Lecture 14 (part 1): Iterative Optimization with Gradient Descent

COMP90049
Introduction to Machine Learning
Semester 1, 2023

Lea Frermann, CIS

Finding Optimal Points I

Finding the parameters that optimize a **target**

Ex1: Estimate the study time which leads to the **best grade** in COMP90049.

Ex2: Find the shoe price which leads to **maximum profit** of our shoe shop.

Ex3: Predicting **housing prices** from a weighted combination of house age and house location

Ex4: Find the parameters θ of a spam classifier which lead to the **lowest error**

Ex5: Find the parameters θ of a spam classifier which lead to the **highest data log likelihood**

Recipe for finding Minima / Maxima

1. Define your function of interest $f(x)$ (e.g., data log likelihood)
2. Compute its first derivative wrt its input x
3. Set the derivative to zero
4. Solve for x

Closed-form vs Iterative Optimization

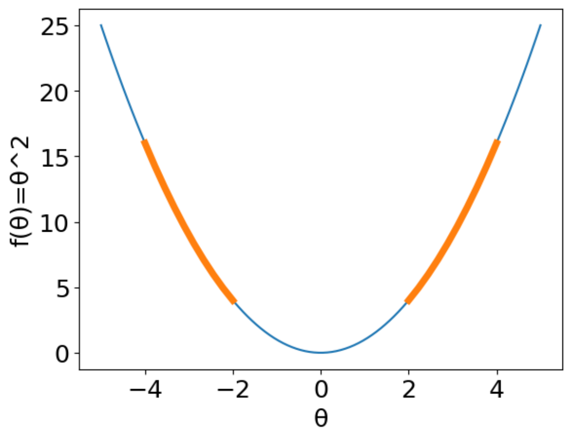
Closed-form solutions

- Previously, we computed the **closed form** solution for the MLE of the binomial distribution
- We follow our recipe, and arrive at a single solution

Unfortunately, life is not always as easy

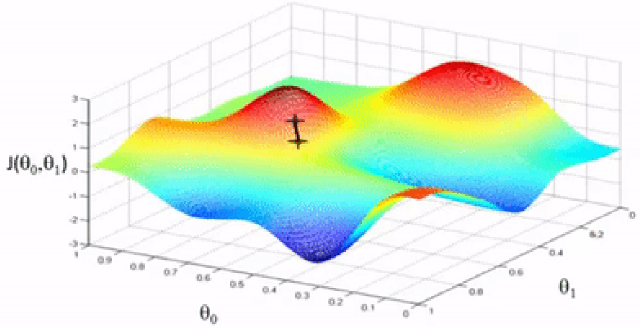
- Often, no closed-form solution exists
- Instead, we have to **iteratively** improve our estimate of $\hat{\theta}$ until we arrive at a satisfactory solution
- Gradient descent is one popular iterative optimization method

'Descending' the function to find the Optimum



- 1-dimensional case: find parameter θ that minimizes the function
- follow the curvature of the line step by step

‘Descending’ the function to find the Optimum



- 2-dimensional case: find parameters $\theta = [\theta_0, \theta_1]$ that minimize the function J
- follow the curvature step by step along the steepest way

Source: `https://medium.com/binaryandmore/beginners-guide-to-deriving-and-implementing-backpropagation-e3c1a5a1e536`

Intuition

- Descending a mountain (aka. our function) as fast as possible: at every position take the next step that takes you most directly into the valley
- We compute a series of solutions $\theta^{(0)}, \theta^{(2)}, \theta^{(3)}, \ldots$ by 'walking' along the function and taking steps in the direction with the steepest local slope (or gradient).
- each solution depends on the current location

Gradient Descent: Details

Learn the model parameters θ

- such that we **minimize the error**
- traverse over the loss function step by step ('descending into a valley')
- we would like an algorithm that tells how to update our parameters

$$\theta \leftarrow \theta + \triangle\theta$$

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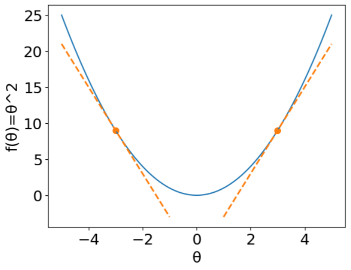
- $\triangle\theta$ is the **derivative** $\frac{\partial f}{\partial \theta}$
- tells us how much f changes in response to a change in θ.
- a measure of the **slope** or **gradient** of a function f at point θ
- the **gradient** points to the greatest **increase** of a function



