

In this project, you will derive the general formulas for the slope and  $y$ -intercept of a least squares line, implement these calculations in Python, and verify results with sample data. This project explores mathematical derivation, Python implementation, and comparison with numerical optimization methods like gradient descent.

**Requirements:** Submit your project in PDF format, including code snippets and explanations.

**Due Date:** December 1st at 5PM

**Preparation:** Complete `PartI_differentiation.ipynb` and `PartII_autograd.ipynb`

### Tasks:

Assume that you have  $n$  data points  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , with the equation of the least squares line given by  $y = b + mx$ .

#### 1. Create Example Data

To create a synthetic dataset, let's generate  $x$ -values and corresponding  $y$ -values with some added noise. Use the code below to create a set of points that should roughly lie on a line. You may choose different values for the true slope and intercept.

```

1      import numpy as np
2      import random
3
4      # Set a seed for reproducibility
5      np.random.seed(42)
6
7      # Generate x-values
8      x = np.linspace(0, 10, 50)
9      # Define the true slope and intercept
10     true_m = 2
11     true_b = 5
12     # Generate y-values with some noise
13     y = true_b + true_m * x + np.random.normal(0, 1, len(x))

```

Write Python code to plot the example data and plot the line given by  $y = \text{true\_b} + \text{true\_m} \times x$ .

#### 2. Modeling the Least Squares Line

- For each data point  $(x_i, y_i)$ , show that the corresponding point on the least squares line has a  $y$ -coordinate of  $b + mx_i$ .
- Implement a Python function, `y_predicted(x, b, m)`, that calculates  $b + mx$  for a given  $x$ ,  $b$ , and  $m$ .

#### 3. Calculating Squared Distances

- Show that for each data point  $(x_i, y_i)$ , the square of the vertical distance from it to the point on the line is  $(y_i - (b + mx_i))^2$ .

- (b) Write a Python function, `squared_distance(y, y_pred)`, to compute  $(y - y_{\text{predicted}})^2$  for values  $y$  and  $y_{\text{predicted}}$ .

#### 4. Defining and Minimizing the Cost Function

- (a) Define the cost function  $f(b, m)$  as the sum of all  $n$  squared distances:

$$f(b, m) = \sum_{i=1}^n (y_i - (b + mx_i))^2.$$

Show that the partial derivatives  $\frac{\partial f}{\partial b}$  and  $\frac{\partial f}{\partial m}$  are:

$$\frac{\partial f}{\partial b} = -2 \sum_{i=1}^n (y_i - (b + mx_i)),$$

$$\frac{\partial f}{\partial m} = -2 \sum_{i=1}^n (y_i - (b + mx_i)) \cdot x_i.$$

- (b) Write three Python functions

i. `sum_of_squared_distances(x, y, b, m)`

ii. `partial_derivative_b`

iii. `partial_derivative_m`

to compute  $f(b, m)$ ,  $\frac{\partial f}{\partial b}$ , and  $\frac{\partial f}{\partial m}$ .

- (c) Write python code to compute  $\frac{\partial f}{\partial b}$ , and  $\frac{\partial f}{\partial m}$  using Symbolic differentiation and Automatic differentiation. Check your answers and compare the computation time.

#### 5. Setting Up and Solving the System of Equations

- (a) Show that setting  $\frac{\partial f}{\partial b} = 0$  and  $\frac{\partial f}{\partial m} = 0$  results in the linear system:

$$nb + \left( \sum_{i=1}^n x_i \right) m = \sum_{i=1}^n y_i,$$

$$\left( \sum_{i=1}^n x_i \right) b + \left( \sum_{i=1}^n x_i^2 \right) m = \sum_{i=1}^n x_i y_i.$$

Explain why solving for  $b$  and  $m$  minimizes the cost function.

- (b) Write a Python function, `solve_least_squares(x, y)`, to solve for  $b$  and  $m$  using this system of linear equations.

#### 6. Deriving Explicit Formulas for $b$ and $m$

- (a) Solve the equations above to derive explicit formulas for  $b$  and  $m$ :

$$b = \frac{(\sum_{i=1}^n x_i^2) \sum_{i=1}^n y_i - (\sum_{i=1}^n x_i) \sum_{i=1}^n x_i y_i}{n \sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2},$$

$$m = \frac{n \sum_{i=1}^n x_i y_i - (\sum_{i=1}^n x_i) \sum_{i=1}^n y_i}{n \sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2}.$$

- (b) Implement `solve_least_squares_formula(x, y)` in Python to calculate  $b$  and  $m$  directly from these formulas. Compare with `solve_least_squares(x, y)` on example data.

7. *Comparing with Gradient Descent*

- (a) Implement gradient descent to minimize  $f(b, m)$  by iteratively updating  $b$  and  $m$  using the partial derivatives.
- (b) Compare results from `solve_least_squares`, `solve_least_squares_formula`, and gradient descent on the example dataset. Discuss any differences in convergence and accuracy.

8. Based on your study of `PartI_differentiation.ipynb` and `PartII_autograd.ipynb`,

- (a) discuss the advantage and limitations of numerical differentiation, symbolic differentiation and automatic differentiation
- (b) summarize the connection of multivariate chain rule and backpropagation, and discuss why is backward differentiation efficient for optimizing neural networks