Lecture 7 (part 1): Iterative Optimization with Gradient Descent

COMP90049
Introduction to Machine Learning
Semester 1, 2020

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Roadmap

So far...

- Naive Bayes Classifier – theory and practice
- MLE estimation of parameters
- Exact optimization

Now: Quick aside on iterative optimization

- Gradient Descent
- Global and local optima

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**

Objective functions

Find parameter values θ that maximize (or minimize) the value of a function $f(\theta)$

- we want to find the **extreme** points of the **objective function**. Depending on our **target**, this could be
- ...the **maximum**
  E.g., the **maximum** profit of our shoe shop
  E.g., the **largest** possible (log) likelihood of the data

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}} f(\theta)$$

- ...or the **minimum** (in which case we often call f a **loss function**)
  E.g., the **smallest** possible classification error

$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}} f(\theta)$$

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

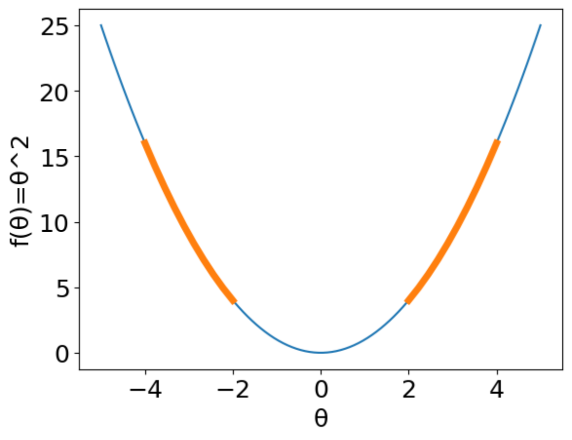
Closed-form solutions

- 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

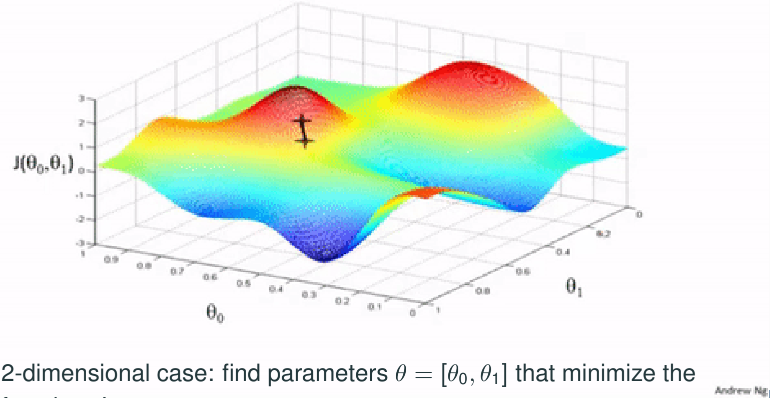
- Often, no closed-form solution exists
- Instead, we have to **iteratively** improve our estimate of $\hat{\theta}$ until we arrive at a satisfactory solution
- Gradient descent is one popular iterative optimization method

‘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`

Gradient Descent: Intuition

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 $\theta^{(0)}, \theta^{(2)}, \theta^{(3)}, ...$ 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

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

Gradient Descent: Details

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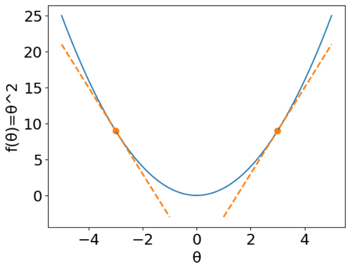
$$\theta \leftarrow \theta + \triangle\theta$$

- $\triangle\theta$ is the **derivative**, a measure of change in the input function given an change in θ
- for a function $f(\theta)$, $\frac{\partial f}{\partial \theta}$ tells us how much f changes in response to a change in θ.
- the derivative measures the **slope** or **gradient** of a function f at point θ



Gradient Descent: Details

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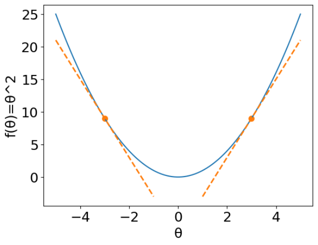
$$\theta \leftarrow \theta + \triangle\theta$$

- if $\frac{\partial f}{\partial x} > 0$: $f(\theta)$ increases as θ increases
- if $\frac{\partial f}{\partial x} < 0$: $f(\theta)$ increases as θ decreases
- if $\frac{\partial f}{\partial x} = 0$: we are at a minimum (or maximum)
- 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 $\frac{\partial f}{\partial \theta_2}$

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- 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**

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

$$\theta_2 \leftarrow \theta_1 + \triangle\theta_2 \quad \text{with } \triangle\,\theta_2 = -\eta\frac{\partial f}{\partial \theta_2}$$

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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)

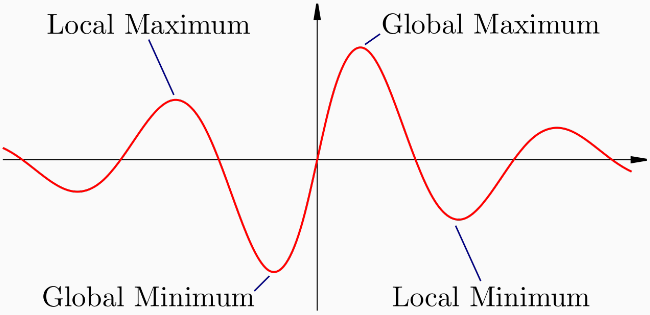
Define objective function $f(\theta)$
Initialize parameters $\{\theta_1^{(0)}, \theta_2^{(0)}, \theta_3^{(0)}, \dots\}$
for iteration $t \in \{0, 1, 2, ...T\}$ **do**
    Initialize vector of *gradients* $\leftarrow$ []
    for parameter $f \in \{1, 2, 3, ...F\}$ **do**
        Compute the first derivative of f at that point $\theta_f^{(t)}$: $\frac{\partial f}{\partial \theta_f^{(t)}}$
        append $\frac{\partial f}{\partial \theta_f^{(t)}}$ 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!

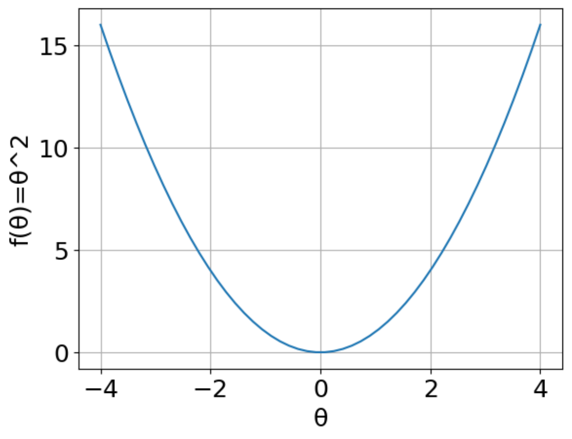
- A function is **convex** if a line between any two points of the function lies above the function
- A global **maximum** is the single highest value of the function
- A global **minimum** is the single lowest value of the function



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

Aside: Global and Local Minima and Maxima

Possible issue: local maxima and minima!



- Convex?
- How many global minima? global maxima?
- How many local minima? local maxima?

Aside: Global and Local Minima and Maxima

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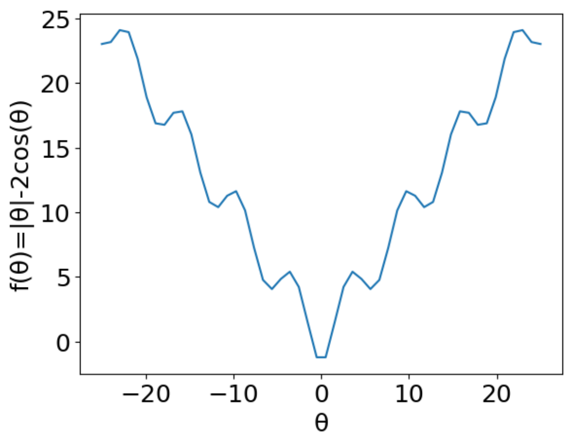

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- How many global minima? global maxima?
- How many local minima? local maxima?

Gradient Descent Guarantees

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

Summary

This aside:

- Iterative optimization
- Gradient descent

Next lecture(s)

- Classifiers which do not have a closed-form solution for their paramters
- Logistic Regresion
- (later) the perceptron, and neural networks