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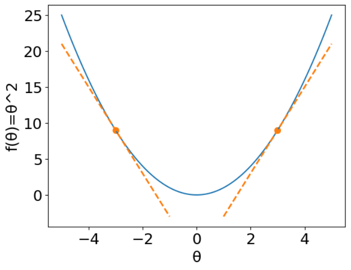
- if $\frac{\partial f}{\partial \theta} > 0$: $f(\theta) : \nearrow$ as $\theta : \nearrow$
- if $\frac{\partial f}{\partial \theta} < 0$: $f(\theta) : \nearrow$ as $\theta : \searrow$
- if $\frac{\partial f}{\partial \theta} = 0$: we are at a minimum
- so, to approach the minimum:

$$\theta \leftarrow \theta - \eta \frac{\partial f}{\partial \theta}$$



Gradient Descent for multiple parameters

- Usually, our models have **several parameters** which need to be optimized to minimize the error
- We compute **partial derivatives** of $f(\theta)$ wrt. individual θ_i
- Partial derivatives measure change in a function of multiple parameters given a change in a single parameter, with all others held constant
- For example for $f(\theta_1, \theta_2)$ we can compute $\frac{\partial f}{\partial \theta_1}$ and $\frac{\partial f}{\partial \theta_2}$
- We then **update each parameter individually**

$$\theta_1 \leftarrow \theta_1 + \triangle\theta_1 \quad \text{with } \triangle\,\theta_1 = -\eta\frac{\partial f}{\partial \theta_1}$$

$$\theta_2 \leftarrow \theta_2 + \triangle\theta_2 \quad \text{with } \triangle\,\theta_2 = -\eta\frac{\partial f}{\partial \theta_2}$$

Gradient Descent: Recipe

Recipe for Gradient Descent (single parameter)

1: Define objective function $f(\theta)$
2: Initialize parameter $\theta^{(0)}$
3: **for** iteration $t \in \{0, 1, 2, \ldots T\}$ **do**
4: Compute the first derivative of f at that point $\theta^{(t)}$: $\frac{\partial f}{\partial \theta^{(t)}}$
5: Update your parameter by subtracting the (scaled) derivative

$$\theta^{(t+1)} \leftarrow \theta^{(t)} - \eta \frac{\partial f}{\partial \theta^{(t)}}$$

- η is the **step size** or **learning rate**, a parameter
- When to stop? Fix number of iterations, or define other criteria

Gradient Descent: Recipe

Recipe for Gradient Descent (multiple parameters)

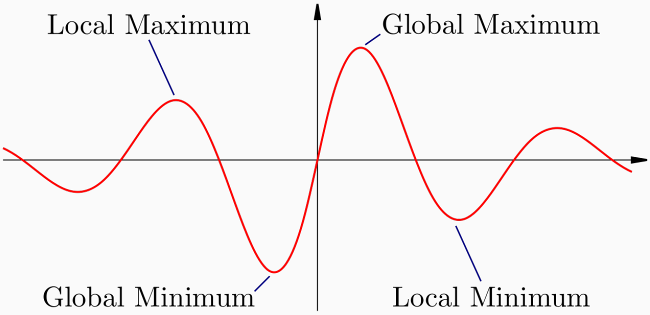
```
Define objective function f(θ)
Initialize parameters {θ_1^(0), θ_2^(0), θ_3^(0), ...}
for iteration t ∈ {0, 1, 2, ...T} do
    Initialize vector of gradients ← []
    for parameter f ∈ {1, 2, 3, ...F} do
        Compute the first derivative of f at that point θ_f^(t) : ∂f/∂θ_f^(t)
        append ∂f/∂θ_f^(t) to gradients
    Update all parameters by subtracting the (scaled) gradient
```

$$\theta^{(t+1)} \leftarrow \theta^{(t)} - \eta \frac{\partial f}{\partial \theta^{(t)}}$$

Aside: Global and Local Minima and Maxima

Possible issue: local maxima and minima!

- A function is **convex** if a line between any two points of the function lies above the function
- A global **maximum** is the single highest value of the function
- A global **minimum** is the single lowest value of the function



https://commons.wikimedia.org/wiki/File:Maxima_and_Minima.svg

Gradient Descent Guarantees

1. with an appropriate learning rate, GD will find the global minimum for differentiable convex functions
2. with an appropriate learning rate, GD will find a local minimum for differentiable non-convex functions

Equivalently, Gradient Ascent ("GA") would find the global maximum (case 1.) and local maximum (case 2.)

Summary

Now you know:

- What optimization is, and why it's important
- How to do closed-form optimization (aka. "set the derivative of $f(\theta)$ to zero and solve for θ)
- That closed-form solutions are not always computable
- In that case, iterative optimization can help us
- Gradient descent is one instance of an iterative optimization method
- How gradient descent works!

Next lecture(s)

- Logistic Regresion
- The perceptron
- Neural networks

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