

# Mathematics for Machine Learning

## — Continuous Optimization: Gradient Descent and Constrained Optimization

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## Credits for the resource

- The slides are based on the textbooks:
  - *Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.*
  - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. Wiley. 2019.*
- We could partially refer to the monograph:  
*Francesco Orabona: A Modern Introduction to Online Learning.*  
<https://arxiv.org/abs/1912.13213>

# Outline

- 1 Preface / Introduction
- 2 Optimization Using Gradient Descent
  - Gradient Descent with Momentum
  - Stochastic Gradient Descent
- 3 Constrained Optimization

# Motivation

- **Machine** learning algorithms are solving mathematical formulations which are expressed as **numerical optimization** methods.
- We focus on basic numerical methods for training machine learning models.
  - This boils down to *finding a “good” set of parameters*.
  - Goodness: determined by the objective function or the probabilistic model.
- Given an objective function, finding the best value of parameters is done using **optimization algorithms**.

# Remark

- We will discuss two branches of continuous optimization:
  - Unconstrained optimization.
  - Constrained optimization.
- Assume that the objective functions are **differentiable**.
- We focus on “minimization” objectives.
- We will make use of the “gradients”.

## Example

Consider the loss function  $\ell(x) = x^4 + 7x^3 + 5x^2 - 17x + 3$ .

The gradient:

$$\frac{d\ell(x)}{dx} = 4x^3 + 21x^2 + 10x - 17.$$

The second derivative:

$$\frac{d^2\ell(x)}{dx^2} = 12x^2 + 42x + 10.$$

Solving  $\frac{d\ell(x)}{dx} = 0$  we get  $x = -4.5, -1.4$ , or  $0.7$ .

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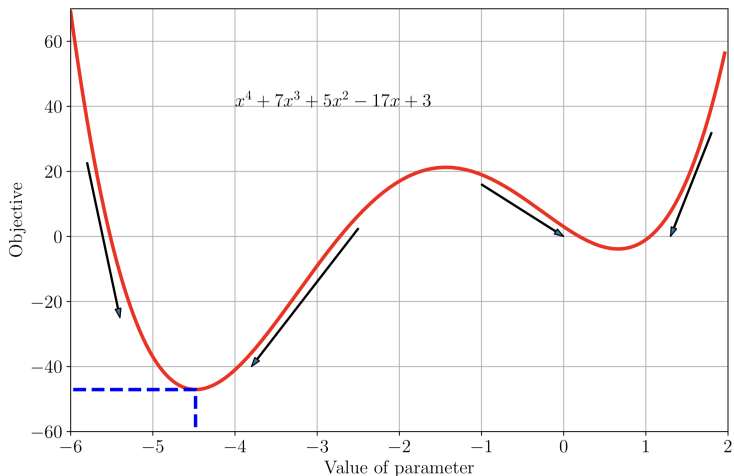
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Solving  $\frac{d\ell(x)}{dx} = 0$  we get  $x = -4.5, -1.4$ , or  $0.7$ .

By checking whether  $\frac{d^2\ell(x)}{dx^2}$  is positive or negative at the stationary point(s), we know  $x = -1.4$  is a (local) maximum.

# Function Plot & Negative Gradients of Univariate $\ell(x)$

Start at some  $x_0$ , and then the negative gradient leads us to some (local) minimum.





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- For **convex functions**, there is no such a tricky dependency on the starting point.
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  - Minimization objective  $\implies$  follows the negative gradient  $\implies$  “gradient descent”.
  - Maximization objective  $\implies$  follows the (positive) gradient  $\implies$  “gradient ascent”.
- For optimization in higher dimensions, it is almost impossible to visualize the idea of gradients, descent directions and optimal values.

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# The Problem

Solving for the minimum of a real-valued function

$$\min_{\mathbf{x}} f(\mathbf{x}),$$

where  $f: \mathbb{R}^d \mapsto \mathbb{R}$  is the objective function which is assumed to be differentiable.

# Gradient Descent

- Gradient descent is a first-order optimization algorithm.

## Gradient Descent

- Starting at a particular location  $\mathbf{x}_0$ .

The algorithm runs iteratively by giving

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t((\nabla f)(\mathbf{x}_t)).$$

where  $\gamma \geq 0$  is called the **step-size** (or **learning rate**).

**Goal:**  $f(\mathbf{x}_0) \geq f(\mathbf{x}_1) \geq \dots$  converges to a **local minimum**.

## Example (1/2)

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Consider

$$f\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \begin{bmatrix} 2 & 1 \\ 1 & 20 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} 5 \\ 3 \end{bmatrix}^\top \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}.$$

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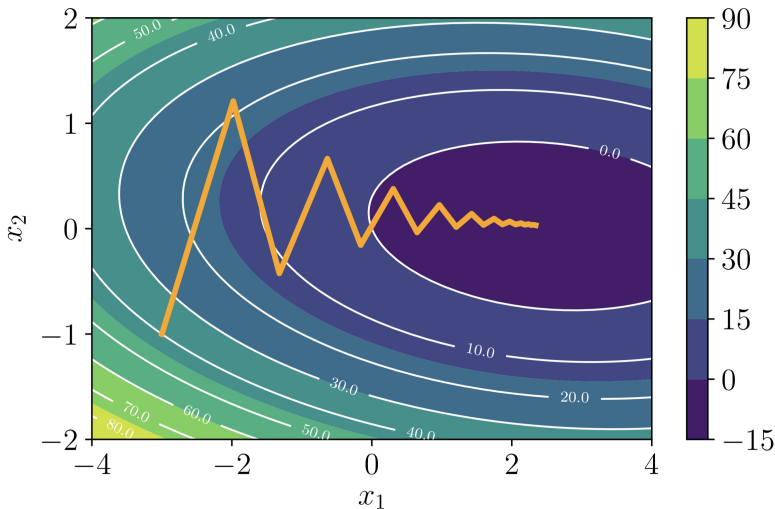
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Running gradient descent and starting at  $\mathbf{x}_0 = [-3, -1]^\top$ , what's  $\mathbf{x}_1$ ?  
And what's  $\mathbf{x}_2$ ?

## Example (2/2)



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$$\frac{df}{dt} = \mathbf{0}.$$

But

$$\frac{df}{dt} = \frac{df}{d\gamma} \frac{d\gamma}{dt} = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \end{bmatrix} \begin{bmatrix} \frac{\partial x}{\partial t} \\ \frac{\partial y}{\partial t} \end{bmatrix} = \langle \nabla_{\gamma} f, \nabla_t \gamma(t) \rangle$$

## On the Step-size

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- Adaptive gradient descent: rescale the step-size  $\gamma$  at each iteration.
- Two simple heuristics:
  - When the function value  $\uparrow$  after a gradient step  $\implies$  undo the step and decrease the step-size.
  - When the function value  $\downarrow$  after a gradient step  $\implies$  try to increase the step-size.



## Another Example: Solving a Linear Equation System

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$$\ell(\mathbf{x}) = \|\mathbf{Ax} - \mathbf{b}\|^2 = (\mathbf{Ax} - \mathbf{b})^\top (\mathbf{Ax} - \mathbf{b})$$

where  $\|\cdot\|$  is the  $\ell_2$ -norm.

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# Gradient Descent with Momentum

- The convergence of gradient descent could be slow due to the curvature of the optimization surface.
- **Idea:** Give gradient descent some *memory*.
  - Introducing an additional term to remember what happened in the previous iteration.
- The steps (for  $\alpha \in [0, 1]$ ):

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t((\nabla f)(\mathbf{x}_t))^T + \alpha \Delta \mathbf{x}_t$$

$$\Delta \mathbf{x}_t = \mathbf{x}_t - \mathbf{x}_{t-1}$$

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# Stochastic Gradient Descent (1/5)

Motivation:

- Computing the gradient can be very time consuming.
- Approximating the gradient is useful.
  - We aim at only knowing a noisy approximation to the gradient.

## Stochastic Gradient Descent (2/5)

The objective function:

$$L(\boldsymbol{\theta}) = \sum_{i=1}^N L_i(\boldsymbol{\theta}),$$

which is sum of losses  $L_i$  incurred by each sample  $i$ .  $\boldsymbol{\theta}$  is the vector of parameters of interest.

- **Goal:** Find  $\boldsymbol{\theta}$  that minimizes  $L$ .

### Example: log-likelihoods

$$L(\boldsymbol{\theta}) = - \sum_{i=1}^N \log p(y_i | \mathbf{x}_i, \boldsymbol{\theta}),$$

for the training inputs  $\mathbf{x}_i \in \mathbb{R}^D$ , training targets  $y_i$ , and the parameters  $\boldsymbol{\theta}$  of the model.

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Updating  $\theta$ :

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### Issues

When training set is enormous or no simple formulas exist for evaluating the (sum of) gradients.

## Stochastic Gradient Descent (4/5)

**Idea:** Consider taking a sum of a **smaller** set of  $L_n$ .

- For  $i = 1, 2, \dots, N$ , randomly choose a subset of  $L_i$  for **mini-batch** gradient descent.

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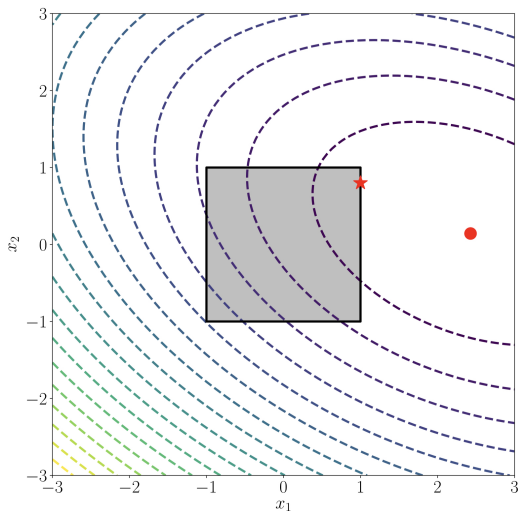
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  - Quick to estimate.
  - Noisy estimate allows us to get out of some bad local optima.
  - Good for generalization.

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The objective function:

$$\begin{aligned} & \min_{\mathbf{x}} f(\mathbf{x}) \\ & \text{subject to } g_i(\mathbf{x}) \leq 0, \text{ for all } i = 1, \dots, m. \end{aligned}$$

**Note:**  $f$  and  $g_i$  could be non-convex in general.

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## An Easy Unconstrained Objective

$$J(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^m \mathbf{1}(g_i(\mathbf{x})),$$

where  $\mathbf{1}(z)$  is an infinite step function  $\mathbf{1}(z) = \begin{cases} 0 & \text{if } z \leq 0 \\ \infty & \text{otherwise} \end{cases}$ .



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The infinite step function is difficult to optimize...

## A Workaround Approach: Lagrange Multipliers

For  $\lambda_i \geq 0$ , define

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \sum_{i=1}^m \lambda_i g_i(\mathbf{x})$$

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- $\mathbf{x}$ : primal variables.
- $\boldsymbol{\lambda}$ : dual variables.

# Primal & Dual Problems

## The primal problem

$$\begin{aligned} & \min_{\mathbf{x}} f(\mathbf{x}) \\ & \text{subject to } g_i(\mathbf{x}) \leq 0, \text{ for } i \in [m]. \end{aligned}$$

## The dual problem

$$\begin{aligned} & \max_{\boldsymbol{\lambda} \in \mathbb{R}^m} \mathcal{D}(\boldsymbol{\lambda}) \\ & \text{subject to } \boldsymbol{\lambda} \geq \mathbf{0}. \end{aligned}$$

$$\mathcal{D}(\boldsymbol{\lambda}) := \min_{\mathbf{x} \in \mathbb{R}^d} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}).$$

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- This is **unconstrained** optimization problem for a **given value of  $\boldsymbol{\lambda}$** .  
 $(\boldsymbol{\lambda} \geq \mathbf{0} \Leftrightarrow \lambda_i \geq 0 \text{ for each } i)$



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( $\boldsymbol{\lambda} \succeq \mathbf{0} \Leftrightarrow \lambda_i \geq 0$  for each  $i \Leftrightarrow \boldsymbol{\lambda} \succeq \mathbf{0}$ )

# Minimax Inequality

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For any function  $\varphi$  with two arguments  $\mathbf{x}, \mathbf{y}$ ,

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- Consider the inequality

$$\text{For all } \mathbf{x}_0, \mathbf{y}_0, \quad \min_{\mathbf{x}} \varphi(\mathbf{x}, \mathbf{y}_0) \leq \max_{\mathbf{y}} \varphi(\mathbf{x}_0, \mathbf{y}).$$

- This implies that

$$\min_{\mathbf{x} \in \mathbb{R}^d} \max_{\lambda \geq 0} \mathcal{L}(\mathbf{x}, \lambda) \geq \max_{\lambda \geq 0} \min_{\mathbf{x} \in \mathbb{R}^d} \mathcal{L}(\mathbf{x}, \lambda).$$

Compare  $J(\mathbf{x})$  with  $\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda})$ 

$$J(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^m \mathbf{1}(g_i(\mathbf{x})), \text{ where } \mathbf{1}(z) = \begin{cases} 0 & \text{if } z \leq 0 \\ \infty & \text{otherwise} \end{cases}$$

v.s.

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# Computation Issues

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  - The outer problem of maximization over  $\boldsymbol{\lambda}$  can be efficiently computed.  
( $\mathcal{D}(\boldsymbol{\lambda})$  is concave so finding the maximum is easy).

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$$h_j(\mathbf{x}) = 0 \implies \begin{cases} h_j(\mathbf{x}) \leq 0 & \text{and} \\ -h_j(\mathbf{x}) \leq 0. \end{cases}$$

# Discussions