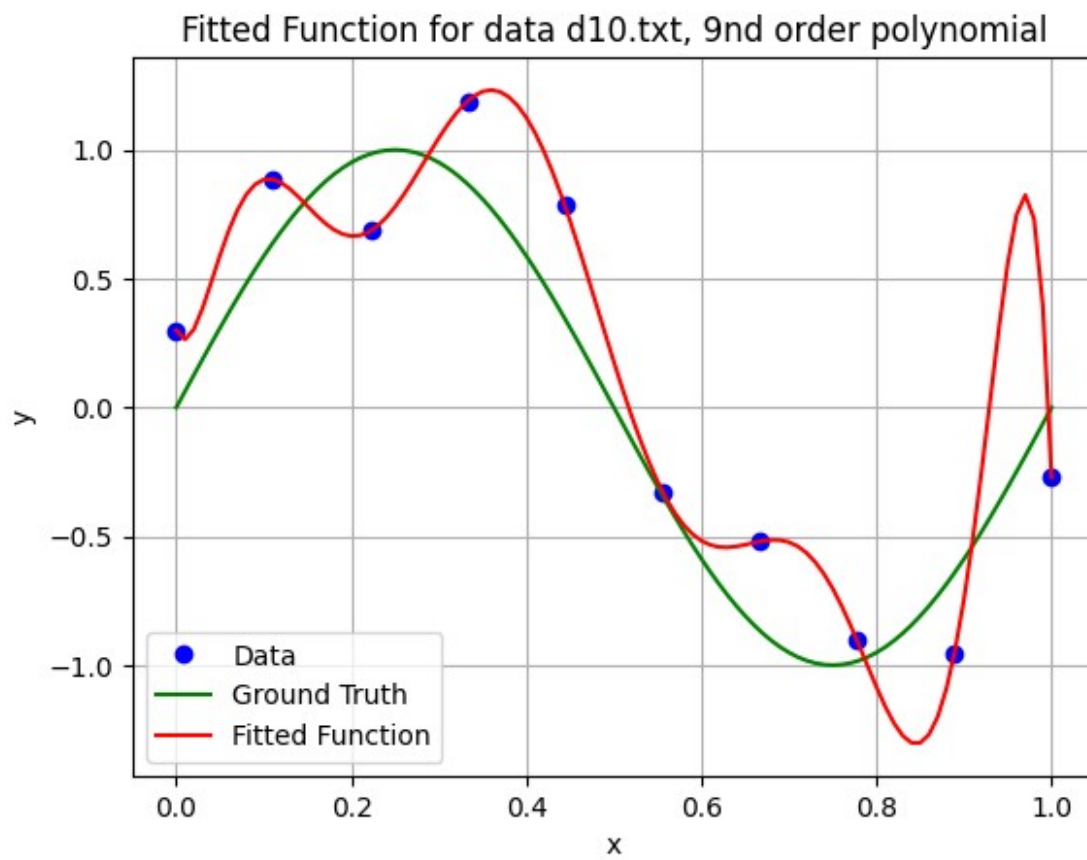


```
Model parameters [w]:  
[[ 0.12128272]  
 [-2.04993418]  
 [ 0.99435046]]
```

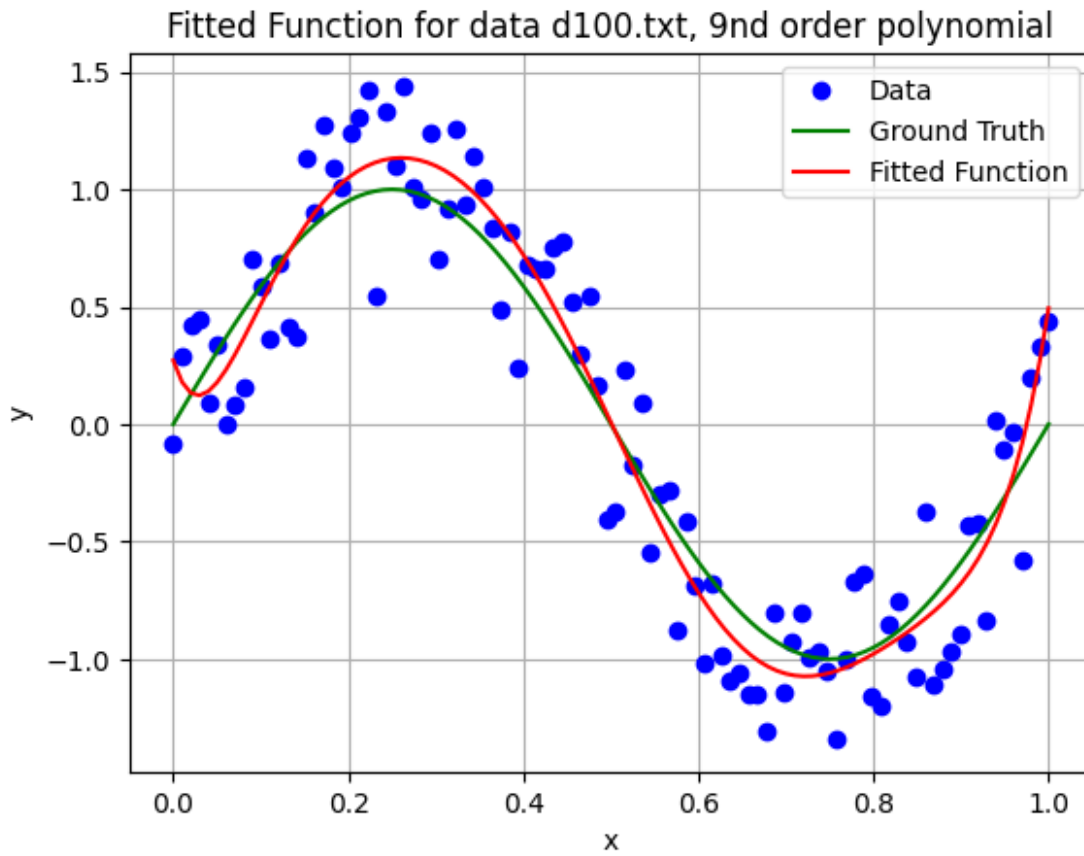


Model parameters [w]:

```
[[-3.92430472e+04]  
[ 1.67896289e+05]  
[-2.96801430e+05]  
[ 2.79608057e+05]  
[-1.50834125e+05]  
[ 4.64985814e+04]  
[-7.69080481e+03]  
[ 5.74539370e+02]  
[-8.63097293e+00]  
[ 3.00002255e-01]]
```

```
Model parameters [w]:  
[[-2.21754283e+03]  
[ 1.15791219e+04]  
[-2.48684201e+04]  
[ 2.86926291e+04]  
[-1.95212853e+04]  
[ 8.13280715e+03]  
[-2.07018765e+03]  
[ 2.84952056e+02]  
[-1.18519096e+01]  
[ 2.71581706e-01]]
```



Discussion:

When the sample size (number of data points) is small, what issues or tendencies do you see with complex models?

Your answer goes here

When the sample size is small, we can observe overfitting with complex models. Furthermore, the model is more sensitive to the given training data and tends to have higher variance in its predictions.

Implement polynomial linear regression with L_2 regularization

You will repeat the previous section, but this time using L_2 regularization. Your regularization term should be $\lambda w' I_m w$, where $\lambda = e^{-10}$, and I_m is the modified identity matrix that masks out the bias term from regularization.

You will consider only two cases:

1. Data: data10.txt, Model: 9th order polynomial (highest power of x in your regression model = 9)
2. Data: data100.txt, Model: 9th order polynomial (highest power of x in your regression model = 9)

For each model:

- Print the learned model parameters `w`
- Use the model parameters `w` to predict `yr` values over a range of x values given by `xr = np.linspace(0,1,101)`
- Plot the data, ground truth function, and regressed model using `plot_model(x,y,xt,yt,xr,yr,title)` with an appropriate title.

```
# YOUR CODE GOES HERE
# linear regression with L2 regularization
def ploy_linear_regression_L2(x,y,deg, L= np.exp(-10)):
    I_m = np.eye(deg+1)
    I_m[-1,-1] = 0
    X = np.vander(x, deg+1)
    regularized_w = np.linalg.inv(X.T @ X + L*I_m) @ X.T @ y.reshape(-1,1)

    # print model parameters (w)
    print('Model parameters [w]: \n', regularized_w)

    # plot the fitted function
    xr = np.linspace(0,1,101)
    XR = np.vander(xr, deg+1)
    yr = XR @ regularized_w
    plot_model(x,y,xt,yt,xr,yr, f'Fitted Function for data {data},
{deg}nd order polynomial with L2 regularization')

    return regularized_w

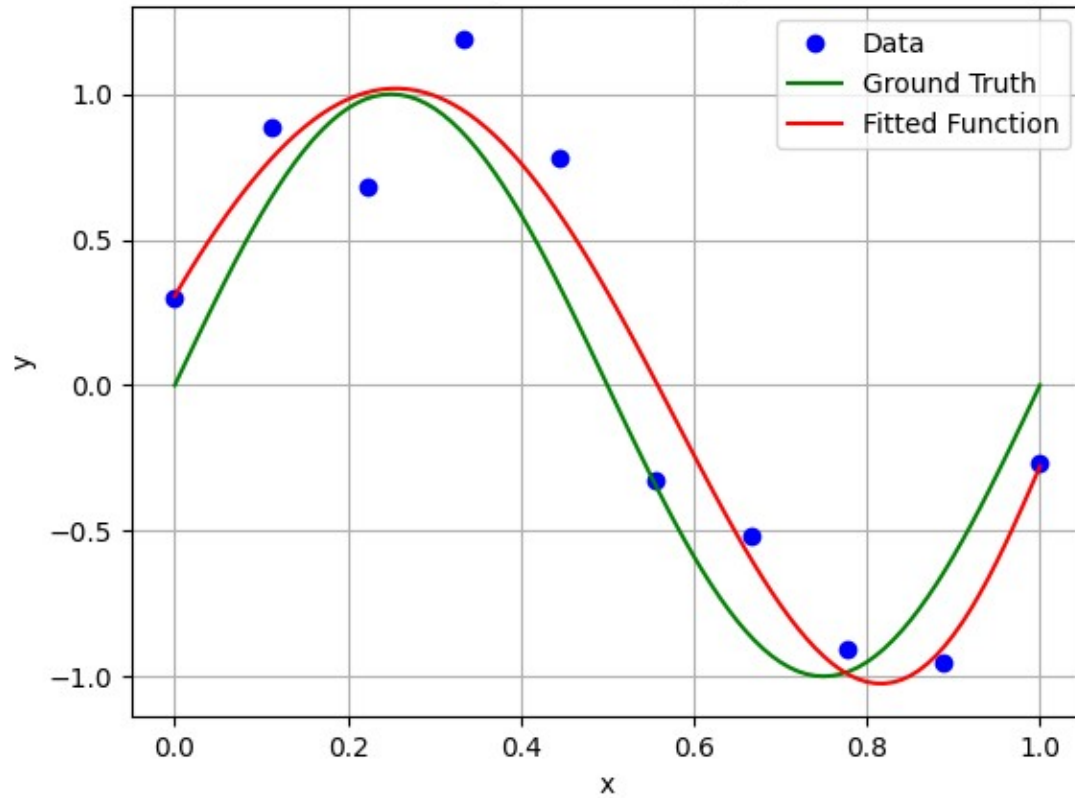
# [case 1] data10.txt, model: 9nd order polynomial
data = 'd10.txt'
deg = 9
w = ploy_linear_regression_L2(x10,y10,deg)

# [case 2] data100.txt, model: 9th order polynomial
data = 'd100.txt'
deg = 9
w = ploy_linear_regression_L2(x100,y100,deg)

Model parameters [w]:
[[-3.5338486 ]
 [-1.84896842]
 [ 2.29997278]
 [ 6.47141056]
 [ 6.80582425]]
```

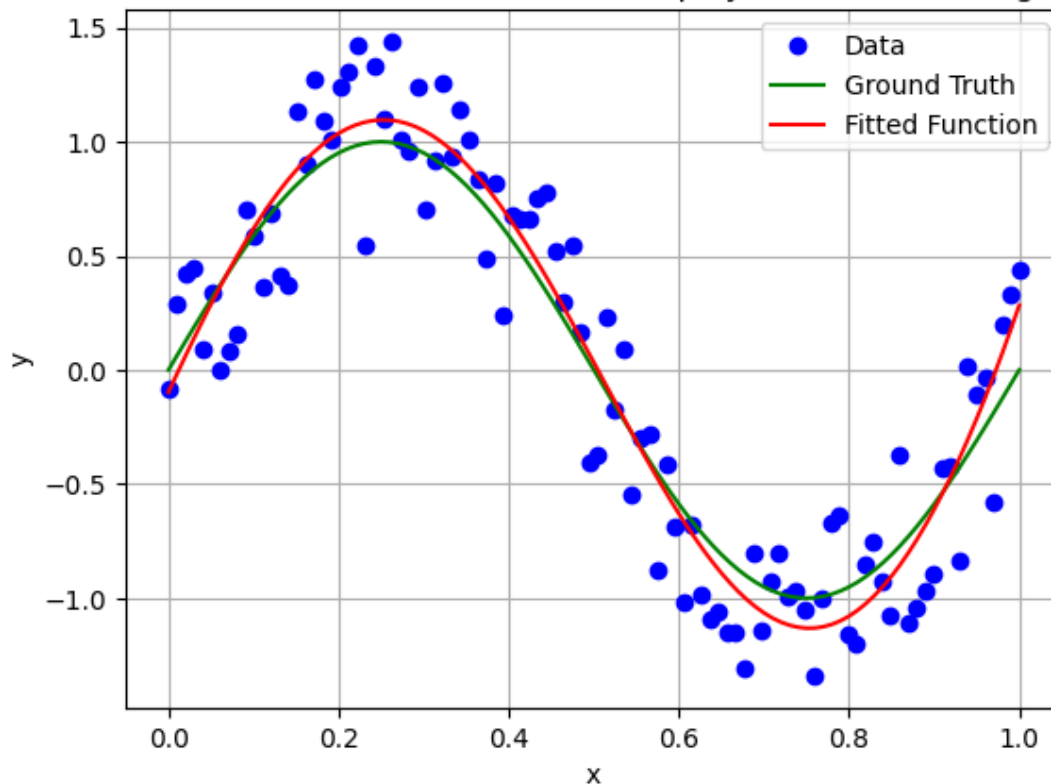
```
[ 0.25321228]
[-9.30526316]
[-6.83132438]
[ 5.10343135]
[ 0.30633599]]
```

Fitted Function for data d10.txt, 9nd order polynomial with L2 regularization



```
Model parameters [w]:
[[ 17.53893754]
 [-22.00647043]
 [-21.06911985]
 [ 7.0398566 ]
 [ 33.8281617 ]
 [ 20.79696185]
 [-38.38285113]
 [-5.43884905]
 [ 8.07411308]
 [-0.0974112 ]]
```

Fitted Function for data d100.txt, 9nd order polynomial with L2 regularization



Discussion:

What differences between the regularized and standard 9th order models fit to d10 do you notice? How does regularization affect the fitted function?

Your answer goes here

The regularized 9th-order model eliminated the overfitting issue faced in the standard 9th-order models. The overall prediction in regularized models is more precise with the ground truth. Regularization will minimize the loss function and prevent models from overfitting/underfitting.

LLS with L_2 regularization and gradient descent

For complex models, the size of $X'X$ can be large, making matrix inversion computationally demanding. Instead, one can use gradient descent to compute w . In our notes, we derived the gradient descent approach both for unregularized as well as L_2 regularized linear regression. The formula for the gradient descent approach with L_2 regularization is:

$$\frac{\partial \text{obj}}{\partial w} = X'Xw - X'y + \lambda \mathbb{I}_m w$$

$$w^{\text{new}} \leftarrow w^{\text{cur}} - \alpha \frac{\partial \text{obj}}{\partial w}$$

In this problem, could gradient descent get stuck in a local minimum? Explain why / why not?

Your answer goes here

In this problem, the gradient descent will not get stuck in a local minimum. The objective function (quadratic) in the given problem is convex, which has no local minimize or saddle points.

You will consider just a single case in the following question:

1. Data: data10.txt, Model: 9th order polynomial.

Starting with a weight vector of zeros as the initial guess, and $\lambda = e^{-10}$, $\alpha = 0.075$, apply 50000 iterations of gradient descent to find the optimal model parameters. In practice, when you train your own models you will have to determine these parameters yourself!

For the trained model:

- Print the learned model parameters `w`
- Use the model parameters `w` to predict `yr` values over a range of `x` values given by `xr = np.linspace(0,1,101)`
- Plot the data, ground truth function, and regressed model using `plot_model(x,y,xt,yt,xr,yr,title)` with an appropriate title.

```
# YOUR CODE GOES HERE
# linear regression with L2 regularization and gradient descent
def ploy_linear_regression_L2_GD(x,y,deg, L= np.exp(-10), a = 0.075,
iterations = 50000):
    I_m = np.eye(deg+1)
    I_m[-1,-1] = 0
    X = np.vander(x, deg+1)
    w = np.zeros((deg+1,1))
    for i in range(iterations):
        grad = X.T @ (X @ w - y.reshape(-1,1)) + L * I_m @ w
        w = w - a * grad

    # plot the fitted function
    xr = np.linspace(0,1,101)
    XR = np.vander(xr, deg+1)
    yr = XR @ w

    # print model parameters (w)
    print('Model parameters [w]: \n', w)

    # print model GD
    # print('Model gradianet: \n', grad)

    # print the predicted yr values
    # print('Predicted yr values: \n', yr)

    plot_model(x,y,xt,yt,xr,yr, f'Fitted Function for data {data},
{deg}nd order polynomial with L2 regularization and gradient descent')
```

```

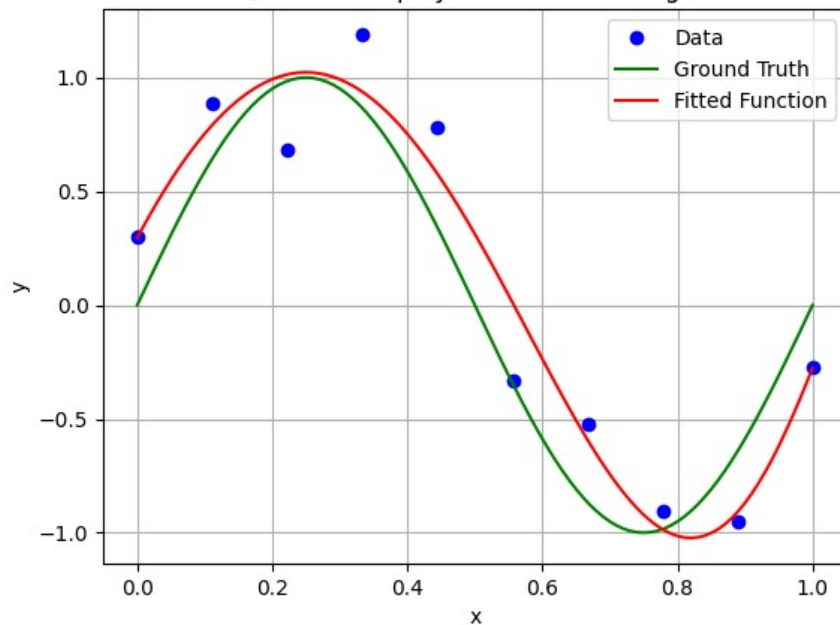
return w

# [case] data10.txt, model: 9nd order polynomial
data = 'd10.txt'
deg = 9
w = ploy_linear_regression_L2_GD(x10,y10,deg)

Model parameters [w]:
[[-3.85457875]
 [-0.40351789]
 [ 2.81217121]
 [ 4.9128699 ]
 [ 4.63900381]
 [ 0.854452 ]
 [-5.76006075]
 [-9.34031661]
 [ 5.56763369]
 [ 0.29561747]]

```

Fitted Function for data d10.txt, 9nd order polynomial with L2 regularization and gradient descent



Discussion:

Visually compare the result you just obtained to the same 9th order polynomial model with L_2 regularization where you solved for w directly in the previous section. They should be very similar. Comment on whether gradient descent has converged.

Your answer goes here

From the model results, the gradient descent has converged. The gradient value has reached near 0, which further proves the previous statement.

m2-hw2

February 4, 2024

1 Problem 2 (30 points)

1.1 Problem Description

In this problem you will use linear least squares to fit a linear function to a 3D temperature field, with x,y,z locations and an associated temperature T .

Fill out the notebook as instructed, making the requested plots and printing necessary values.

You are welcome to use any of the code provided in the lecture activities.

Summary of deliverables: Results: - Predicted temperature $T(5,5,5)$ using a hand-coded LLS squares model with a linear function - Direction of travel from $(5,5,5)$ to experience the greatest decrease in temperature

Discussion: - Reasoning for how we can use our fitted function to determine the direction of greatest decrease in temperature

Imports and Utility Functions:

```
[12]: import numpy as np
```

1.2 Load the data

The data is contained in `tempfield.npy` and can be loaded with `np.load(tempfield.npy)`. The first three columns correspond to the x , y , and z locations of the data points, and the 4th column corresponds to the temperature T at the respective point. Store the data as you see fit.

```
[13]: # YOUR CODE GOES HERE
tempfield_data = np.load("tempfield.npy")
x = np.array(tempfield_data[:,0])
y = np.array(tempfield_data[:,1])
z = np.array(tempfield_data[:,2])
T = np.array(tempfield_data[:,3])
```

1.3 LLS Regression in 3D

Now fit a linear function to the data using the closed form of LLS regression. Use your fitted function to report the predicted temperature at $x = 5$, $y = 5$, $z = 5$. You are free to add regularization to your model, but this is not required and will not be graded.


```
[14]: # YOUR CODE GOES HERE
X = np.c_[x, y, z, np.ones(len(x))]
w = np.linalg.inv(X.T @ X) @ X.T @ T.reshape(-1, 1)
# Given x, y, z coordinates, predict the temperature at that point
x_pred, y_pred, z_pred = 5, 5, 5

# temperature prediction logic
T_pred = np.array([x_pred, y_pred, z_pred, 1]) @ w
print(f'The predicted temperature at ({x_pred}, {y_pred}, {z_pred}) is:␣
↪{T_pred[0]}')

# direction of travel logic
direction = -1*w[0:3].flatten()
direction/np.linalg.norm(direction)
print(f'The direction of travel to experience the greatest decrease in␣
↪temperature is: {direction}')
```

The predicted temperature at (5, 5, 5) is: 21.389073383508922

The direction of travel to experience the greatest decrease in temperature is: [0.13421269 -0.11741862 -0.72677374]

1.4 Gradient Intuition

Using the function you fit in the previous part, in which direction should one move from the point $p = (5, 5, 5)$ to experience the largest decrease in temperature in the immediate neighborhood of the point? Report the specific direction, along with your reasoning.

1.4.1 Your answer goes here

The negative of the gradient moves you in the direction of the maximum decreasing rate of a function. One should move in the direction of [0.13421269 -0.11741862 -0.72677374] from the point $p = (5, 5, 5)$ to experience the largest decrease in temperature.

m2-l1-p1

February 3, 2024

1 M2-L1 Problem 1 (5 points)

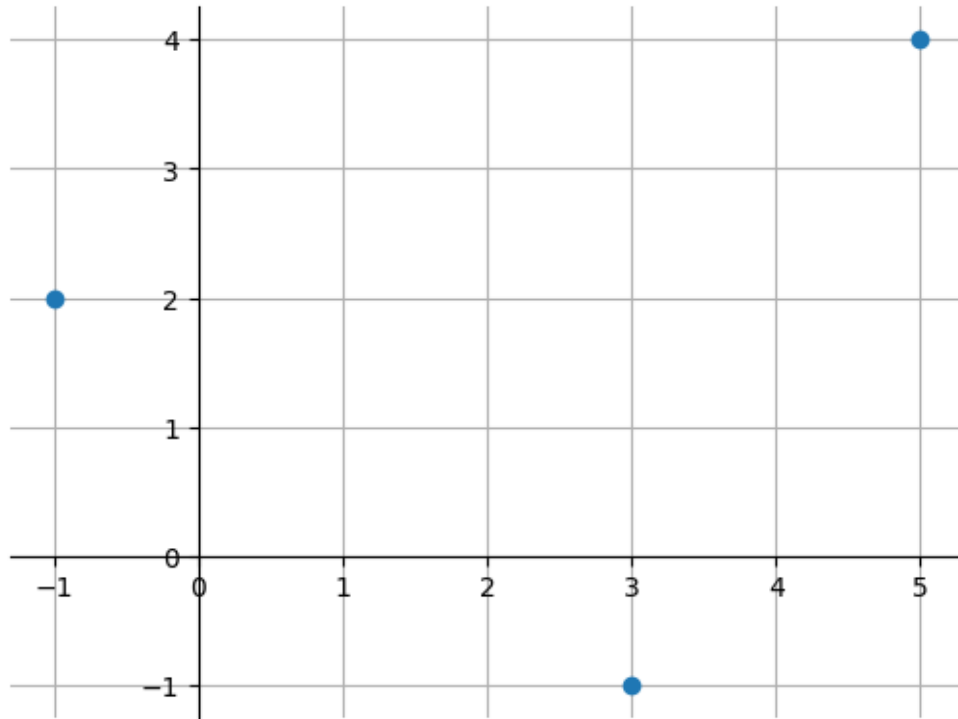
In this question you will perform linear least squares regression on a very small dataset of 3 points. First, load and plot the data by running the following cell.

The variables provided are: - x: 3x1 input data - y: 3x1 output data

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

x = np.array([[-1, 3, 5]]).T
y = np.array([[2, -1, 4]]).T

fig, ax = plt.subplots()
plt.plot(x, y, 'o')
ax.spines['left'].set_position(('data', 0))
ax.spines['bottom'].set_position(('data', 0))
sns.despine()
plt.grid()
plt.show()
```



1.1 Construct a design matrix

For 1-D linear regression, the design matrix must contain not only a column of input x -values, but also a ‘bias column’ – a column of ones (to allow the regression line to have an intercept).

The next step is to construct the design matrix X by concatenating a column of ones to the given input x . This has been done for you below:

```
[14]: bias = np.ones_like(x)

X = np.concatenate([x,bias],1)

print("Design Matrix:\n",X)
```

Design Matrix:

```
[[ -1  1]
 [  3  1]
 [  5  1]]
```

1.2 Solving for regression coefficients

Now that we have the design matrix X and the output y , we can solve for the coefficients w such that $Xw \approx y$ using:

$$w = (X'X)^{-1}X'y$$

Note that you can use the following in Python: - `@` for matrix multiplication - `np.linalg.inv(A)` for inversion of matrix `A` - `A.T` for transpose of a matrix `A` - `b.reshape(-1,1)` to treat 1D array `b` as a column (you will need to do this for `y`)

Your line's slope should be ≈ 0.18 and your y-intercept should be ≈ 1.25 .

```
[15]: # YOUR CODE GOES HERE
      # Get coefficients w
      w = np.linalg.inv(X.T @ X) @ X.T @ y.reshape(-1,1)
      print("Linear Coefficients:\n", w)
```

```
Linear Coefficients:
[[0.17857143]
 [1.25      ]]
```

1.3 Making predictions

Now that we have the coefficients, we can make predictions on new data with the model.

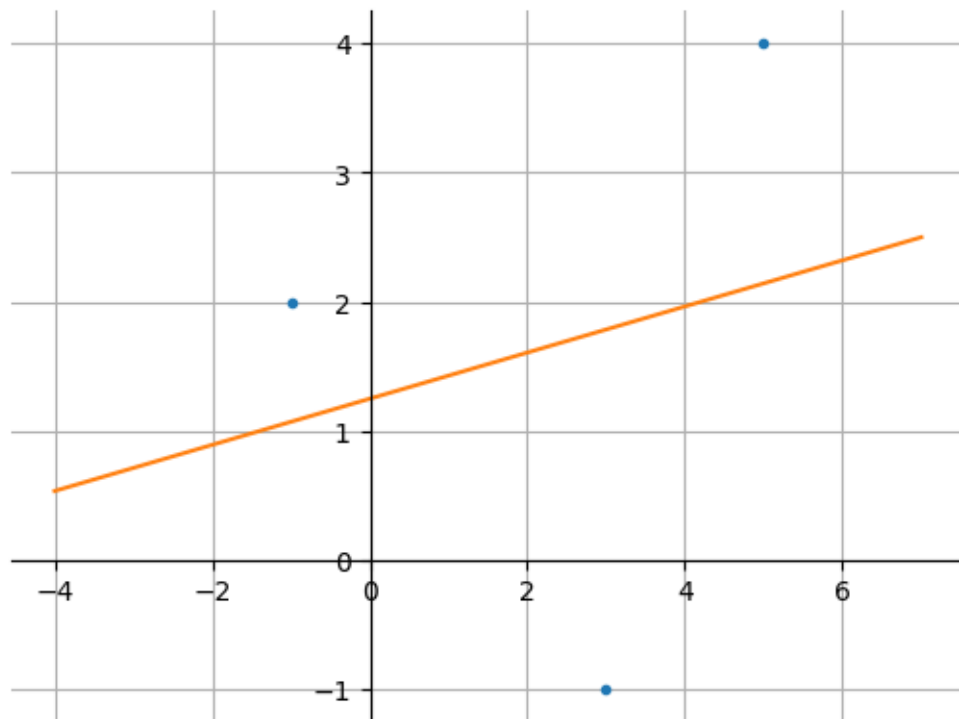
Do the following steps: - [Given] Sample 40 points on the interval $[-3,7]$, such as by using `np.linspace()` (Append `.reshape(-1,1)` to convert to a column) - [Given] Create a design matrix by adding a column of ones as done previously - Make a prediction by multiplying your new design matrix by `w`. You can do matrix multiplication with the `@` symbol

- [Given] Add a line to the plot showing these predictions

```
[16]: n = 40
      x_test = np.linspace(-4,7,n).reshape(-1,1)
      bias_test = np.ones_like(x_test)
      X_test = np.concatenate([x_test, bias_test], 1)

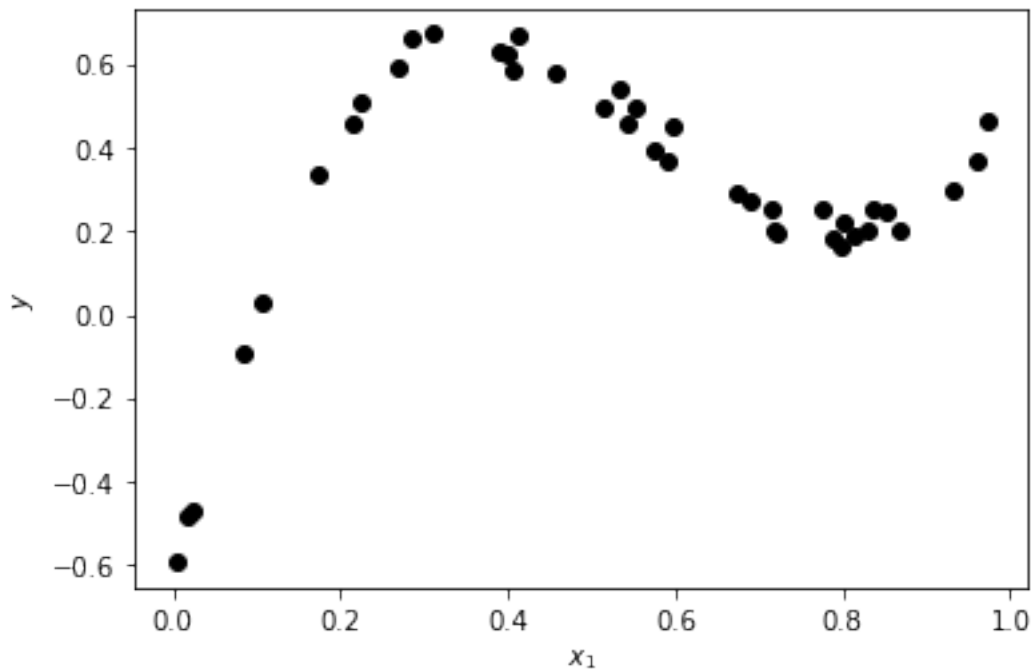
      # YOUR CODE GOES HERE
      # Predict y_test
      y_test = X_test @ w

      fig, ax = plt.subplots()
      plt.plot(x, y, '.')
      plt.plot(x_test, y_test)
      ax.spines['left'].set_position(('data', 0))
      ax.spines['bottom'].set_position(('data', 0))
      sns.despine()
      plt.grid()
      plt.show()
```



M2-L1 Problem 2 (5 points)

Consider the following data:



We will perform these steps:

1. Load the data
2. Generate a design matrix
3. Solve for the regression coefficients
4. Create and plot a curve using these coefficients

First, we demonstrate the above for a linear (1st order) model. First, run each cell in the demo and follow along with each step. Your job is then to make 2nd and 3rd order models for the same data using similar techniques.

Demonstration: Linear fit

First, we load the data in to x and y :

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

x = np.array([0.2855, 0.0033, 0.8307, 0.9606, 0.8153, 0.5539, 0.5152,
0.7761,
0.5763, 0.2697, 0.6744, 0.7998, 0.1052, 0.8674, 0.598 , 0.3985,
0.0171, 0.1732, 0.7976, 0.4137, 0.7161, 0.7225, 0.3892, 0.0834,
```

```

0.9733, 0.3097, 0.8509, 0.0226, 0.6901, 0.2235, 0.5914, 0.5436,
0.7189, 0.4558, 0.8366, 0.534 , 0.214 , 0.9314, 0.4065,
0.788 ])

y = np.array([ 0.6603, -0.5925, 0.2045, 0.3698, 0.191 , 0.496 ,
0.4986,
0.2516, 0.3905, 0.5932, 0.2924, 0.219 , 0.0287, 0.2024,
0.4489, 0.6237, -0.4857, 0.3384, 0.162 , 0.6694, 0.2539,
0.1936, 0.6322, -0.0953, 0.4632, 0.6721, 0.2464, -0.4672,
0.2746, 0.5087, 0.3691, 0.4559, 0.2021, 0.5797, 0.2531,
0.5417, 0.4577, 0.2952, 0.5856, 0.1818])

```

Now we generate a linear design matrix for the data:

```

# Function to get a linear design matrix for 1D data
def get_linear_design_matrix(x):
    x = x.reshape(-1, 1)          # Turn x into a column array
    columns = [x, np.ones_like(x)] # Linear design matrix has a
    column of x and a column of ones
    X = np.concatenate(columns, axis=1) # Combine each column
    horizontally to make a matrix
    return X

X = get_linear_design_matrix(x)
print("First four rows of X:")
print(X[:4,:])

First four rows of X:
[[0.2855 1.    ]
 [0.0033 1.    ]
 [0.8307 1.    ]
 [0.9606 1.    ]]

```

Now that we have the design matrix X and the output y , we can solve for the coefficients w such that $Xw \approx y$ using:

$$w = (X'X)^{-1}X'y$$

Note the use of the following in Python:

- `@` for matrix multiplication
- `np.linalg.inv(A)` for inversion of matrix `A`
- `A.T` for transpose of a matrix `A`
- `b.reshape(-1,1)` to treat 1D array `b` as a column

```

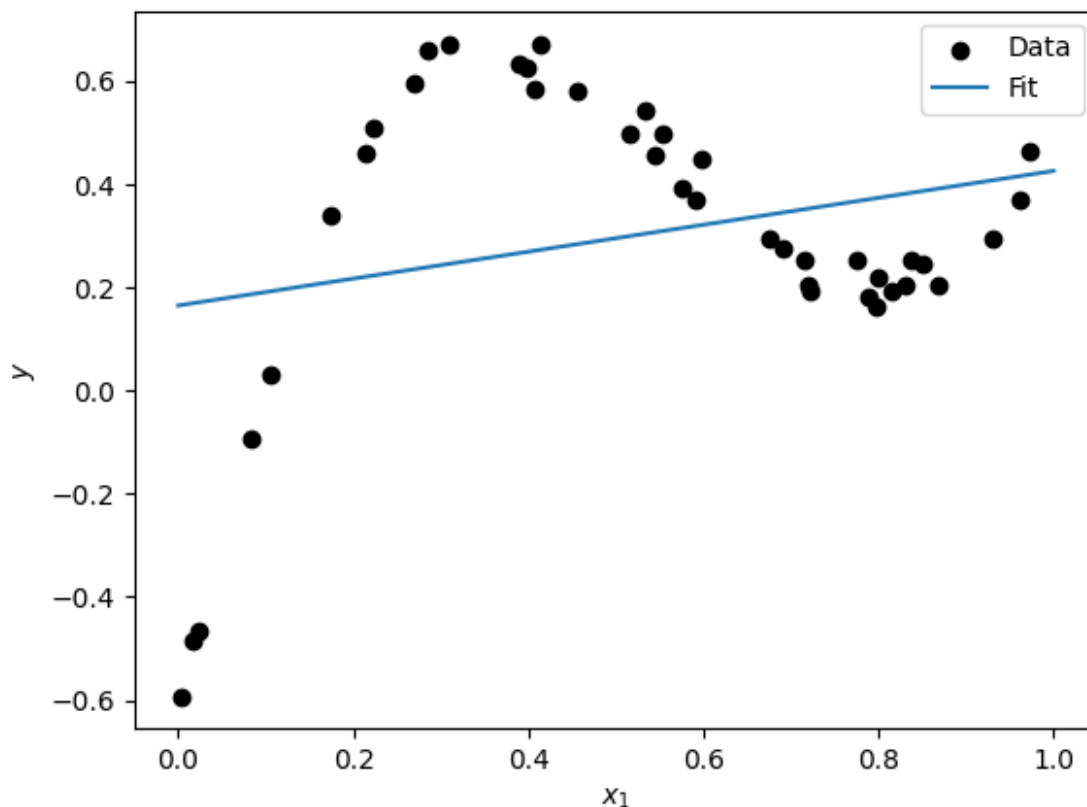
# Get coefficients
w = np.linalg.inv(X.T @ X) @ X.T @ y.reshape(-1,1)
print("Linear Coefficients:", w.flatten())

Linear Coefficients: [0.26080739 0.16441038]

```

Next, we write a plotting function to plot data and our least squares regression on the same axes. To apply our regression we can call the `get_linear_design_matrix()` function on a new set of x values and multiply the result by our coefficients w .

```
def plot_data_with_regression(x_data, y_data, x_reg, y_reg):  
    plt.figure()  
  
    plt.scatter(x_data, y_data, label="Data", c="black")  
    plt.plot(x_reg, y_reg, label="Fit")  
  
    plt.legend()  
    plt.xlabel(r"$x_1$")  
    plt.ylabel(r"$y$")  
    plt.show()  
  
x_fit = np.linspace(0, 1, 100) # x values for fit line  
y_fit = get_linear_design_matrix(x_fit) @ w # y values for fit line  
plot_data_with_regression(x, y, x_fit, y_fit)
```



Your turn: Second order polynomial

Now you will solve the same problem, but with a quadratic polynomial instead of linear. We need to write a new function to generate a design matrix.

Replace the commented code below:

```
def get_quadratic_design_matrix(x):  
    # YOUR CODE GOES HERE  
    # GENERATE A DESIGN MATRIX WITH 2ND ORDER FEATURES: X  
    x = x.reshape(-1, 1)  
    columns = [x**2, x, np.ones_like(x)]  
    X = np.concatenate(columns, axis=1)  
    return X
```

```
X = get_quadratic_design_matrix(x)  
print("First four rows of X:")  
print(X[:4,:])
```

First four rows of X:

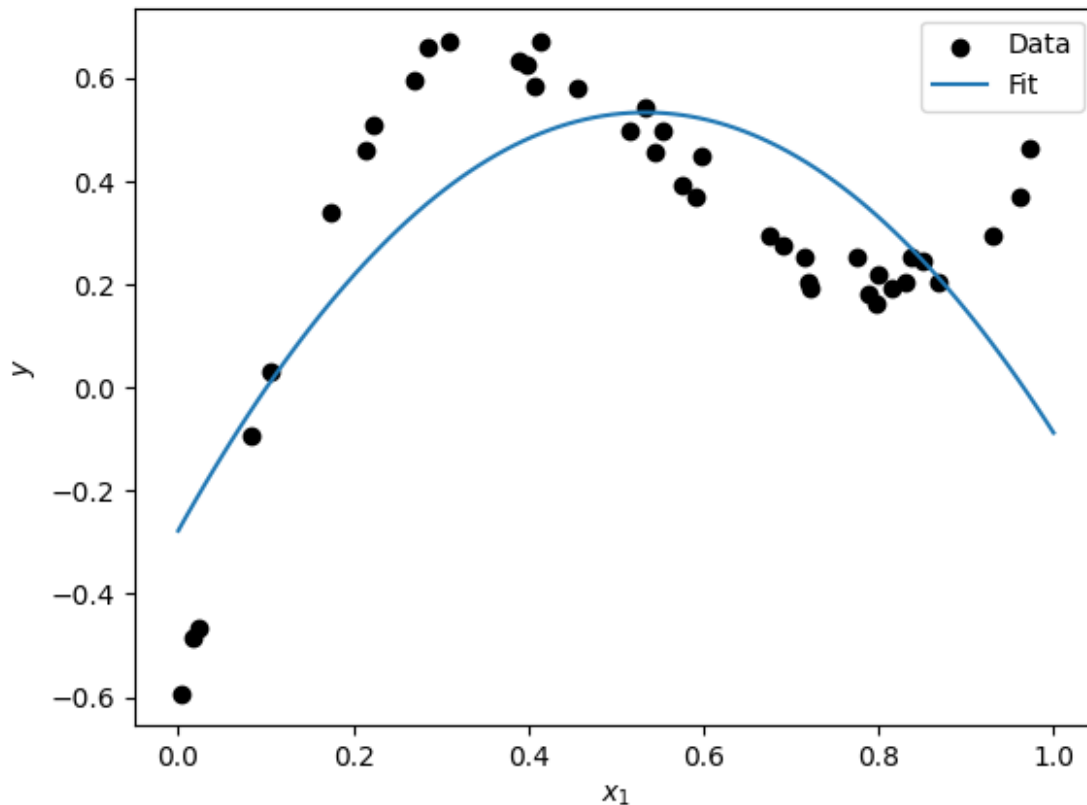
```
[[8.1510250e-02 2.8550000e-01 1.0000000e+00]  
 [1.0890000e-05 3.3000000e-03 1.0000000e+00]  
 [6.9006249e-01 8.3070000e-01 1.0000000e+00]  
 [9.2275236e-01 9.6060000e-01 1.0000000e+00]]
```

Compute the w coefficients with a pseudo-inverse as in the example:

```
# YOUR CODE GOES HERE  
# COMPUTE COEFFICIENTS w  
w = np.linalg.inv(X.T @ X) @ X.T @ y.reshape(-1,1)  
print("Quadratic Coefficients:", w.flatten())  
  
Quadratic Coefficients: [-2.84999306  3.03972629 -0.27780147]
```

Now plot by generating a regression curve and calling the `plot_data_with_regression()` function:

```
# YOUR CODE GOES HERE  
# PLOT  
x_fit = np.linspace(0, 1, 100)  
y_fit = get_quadratic_design_matrix(x_fit) @ w  
  
plot_data_with_regression(x, y, x_fit, y_fit)
```



3rd Order Polynomial

Here we go through the same steps as above, but this time we perform a cubic polynomial fit. Once again, fill in the necessary code:

```
def get_cubic_design_matrix(x):
    # YOUR CODE GOES HERE
    # GENERATE A DESIGN MATRIX WITH 3RD ORDER FEATURES: X
    x = x.reshape(-1, 1)
    columns = [x**3, x**2, x, np.ones_like(x)]
    X = np.concatenate(columns, axis=1)
    return X

X = get_cubic_design_matrix(x)
print("First four rows of X:")
print(X[:4,:])
```

