Weeks 2 and 3: Optimization Problems in Machine Learning and Linear Regression via Gradient Descent

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Introduction

This document explores fundamental optimization problems in machine learning:

- **Formulating the Mean as an Optimization Problem**: We derive the arithmetic mean by minimizing the sum of squared errors for a set of data points.
- **Optimization of a Quadratic Function Using Gradient Descent**: We minimize a quadratic cost function using the gradient descent algorithm, demonstrating its convergence properties.
- **Linear Regression via Gradient Descent**: We optimize a linear regression model using gradient descent for a simple dataset.

Formulating the Mean as an Optimization Problem

We are given four data points:

$$x_1 = 2, \quad x_2 = 4, \quad x_3 = 6, \quad x_4 = 8.$$

1. Define the Parameter

Let

$$\theta \in \mathbb{R}$$

be a parameter representing a candidate estimate of the central value (mean) of the data.

2. Define the Cost Function

We define the objective (cost) function as the sum of squared errors:

$$J(\theta) = \sum_{i=1}^{4} (x_i - \theta)^2.$$

Substituting the data values explicitly,

$$J(\theta) = (2-\theta)^2 + (4-\theta)^2 + (6-\theta)^2 + (8-\theta)^2.$$

3. Expand the Cost Function

$$\begin{aligned} J(\theta) &= (\theta^2 - 4\theta + 4) + (\theta^2 - 8\theta + 16) + (\theta^2 - 12\theta + 36) + (\theta^2 - 16\theta + 64) \\ &= 4\theta^2 - 40\theta + 120. \end{aligned}$$

4. Compute the First Derivative

We differentiate the cost function with respect to θ:
Since $J(\theta) = 4\theta^2 - 40\theta + 120$,

$$\frac{dJ}{d\theta} = \frac{d}{d\theta}(4\theta^2 - 40\theta + 120) = 8\theta - 40.$$

5. Find the Critical Point

Setting the derivative equal to zero,

$$8\theta - 40 = 0,$$

which yields

$$\theta^* = 5.$$

6. Final Result

$$\boxed{\theta^* = 5}$$

This value coincides with the arithmetic mean of the data:

$$\frac{2+4+6+8}{4} = 5.$$

Optimization of a Quadratic Function Using Gradient Descent

We consider the problem of finding the minimum of the function

$$y = x^2 + 2x + 5.$$

This problem is solved by formulating it as an optimization problem and applying the gradient descent method.

1. Define the Optimization Problem

Let

$$\theta \in \mathbb{R}$$

be the optimization parameter.

Define the cost function:

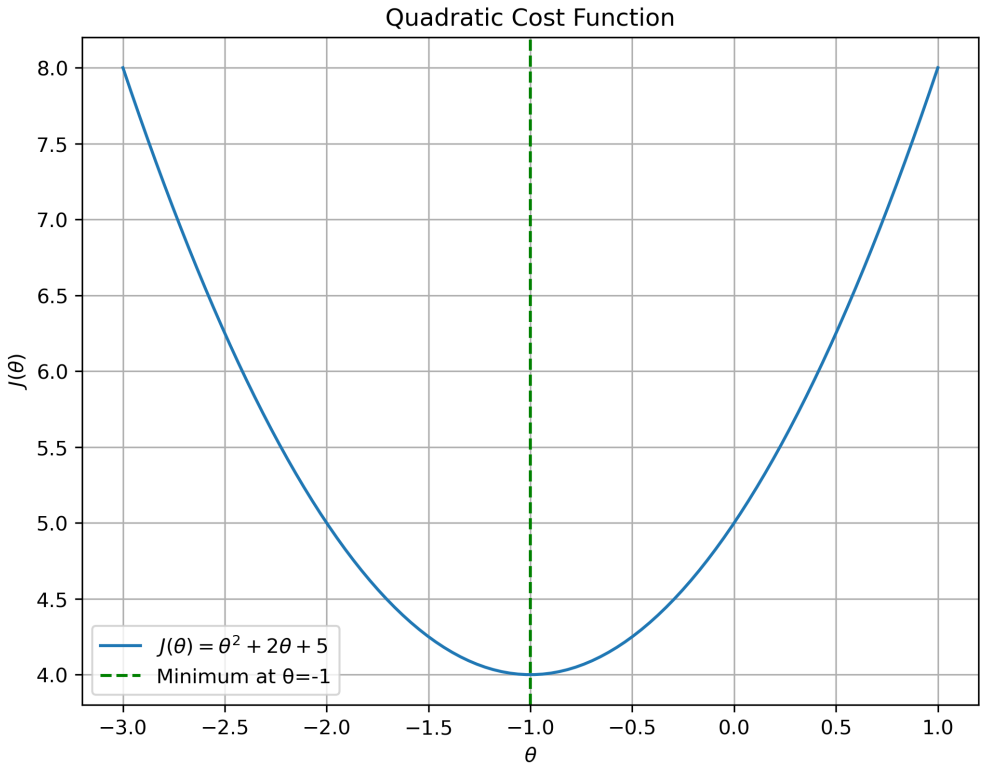
$$J(\theta) = \theta^2 + 2\theta + 5.$$

Our goal is to find the value of θ that minimizes $J(\theta)$.

2. Plotting $J(\theta)$ vs. θ

The function $J(\theta)$ is a quadratic polynomial with a positive coefficient on θ^2, so its graph is a parabola that opens upward and has a single global minimum.

From the graph, we can see that the minimum occurs at $\theta = -1$ with $J(-1) = 4$. We are now going to setup and solve for these using gradient descent.



3. Gradient Descent Solution

Compute the Gradient

Differentiate the cost function with respect to θ:

Since $J(\theta) = \theta^2 + 2\theta + 5$,

$$\frac{dJ}{d\theta} = \frac{d}{d\theta}(\theta^2 + 2\theta + 5) = 2\theta + 2.$$

Gradient Descent Update Equation

The gradient descent update rule is given by:

$$\theta_{k+1} = \theta_k - \alpha \frac{dJ}{d\theta}\bigg|_{\theta=\theta_k}.$$

Here, α is the learning rate that determines the step size in each iteration, and $\frac{dJ}{d\theta}$ is the gradient of the cost function, which points in the direction of the steepest ascent. Subtracting it moves us towards the minimum.

Substituting the gradient expression, we obtain:

$$\theta_{k+1} = \theta_k - \alpha(2\theta_k + 2).$$

Choose Parameters

The gradient descent parameters are:

- Initial value: $\theta_0 = 0$
- Learning rate: $\alpha = 0.4$

Iteration 1

Using the update equation,

$$\theta_1 = \theta_0 - 0.4(2\theta_0 + 2).$$

Substituting $\theta_0 = 0$,

$$\theta_1 = 0 - 0.4(2) = -0.8.$$

Iteration 2

$$\theta_2 = \theta_1 - 0.4(2\theta_1 + 2).$$

Substituting $\theta_1 = -0.8$,

$$\theta_2 = -0.8 - 0.4(0.4) = -0.96.$$

Iteration 3

$$\theta_3 = \theta_2 - 0.4(2\theta_2 + 2).$$

Substituting $\theta_2 = -0.96$,

$$\theta_3 = -0.96 - 0.4(0.08) = -0.992.$$

4. Conclusion

After three iterations of gradient descent, the parameter value is:

$$\theta \approx -0.992,$$

which is very close to the exact analytical minimum:

$$\boxed{\theta^* = -1}$$

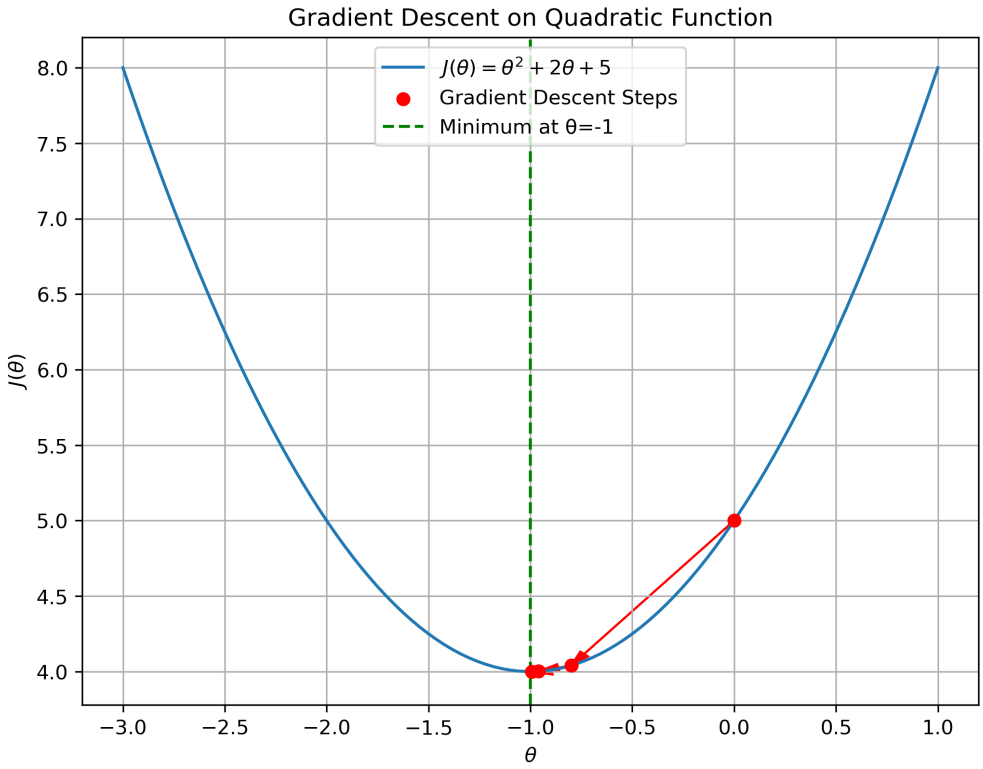
The minimum value of the function is:

$$\boxed{J(\theta^*) = 4}$$

This demonstrates that gradient descent with a sufficiently large learning rate can converge rapidly for a convex quadratic function.

5. Visualization of Gradient Descent

The following plot illustrates the gradient descent iterations on the cost function:



Linear Regression via Gradient Descent

Introduction

This section explores linear regression optimization using gradient descent for a simple dataset of three data points.

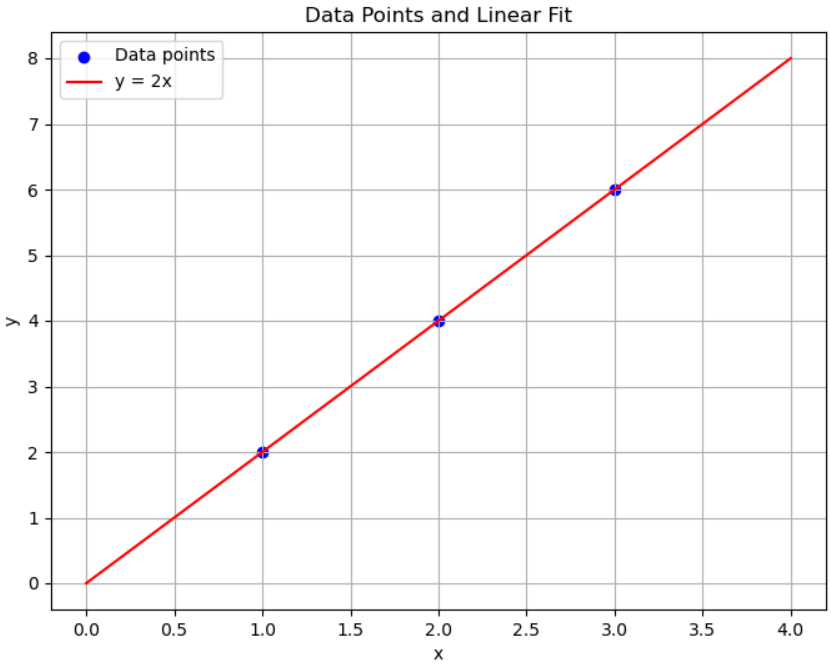
We are given the data points

$$(x, y) = (1, 2),\ (2, 4),\ (3, 6).$$

From inspection, the output variable y is exactly twice the input variable x for all data points. Therefore, we expect the optimal linear relationship to be

$$y = 2x,$$

which suggests that the optimal parameter value should be $\theta = 2$. Next we will verify this result by explicitly formulating and solving a linear regression optimization problem using gradient descent.