First four rows of X:

```
[[2.32711764e-02  8.15102500e-02  2.85500000e-01  1.00000000e+00]
 [3.59370000e-08  1.08900000e-05  3.30000000e-03  1.00000000e+00]
 [5.73234910e-01  6.90062490e-01  8.30700000e-01  1.00000000e+00]
 [8.86395917e-01  9.22752360e-01  9.60600000e-01  1.00000000e+00]]
```

```

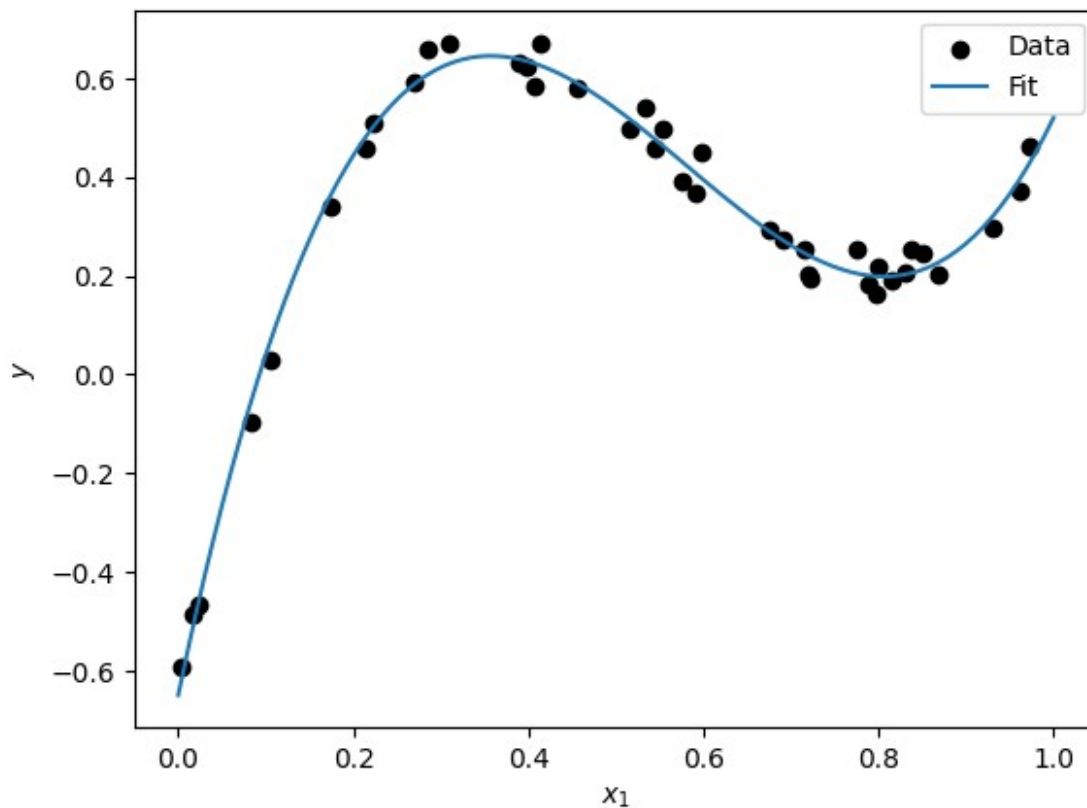
# YOUR CODE GOES HERE
# COMPUTE COEFFICIENTS w
w = np.linalg.inv(X.T @ X) @ X.T @ y.reshape(-1,1)
print("Cubic Coefficients:", w.flatten())

Cubic Coefficients: [  9.86043282 -17.20179622  8.51092348 -
0.64960983]

# YOUR CODE GOES HERE
# PLOT
x_fit = np.linspace(0, 1, 100)
y_fit = get_cubic_design_matrix(x_fit) @ w

plot_data_with_regression(x, y, x_fit, y_fit)

```



m2-l1-p3

February 3, 2024

1 M2-L1 Problem 3 (5 points)

In this question you will perform regression on 2D data. A linear fit will be demonstrated, and afterward you will extend the code to perform a second-order fit. First, run the Setup cells.

1.1 Setup

1.1.1 Generating data

```
[12]: # Generating data for the problem
import numpy as np
import matplotlib.pyplot as plt

def gaussian2d(A, mx, my, sx, sy):
    F = lambda xy: A*np.exp(-((xy[:,0]-mx)**2/(2*sx*sx)
                               + (xy[:,1]-my)**2/(2*sy*sy)))
    return F

def get_data_function():
    f1 = gaussian2d(A=0.7, mx = 0.25,my=0.25,sx=0.25,sy=0.25)
    f2 = gaussian2d(A=0.7, mx = 0.75,my=0.75,sx=0.25,sy=0.45)
    f = lambda xy: f1(xy) + f2(xy)
    return f

np.random.seed(0)
x = np.random.rand(60,2)
f = get_data_function()
y = f(x)
```

1.1.2 Function for 3D plotting

```
[13]: from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm

# Writing a 3D Plotting function. Inputs data points and regression function
def plot_data_with_regression(x_data, y_data, regfun=None):
    plt.figure(figsize=(8,8))
    fig = plt.gcf()
```

```

ax = fig.add_subplot(111, projection='3d')
ax.scatter(x_data[:,0], x_data[:,1], 0*y_data,s=13,c=y_data,zorder=-1,cmap="coolwarm", alpha=1,
↪edgecolor="black", linewidth=0.2)
ax.scatter(x_data[:,0], x_data[:,1], y_data,s=20,c="black",zorder=-1)
for i in range(len(y_data)):
    ax.
↪plot([x_data[i,0],x_data[i,0]],[x_data[i,1],x_data[i,1]],[0,y_data[i]], 'k:
↪',linewidth=0.3)

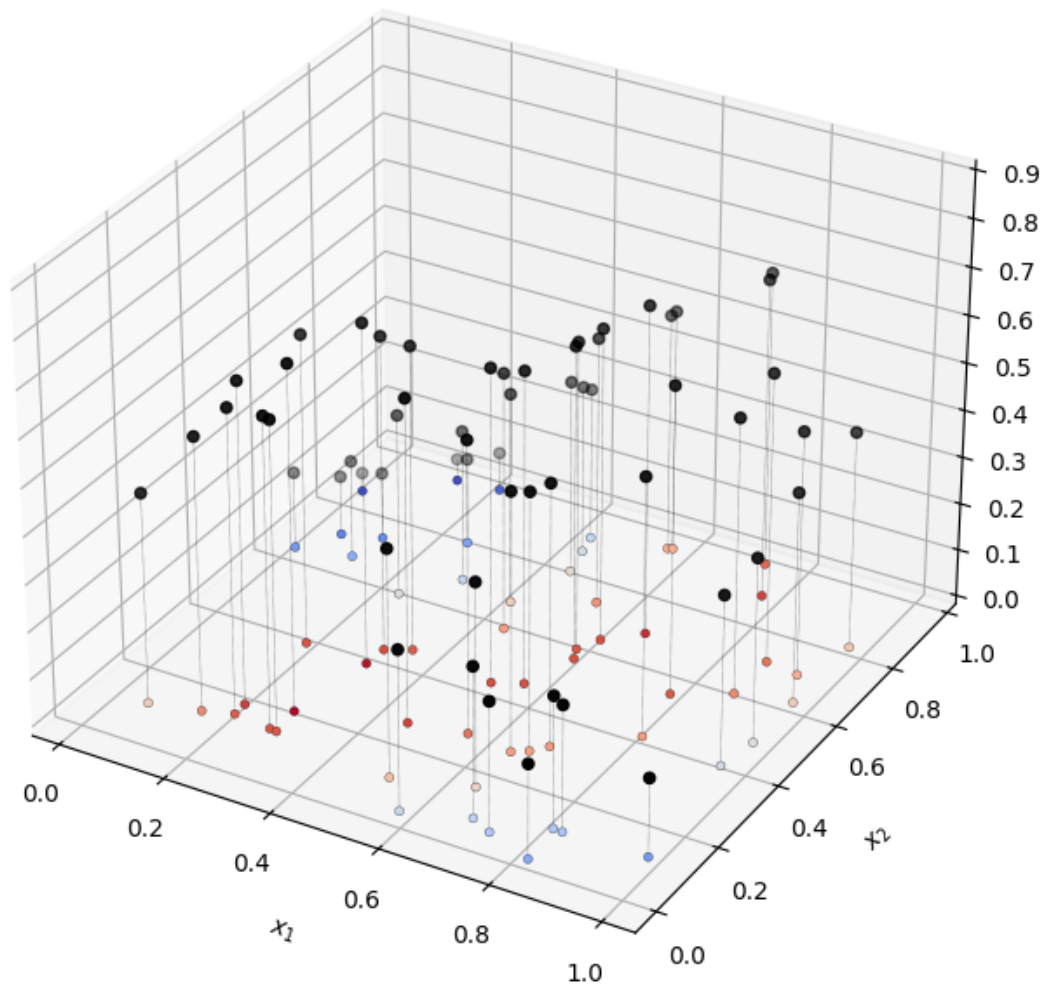
ax.set_xlabel('\n' + r"$x_1$")
ax.set_ylabel('\n' + r"$x_2$")
ax.set_zlabel('\n'+r"$y$")
ax.set_zlim(0,0.9)

if regfun is not None:
    vals = np.linspace(0, 1, 100)
    x1grid, x2grid = np.meshgrid(vals, vals)
    y = regfun(np.concatenate((x1grid.reshape(-1,1),x2grid.
↪reshape(-1,1)),1)).reshape(*np.shape(x1grid))
    ax.plot_surface(x1grid, x2grid, y.reshape(x1grid.shape), alpha = 0.8,
↪cmap = cm.coolwarm)
plt.show()

```

1.1.3 Data visualized

```
[14]: plot_data_with_regression(x,y)
```



1.2 Demonstration: 2D Linear Regression

First, I generate a design matrix within a function called `get_linear_design_matrix()`

```
[15]: def get_linear_design_matrix(x):
    x1 = x[:,0].reshape(-1, 1)
    x2 = x[:,1].reshape(-1, 1)
    columns = [x1, x2, np.ones_like(x1)]    # Linear design matrix has a column
    ↪ of x1, column of x2, and a column of ones
    X = np.concatenate(columns, axis=1)    # Combine each column horizontally to
    ↪ make a matrix
    return X
```

```
[16]: X = get_linear_design_matrix(x)
print("First four rows of X:")
print(X[:4,:])
```

First four rows of X:

```
[[0.5488135  0.71518937 1.          ]
 [0.60276338 0.54488318 1.          ]
 [0.4236548  0.64589411 1.          ]
 [0.43758721 0.891773   1.          ]]
```

Next, get the coefficients of the regression:

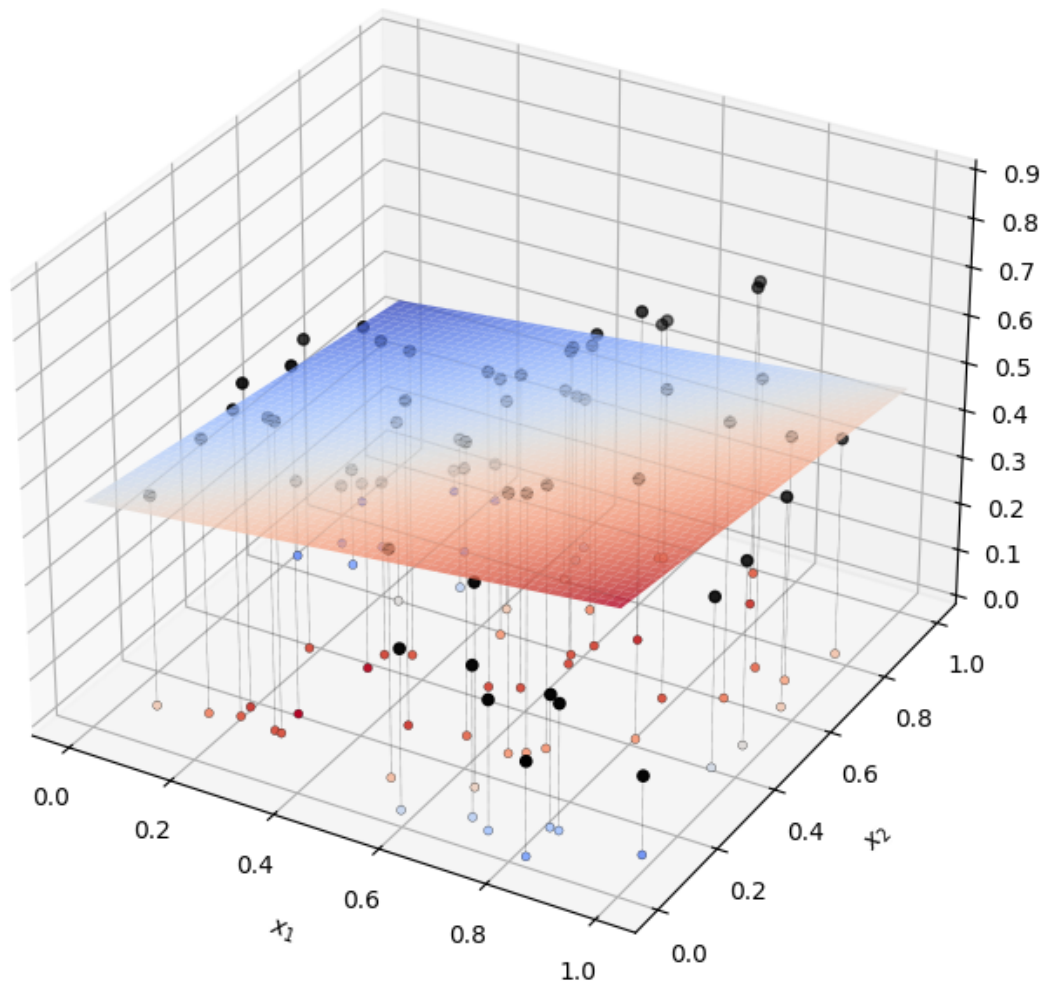
```
[17]: # Get coefficients
w1 = np.linalg.inv(X.T @ X) @ X.T @ y.reshape(-1,1)
print("Linear Coefficients:", w1.flatten())
```

Linear Coefficients: [0.11233939 -0.10638434 0.45720916]

Finally, we plot the result. Here, `plot_data_with_regression()` takes as input the `x` input data, `y` output data, and a function which performs the desired regression. Therefore I first define said regression function, and plug it in as an argument to the plotting function:

```
[18]: def do_2d_linear_regression(x):
        y_fit = get_linear_design_matrix(x) @ w1
        return y_fit

plot_data_with_regression(x, y, do_2d_linear_regression)
```



1.3 Your Turn: 2D Quadratic Regression

The linear regression results are clearly not a great fit. You will see if a 2nd order fit can do any better. Fill in the missing code below to generate a quadratic design matrix and plot the results:

```
[19]: def get_quadratic_design_matrix(x):
    x1 = x[:,0].reshape(-1, 1)
    x2 = x[:,1].reshape(-1, 1)

    # YOUR CODE GOES HERE
    # 2ND ORDER, 2-D DESIGN MATRIX NEEDS 6 TOTAL COLUMNS
    columns = [x1**2, x2**2, x1*x2, x1, x2, np.ones_like(x1)]
    X = np.concatenate(columns, axis=1)
```



```
return X
```

```
[20]: X = get_quadratic_design_matrix(x)
print("First four rows of X:")
print(X[:4,:])
```

First four rows of X:

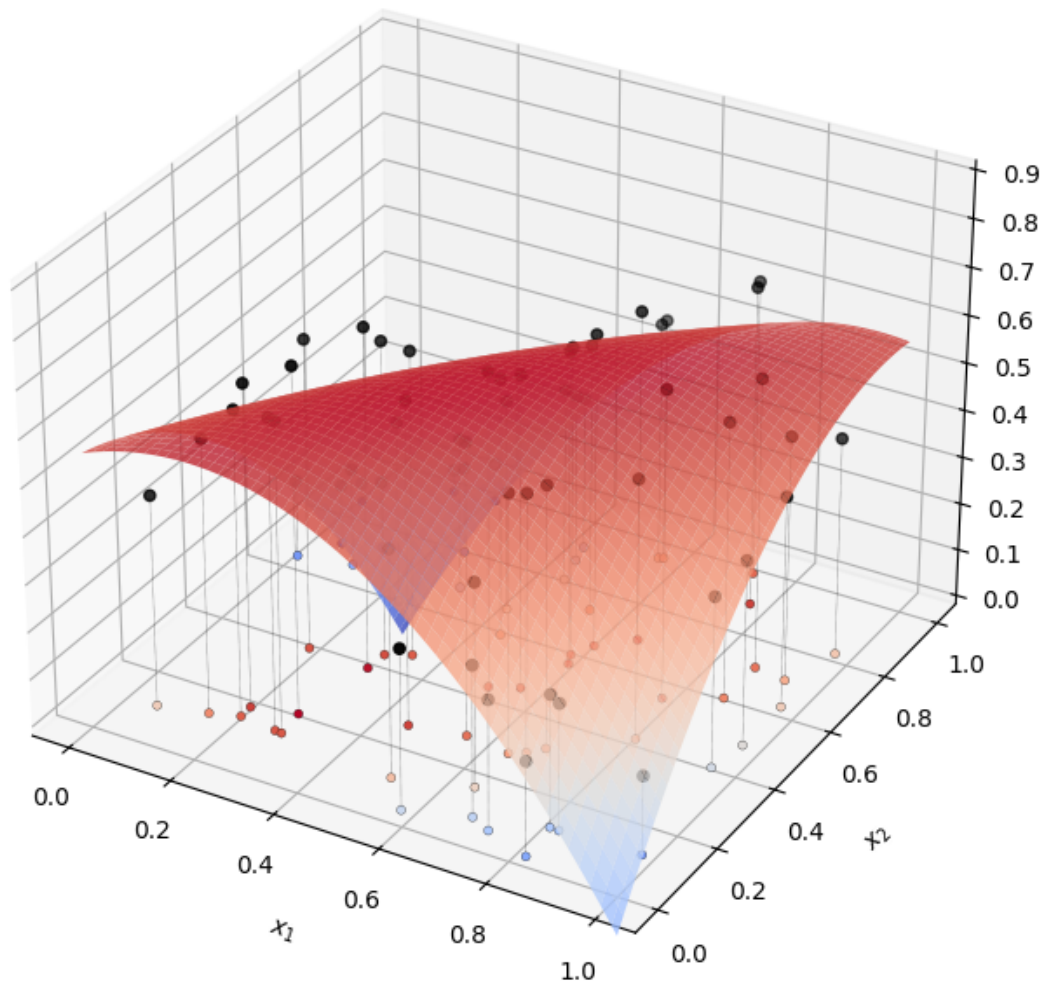
```
[[0.30119626 0.51149583 0.39250558 0.5488135  0.71518937 1.         ]
 [0.36332369 0.29689768 0.32843563 0.60276338 0.54488318 1.         ]
 [0.17948339 0.41717921 0.27363614 0.4236548  0.64589411 1.         ]
 [0.19148257 0.79525908 0.39022846 0.43758721 0.891773   1.         ]]
```

```
[21]: # Get coefficients
w2 = np.linalg.inv(X.T @ X) @ X.T @ y.reshape(-1,1)
print("Quadratic Coefficients:", w2.flatten())
```

Quadratic Coefficients: [-1.09949493 -0.78655383 1.62592273 0.44193704
-0.17753776 0.55677679]

```
[22]: def do_2d_quadratic_regression(x):
        y_fit = get_quadratic_design_matrix(x) @ w2
        return y_fit

plot_data_with_regression(x, y, do_2d_quadratic_regression)
```



m2-l2-p1

February 3, 2024

1 M2-L2 Problem 1 (5 points)

In this problem you will perform cubic least squares regression using gradient descent. Starting with an initial guess, you will plot the regression curve as you perform many iterations of gradient descent, and observe how the regression performance improves.

Start by running the following cell to load data and define helpful functions. Data is loaded into 'x' and 'y', with a cubic design matrix as 'X'.

```
[1]: import numpy as np
import matplotlib.pyplot as plt

def plot_data_with_regression(x_data, y_data, x_reg, y_reg, title=""):
    plt.figure()

    plt.scatter(x_data.flatten(), y_data.flatten(), label="Data", c="black")
    plt.plot(x_reg.flatten(), y_reg.flatten(), label="Fit")

    plt.legend()
    plt.xlabel(r"$x_1$")
    plt.ylabel(r"$y$")
    plt.xlim(-2,2)
    plt.ylim(-2,2)
    plt.title(title)
    plt.show()

x = np.array([-1.52362349, -1.60576489, -1.34827768, -1.45340266, -1.42652973,
↪ -1.20489448, -1.34662672, -0.77989399, -1.02479866, -1.18388425, -0.63601103,
↪ -1.06184469, -0.81853545, -0.98253754, -0.41599291, -0.39373095, -0.49828026,
↪ -0.50820654, -0.33545205, -0.17745781, -0.11232523, -0.1065807 , -0.28129177,
↪ -0.27996129, -0.30355288, 0.32030413, -0.10195465, 0.44533511, 0.43274828,
↪ 0.35343658, 0.10612364, 0.22594603, 0.72121097, 0.81574553, 0.50008731, 0.
↪ 61311114, 0.65468014, 0.60571755, 0.67438719, 0.67226667, 0.82554208, 0.
↪ 99744723, 1.04085817, 1.26282573, 1.14517384, 1.22017733, 1.28481911, 1.
↪ 29034024, 1.66304968, 1.49217068])
```

```

y = np.array([ 1.65517515,  1.33249684,  1.38328432,  1.1531808 ,  0.89478436,0.
↪66783182,  0.59841012,  0.64060691,  0.73930904,  0.91751879,0.52952715,  0.
↪30183071,  0.31052792,  0.3684916 ,  0.6584406 , 0.72407787,  0.83710857,  0.
↪74432213,  0.80478856,  0.6755436 ,0.47643214,  0.50833171,  0.7731494 ,  0.
↪60172717,  0.39123432, 0.69418038,  0.59625493,  0.90711162,  1.01760262,  0.
↪98348453, 0.78208567,  0.76030704,  0.55105897,  0.7830408 ,  0.86284938, 0.
↪88284709,  0.35630757,  0.7237893 ,  0.66325283,  0.23944077,-0.04822037,  0.
↪16059611, -0.14460941, -0.38449511, -0.54652704, -0.85011695, -0.84597649,
↪-0.90989068, -1.06840649, -1.77916364])
X = np.vstack([x*x*x, x*x, x, np.ones_like(x)]).T

xreg = np.linspace(-2,2)
Xreg = np.vstack([xreg*xreg*xreg, xreg*xreg, xreg, np.ones_like(xreg)]).T

```

1.1 Gradient function

We need to define a function for the gradient of our objective function. In the lecture, this gradient was:

$$\frac{\partial \text{obj}}{\partial w} = 2X'(Xw - y)$$

Please complete the function below to compute the gradient. Recall that the design matrix is the global variable X, and you may need to reshape the output y as a column vector.

```

[2]: def grad(w):
      # YOUR CODE GOES HERE
      # Return the gradient of the objective function
      gradient = 2*X.T.dot(X.dot(w)-y.reshape(-1,1))
      return gradient

```

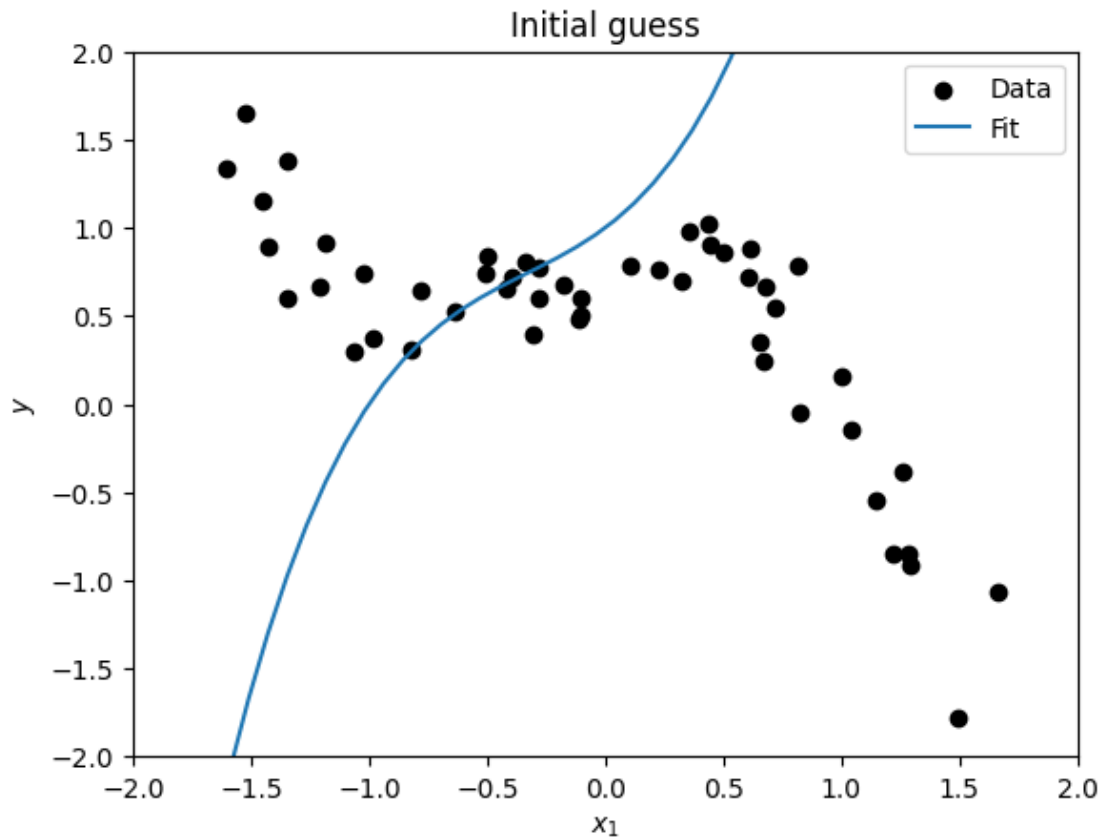
1.2 Initial guess

Let's define an initial guess for w and visualize the resulting curve:

```

[3]: w = np.array([[1,1,1,1]]).T
      yreg = Xreg @ w
      plot_data_with_regression(x,y,xreg, yreg, "Initial guess")

```



2 Gradient Descent Loop

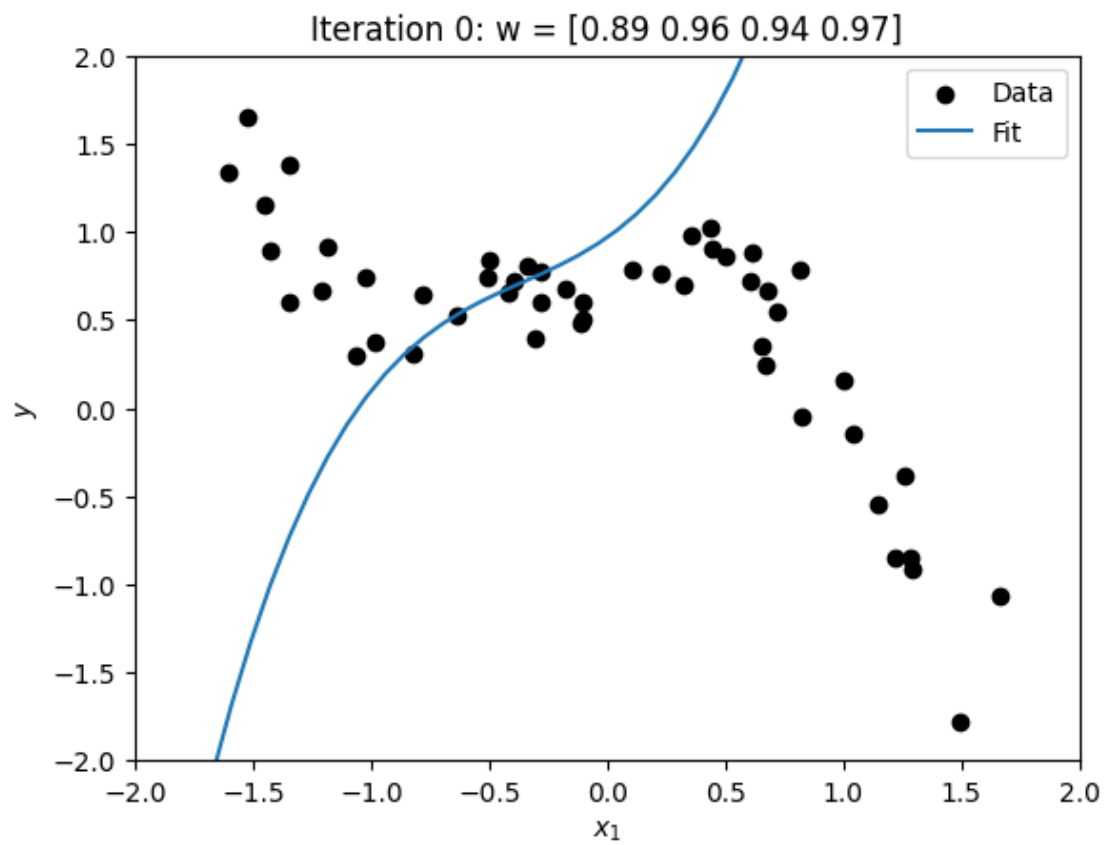
Now complete the gradient descent loop below. You should call your gradient function, update w by subtracting η (the step size) times the gradient.

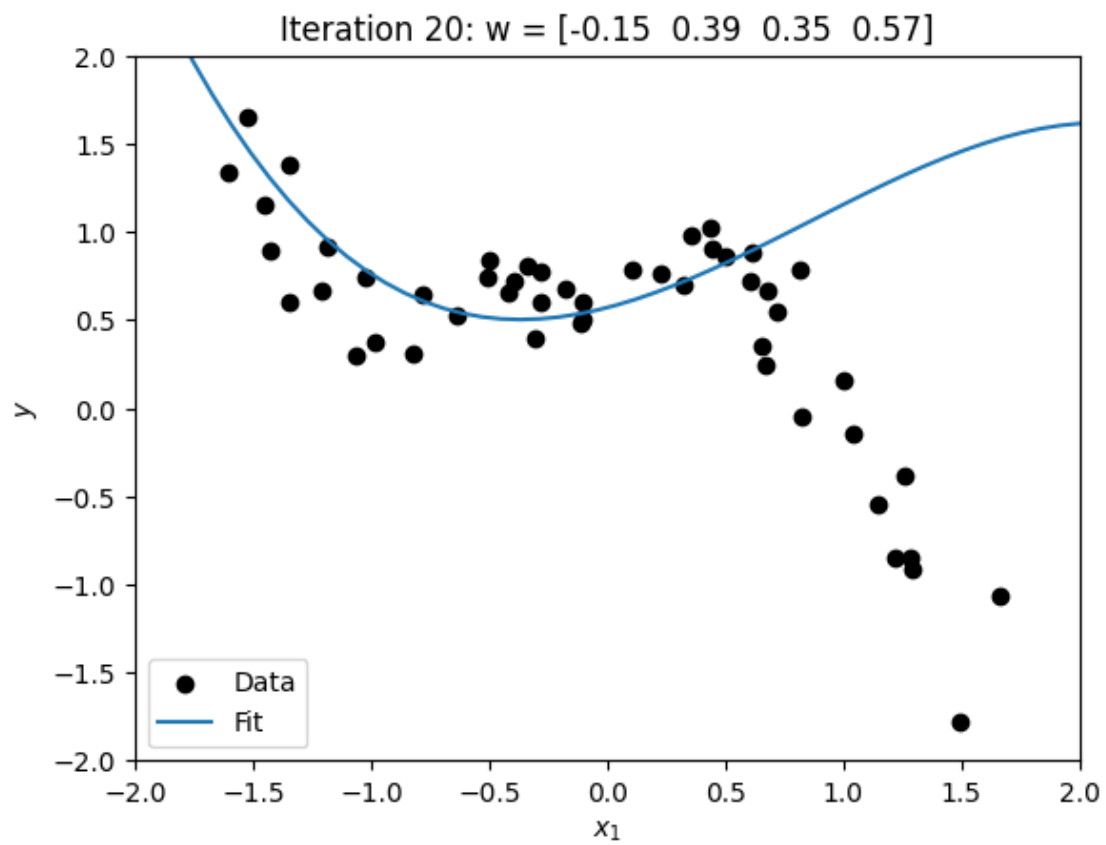
Every several iterations, the result is plotted. You should observe the gradual improvement of the model.

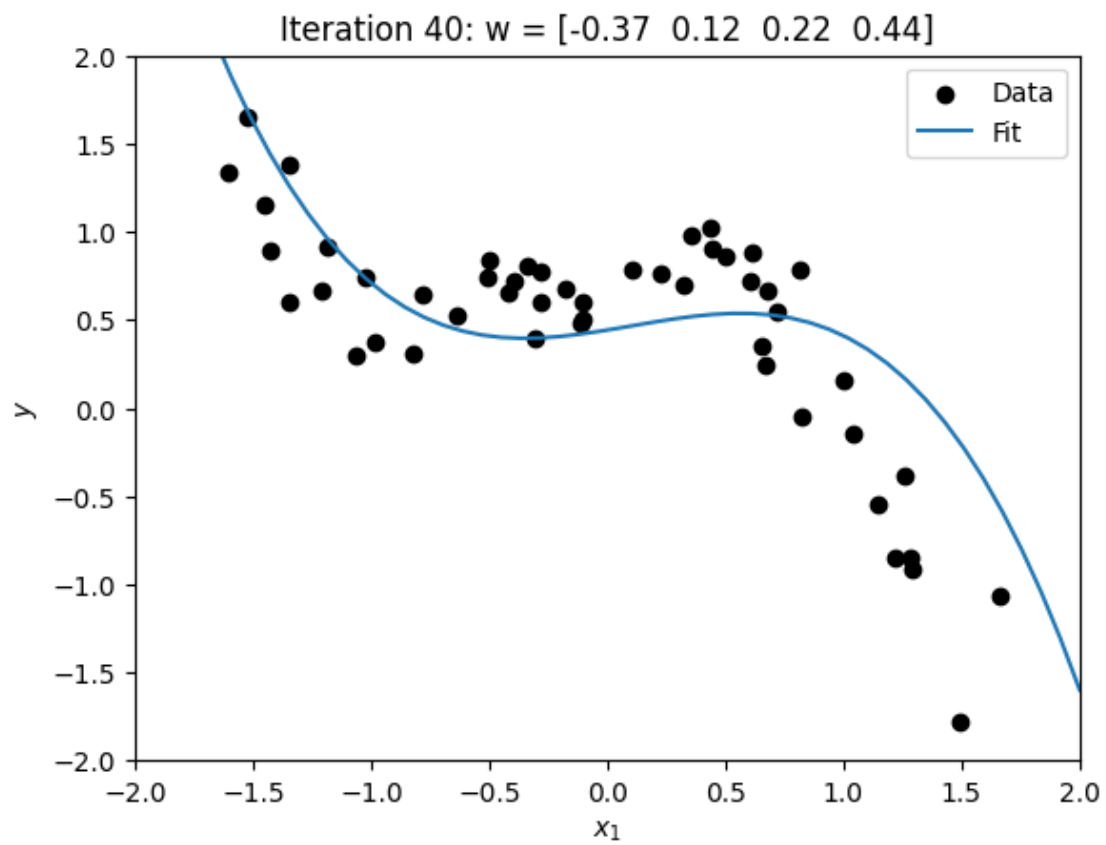
```
[4]: eta = 0.00025
for i in range(101):

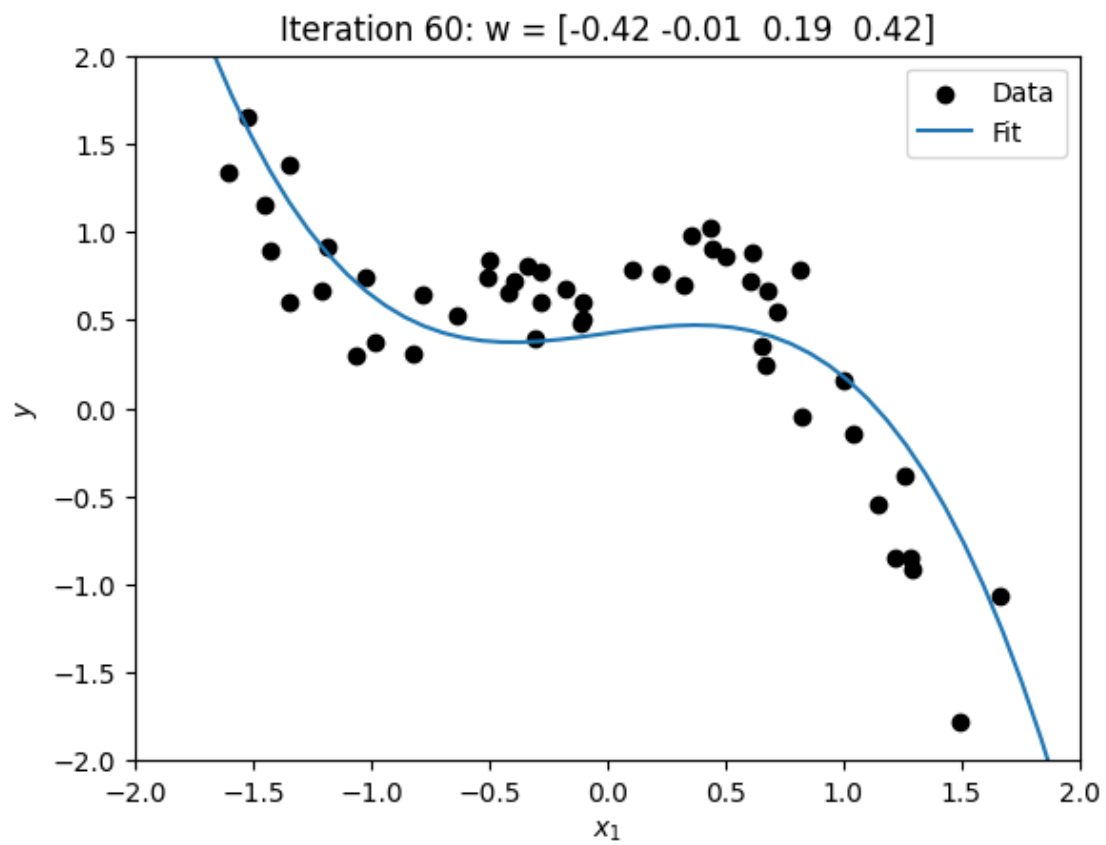
    # YOUR CODE GOES HERE
    # Update w
    w = w - eta * grad(w)

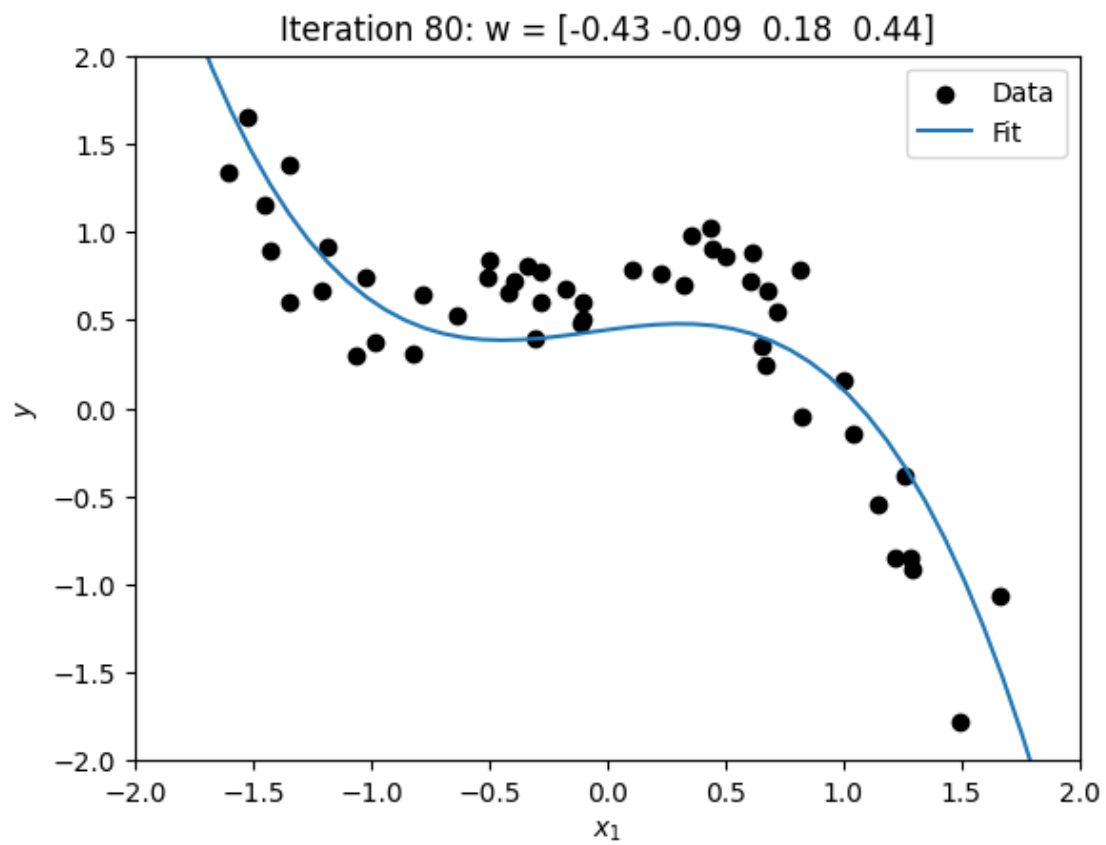
    if 0 == i%20:
        yreg = Xreg @ w
        plot_data_with_regression(x,y,xreg, yreg, f"Iteration {i}: w = {np.
↪round(w.flatten(),2)}")
```

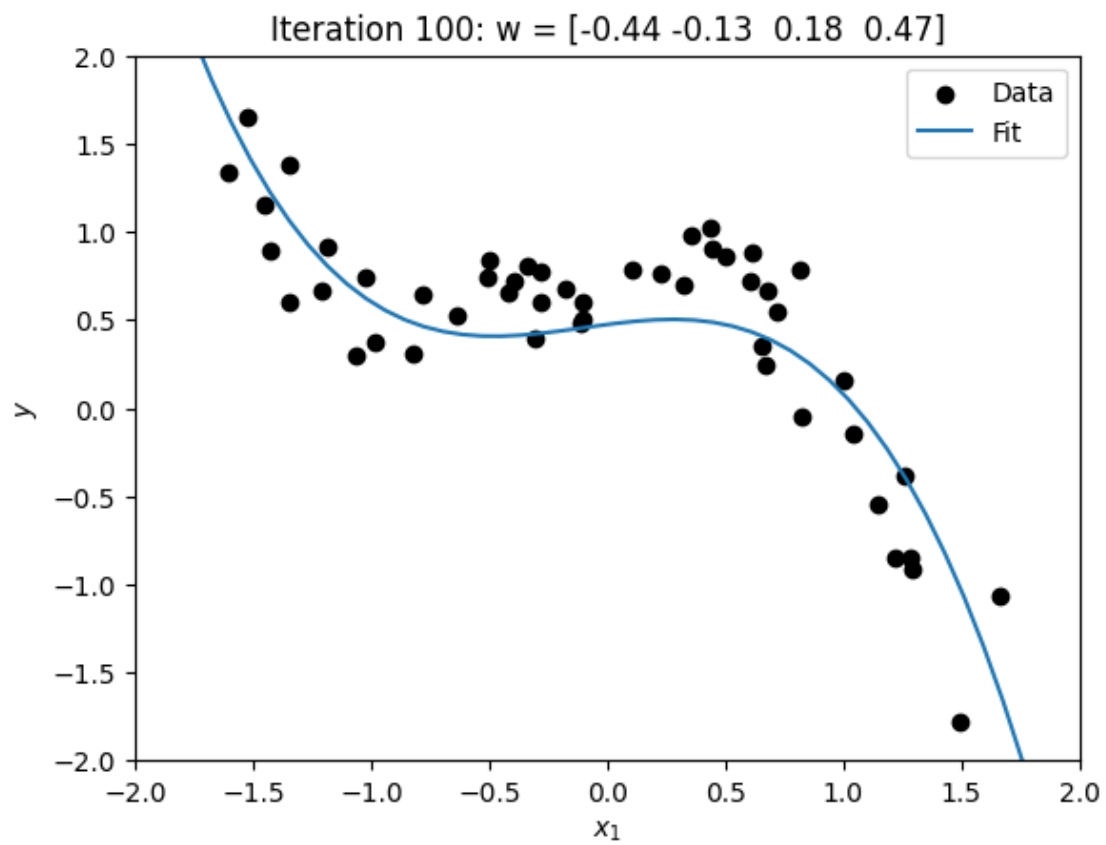












m2-l2-p2

February 3, 2024

1 M2-L2 Problem 2 (5 points)

In this problem we will perform least-squares regression using sklearn's built-in tools.

First, you will generate a standard linear least squares regression model with `LinearRegression`.

Next, you will use stochastic gradient descent to train another model with `SGDRegressor`.

Run this cell to perform the required imports and load the data:

```
[1]: import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import LinearRegression
from sklearn.linear_model import SGDRegressor

def plot_data_with_regression(x_data, y_data, x_reg, y_reg, title=""):
    plt.figure()

    plt.scatter(x_data.flatten(), y_data.flatten(), label="Data", c="black")
    plt.plot(x_reg.flatten(), y_reg.flatten(), label="Fit")

    plt.legend()
    plt.xlabel(r"$x_1$")
    plt.ylabel(r"$y$")
    plt.xlim(-2,2)
    plt.ylim(-2,2)
    plt.title(title)
    plt.show()

x = np.array([-1.52362349, -1.60576489, -1.34827768, -1.45340266, -1.42652973,
↪ -1.20489448, -1.34662672, -0.77989399, -1.02479866, -1.18388425, -0.63601103,
↪ -1.06184469, -0.81853545, -0.98253754, -0.41599291, -0.39373095, -0.49828026,
↪ -0.50820654, -0.33545205, -0.17745781, -0.11232523, -0.1065807, -0.28129177,
↪ -0.27996129, -0.30355288, 0.32030413, -0.10195465, 0.44533511, 0.43274828,
↪ 0.35343658, 0.10612364, 0.22594603, 0.72121097, 0.81574553, 0.50008731, 0.
↪ 61311114, 0.65468014, 0.60571755, 0.67438719, 0.67226667, 0.82554208, 0.
↪ 99744723, 1.04085817, 1.26282573, 1.14517384, 1.22017733, 1.28481911, 1.
↪ 29034024, 1.66304968, 1.49217068])
```

```

y = np.array([ 1.65517515,  1.33249684,  1.38328432,  1.1531808 ,  0.89478436,0.
↪66783182,  0.59841012,  0.64060691,  0.73930904,  0.91751879,0.52952715,  0.
↪30183071,  0.31052792,  0.3684916 ,  0.6584406 , 0.72407787,  0.83710857,  0.
↪74432213,  0.80478856,  0.6755436 ,0.47643214,  0.50833171,  0.7731494 ,  0.
↪60172717,  0.39123432, 0.69418038,  0.59625493,  0.90711162,  1.01760262,  0.
↪98348453, 0.78208567,  0.76030704,  0.55105897,  0.7830408 ,  0.86284938, 0.
↪88284709,  0.35630757,  0.7237893 ,  0.66325283,  0.23944077,-0.04822037,  0.
↪16059611, -0.14460941, -0.38449511, -0.54652704, -0.85011695, -0.84597649,↪
↪-0.90989068, -1.06840649, -1.77916364])
X = np.vstack([x*x*x, x*x, x, np.ones_like(x)]).T

xreg = np.linspace(-2,2)
Xreg = np.vstack([xreg*xreg*xreg, xreg*xreg, xreg, np.ones_like(xreg)]).T

```

1.1 Least Squares Regression

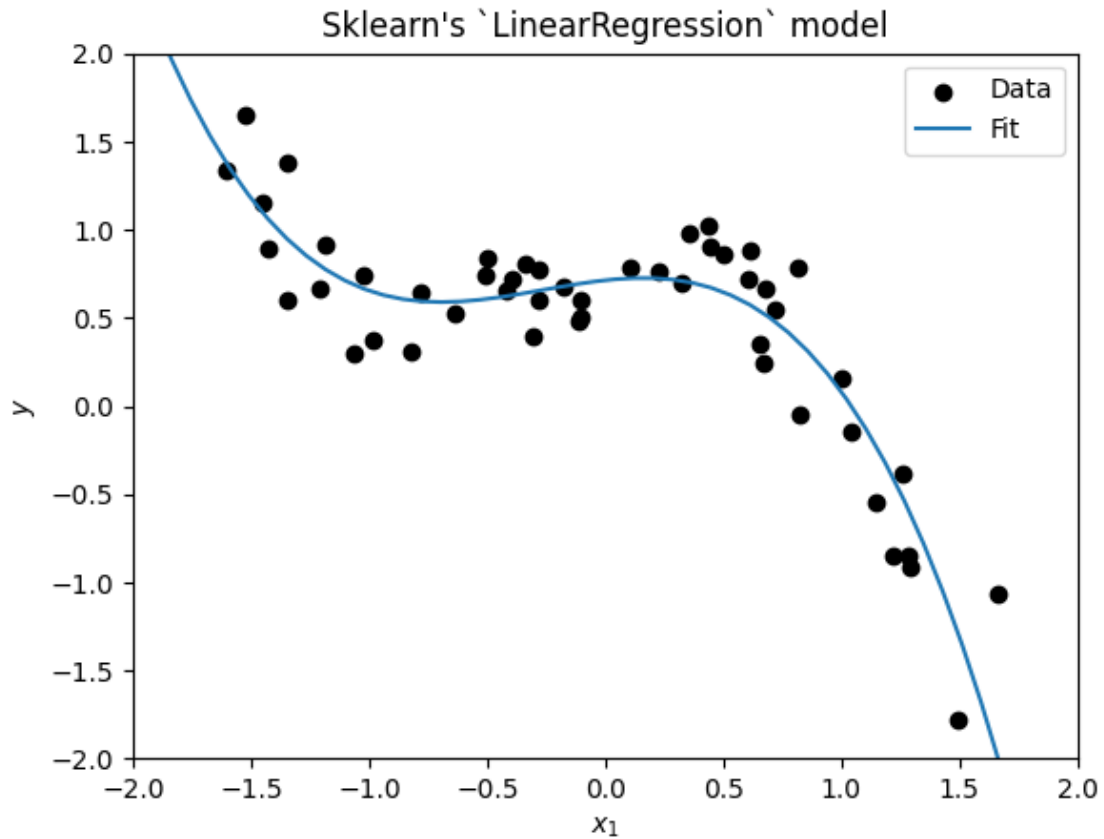
We have provided a demonstration of least squares regression using sklearn:

```

[2]: model = LinearRegression()
model.fit(X,y)

yreg = model.predict(Xreg)
plot_data_with_regression(x, y, xreg, yreg, "Sklearn's `LinearRegression`↪
↪model")

```

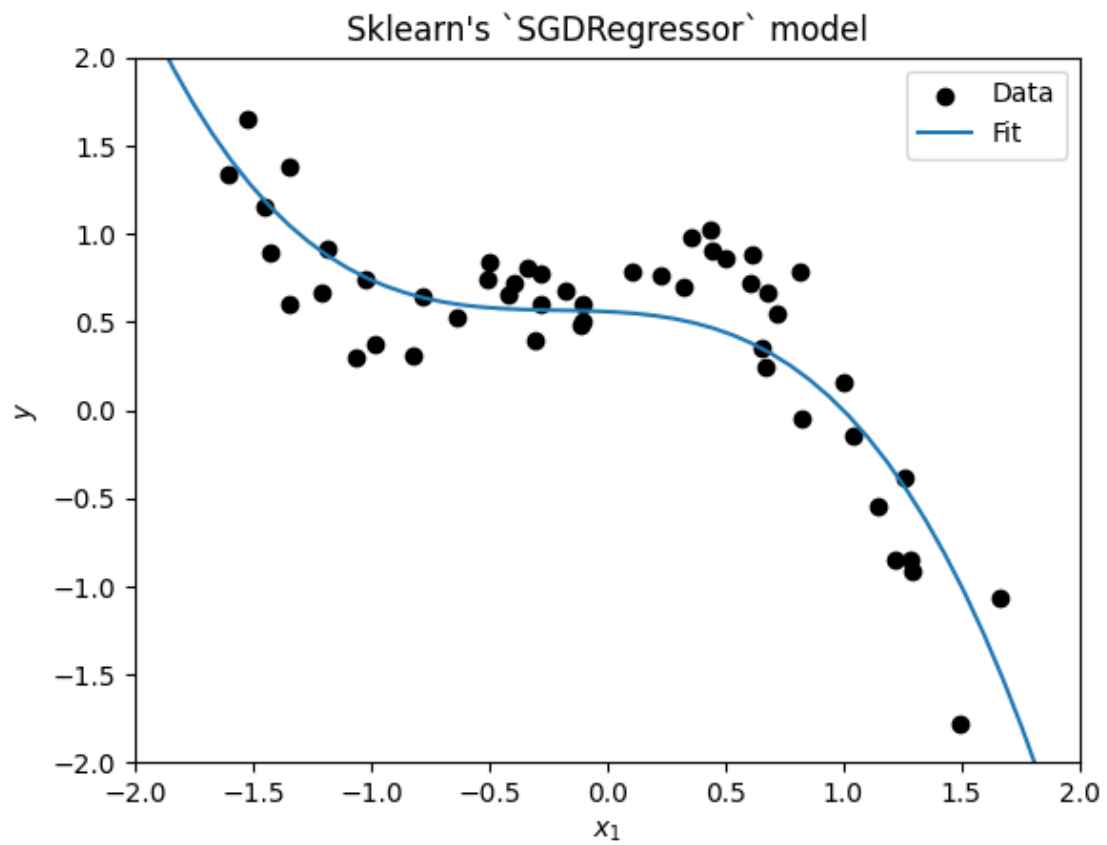


1.2 Using SGD

Now use stochastic gradient descent to solve the same problem and make a similar plot, but for a `SGDRegressor` model instead of `LinearRegression`:

```
[3]: # YOUR CODE GOES HERE
model = SGDRegressor()
model.fit(X,y)

yreg = model.predict(Xreg)
plot_data_with_regression(x, y, xreg, yreg, "Sklearn's `SGDRegressor` model")
```



m2-l2-p3

February 3, 2024

1 M2-L2 Problem 3 (5 points)

When flow is directed across a pin fin heat sink, increasing fluid velocity can improve the heat transfer, making the heat sink more effective.

You have been given a dataset containing measurements for such a scenario, which contains the following: - Input: Reynolds Number of air flowing past the heat sink - Output: Heat transfer coefficient of the heat sink, in $\text{W}/(\text{m}^2 \text{ K})$

Your job is to train a model on this data to predict the heat transfer coefficient, given Reynolds number as input. You will use a high-order polynomial

Start by loading the data in the following cell:

```
[5]: import numpy as np
import matplotlib.pyplot as plt

def plot_data_with_regression(x_data, y_data, x_reg, y_reg, title=""):
    plt.figure()

    plt.scatter(x_data.flatten(), y_data.flatten(), label="Data", c="black")
    plt.plot(x_reg.flatten(), y_reg.flatten(), label="Fit")

    plt.legend(loc="upper left")
    plt.xlabel(r"$Re / 1000$")
    plt.ylabel(r"$h, \text{W}/\text{m}^2 \text{ K}$")
    plt.xlim(0,6)
    plt.ylim(50,200)
    plt.title(title)
    plt.show()

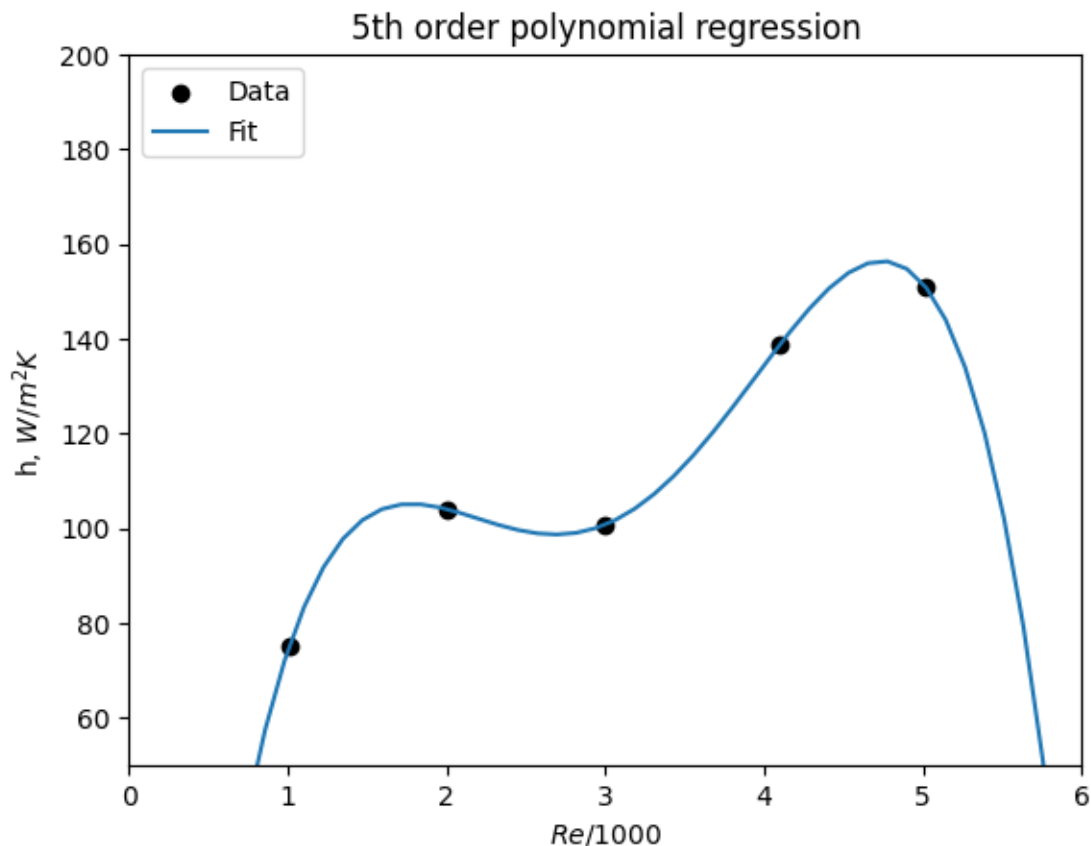
deg = 5
x = np.array([1.010, 2.000, 2.990, 4.100, 5.020])
y = np.array([75.1, 104.0, 100.6, 138.8, 150.8])
X = np.vander(x, deg)

xreg = np.linspace(0,6)
Xreg = np.vander(xreg, deg)
```


1.1 Least Squares Regression

As we have done for previous problems, we can do least squares regression by computing the pseudo-inverse of the design matrix. Notice how the model performs beyond the training data.

```
[6]: w = np.linalg.inv(X.T @ X) @ X.T @ y.reshape(-1,1)
yreg = Xreg @ w
plot_data_with_regression(x, y, xreg, yreg, "5th order polynomial regression")
```



1.2 L2 Regularization

Notice that the plot above reveals that our fifth-order model is overfitting to the data. Let's try applying L2 regularization to fix this. In the lecture, the closed-form solution to least squares with L2 regularization was:

$$w = (X'X + \lambda I_m)^{-1} X'y$$

where I_m is the identity matrix, but with zero in the bias row/column instead of 1; λ is regularization strength; X' is the design matrix and y column vector output.

Complete the function below to compute this w for a given λ :

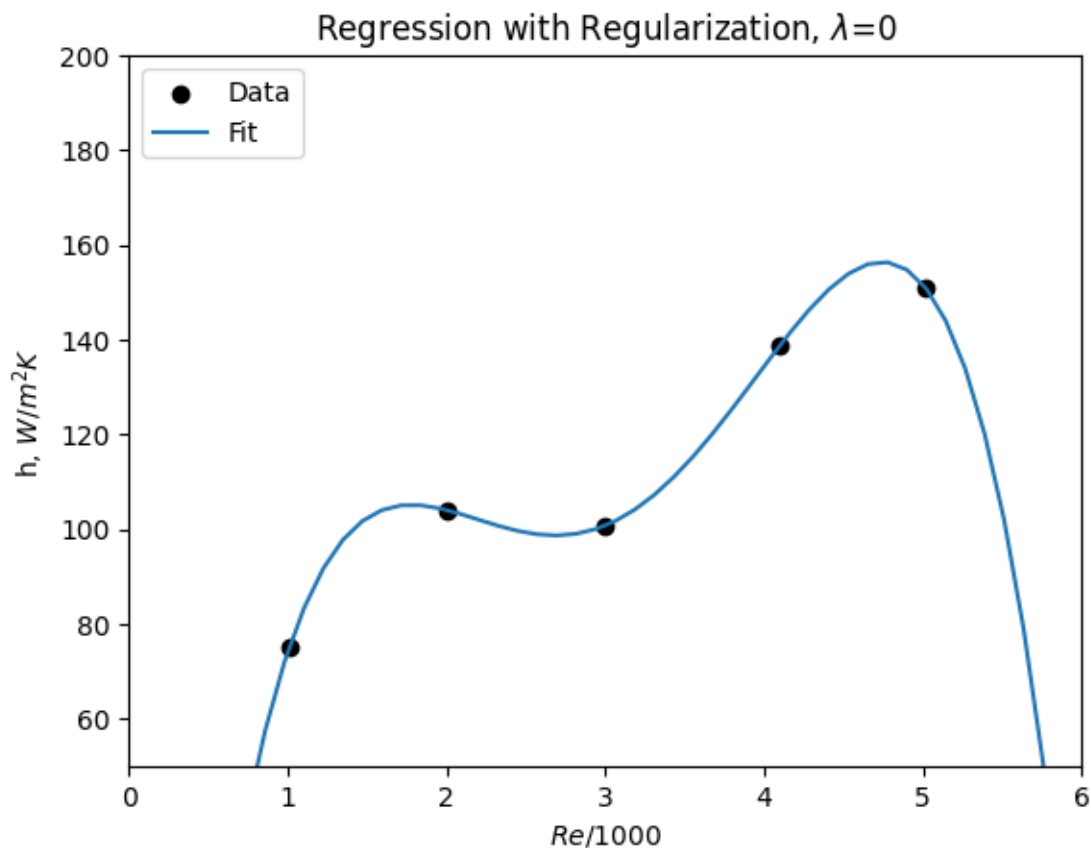
```
[7]: def get_regularized_w(L):
    I_m = np.eye(deg)
    I_m[-1,-1] = 0

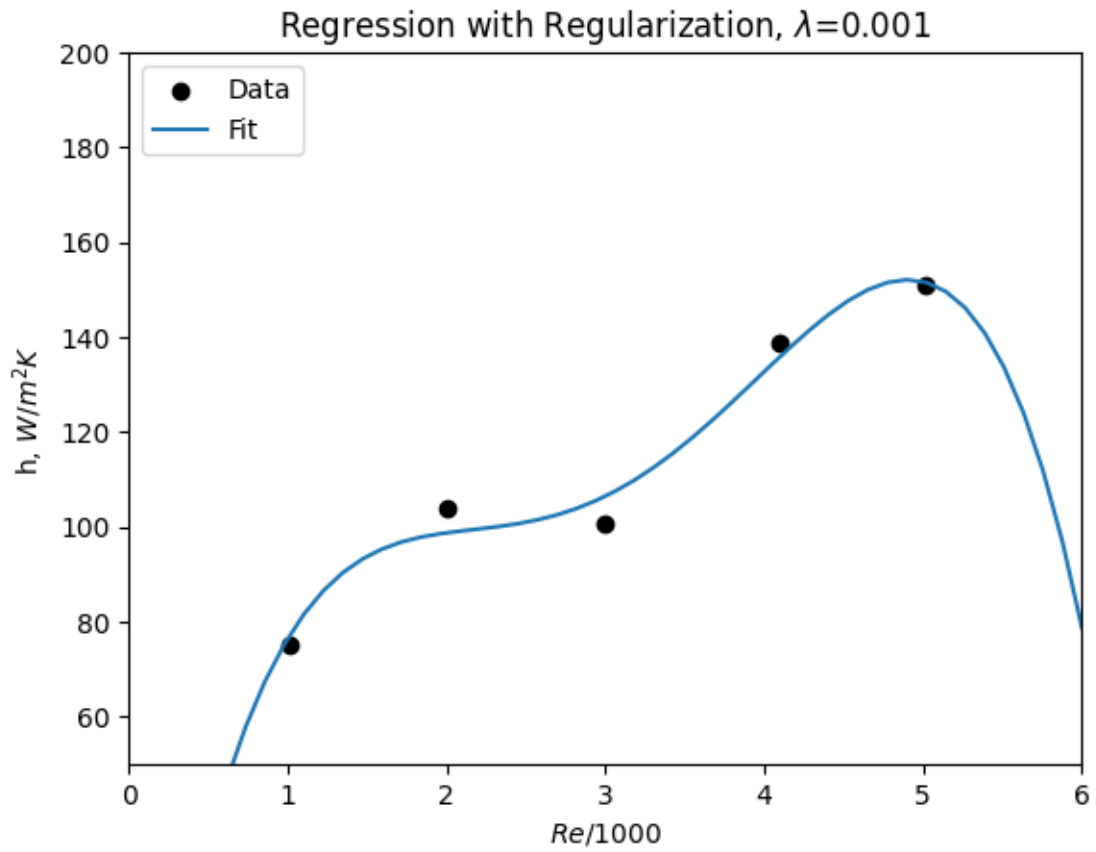
    # YOUR CODE GOES HERE
    # return regularized w
    regularized_w = np.linalg.inv(X.T @ X + L*I_m) @ X.T @ y.reshape(-1,1)
    return regularized_w
```

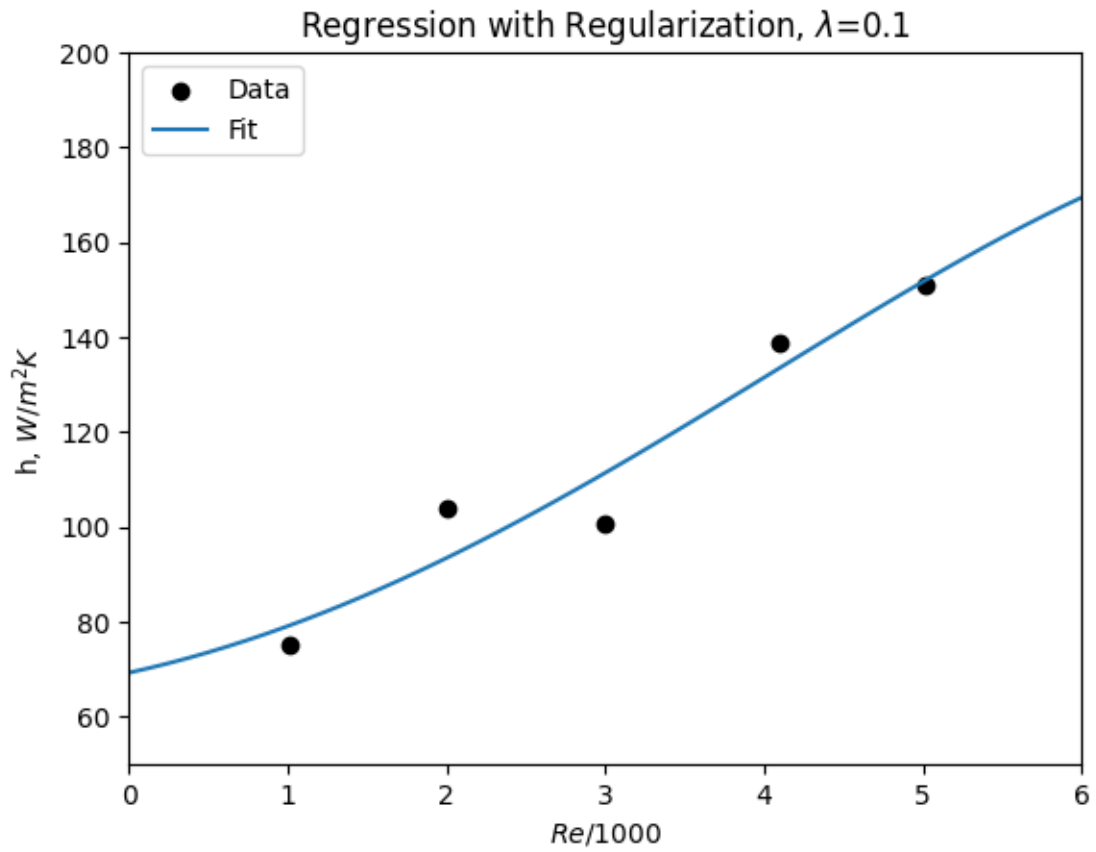
1.3 Testing different lambda values

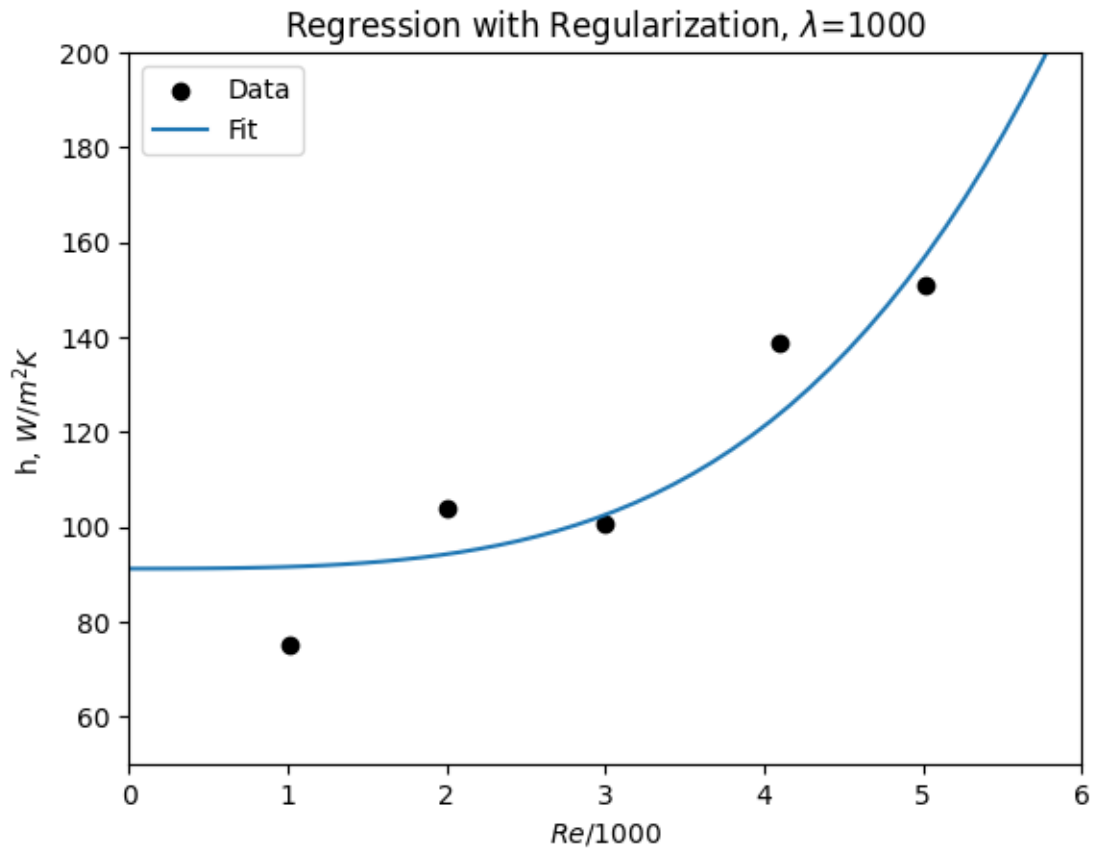
With the above function written, we can compute w for some different values of λ and decide which is qualitatively best.

```
[8]: for L in [0,.001,0.1,1000]:
    w = get_regularized_w(L)
    yreg = Xreg @ w
    plot_data_with_regression(x, y, xreg, yreg,
                             f"Regression with Regularization,  $\lambda$ ={L}")
```









1.4 Model Selection

Which value of lambda appears to yield the “best” model?

When lambda is 0.1, the model appears to yield the best.