1. Model Assumption

We use a linear model *without an intercept*:

$$h_\theta(x) = \theta x.$$

No intercept term is included because the data lie exactly on a line passing through the origin (and it makes the math a bit easier for this example). For a more complex or completed problem you would be expected to include the intercept

2. Define the Cost Function

We use the mean squared error cost function:

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x_i) - y_i)^2,$$

where $m = 3$ is the number of data points.

Substituting the data,

$$J(\theta) = \frac{1}{6} \Big[(\theta - 2)^2 + (2\theta - 4)^2 + (3\theta - 6)^2 \Big].$$

3. Gradient Descent Solution

Compute the Gradient

To compute the gradient, we need to find the derivative of the cost function $J(\theta)$ with respect to θ.

The cost function is:

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x_i) - y_i)^2,$$

where $h_\theta(x_i) = \theta x_i$ is our linear model.

To find $\frac{dJ}{d\theta}$, we differentiate each term in the sum using the chain rule:

$$\frac{d}{d\theta} (h_\theta(x_i) - y_i)^2 = 2(h_\theta(x_i) - y_i) \cdot \frac{d}{d\theta}(\theta x_i) = 2(h_\theta(x_i) - y_i)x_i.$$

Differentiating the entire cost function:

$$\frac{dJ}{d\theta} = \frac{1}{2m} \cdot 2 \sum_{i=1}^{m} (h_\theta(x_i) - y_i)x_i = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x_i) - y_i)x_i.$$

For our data with $m = 3$, this becomes

$$\frac{dJ}{d\theta} = \frac{1}{3} \left[(\theta x_1 - y_1)x_1 + (\theta x_2 - y_2)x_2 + (\theta x_3 - y_3)x_3 \right].$$

Substituting the data,

$$\frac{dJ}{d\theta} = \frac{1}{3} \left[(\theta \cdot 1 - 2) \cdot 1 + (\theta \cdot 2 - 4) \cdot 2 + (\theta \cdot 3 - 6) \cdot 3 \right].$$

Simplifying each term:

$$\begin{aligned} (\theta - 2) \cdot 1 &= \theta - 2, \\ (2\theta - 4) \cdot 2 &= 4\theta - 8, \\ (3\theta - 6) \cdot 3 &= 9\theta - 18. \end{aligned}$$

Summing these terms:

$$(\theta - 2) + (4\theta - 8) + (9\theta - 18) = 14\theta - 28.$$

Dividing by $m = 3$:

$$\frac{dJ}{d\theta} = \frac{14\theta - 28}{3} = \frac{14}{3}\theta - \frac{28}{3} = \frac{14}{3}(\theta - 2).$$

Gradient Descent Update Rule

The gradient descent update equation is

$$\theta_{k+1} = \theta_k - \alpha \frac{dJ}{d\theta}\bigg|_{\theta=\theta_k}.$$

Substituting the gradient expression,

$$\theta_{k+1} = \theta_k - \alpha \frac{14}{3}(\theta_k - 2).$$

Choose Parameters

We choose:

- Initial value: $\theta_0 = 0$
- Learning rate: $\alpha = 0.3$

Iteration 1

$$\theta_1 = 0 - 0.3\left(\frac{14}{3}(0 - 2)\right) = 2.8.$$

Iteration 2

$$\theta_2 = 2.8 - 0.3\left(\frac{14}{3}(2.8 - 2)\right) = 1.68.$$

Iteration 3

$$\theta_3 = 1.68 - 0.3\left(\frac{14}{3}(1.68 - 2)\right) \approx 2.13.$$

4. Conclusion

After three iterations of gradient descent, the parameter value is

$$\theta \approx 2.13,$$

which is clearly converging toward the expected optimal value

$$\theta^* = 2.$$

The resulting model,

$$h(x) = 2x,$$

exactly captures the linear relationship in the data, yielding zero prediction error.

5. Visualization of Gradient Descent

The following plot illustrates the gradient descent iterations on the cost function: