

Mathematics for Machine Learning

— Continuous Optimization

Gradient Descent and Constrained Optimization

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Fall 2025

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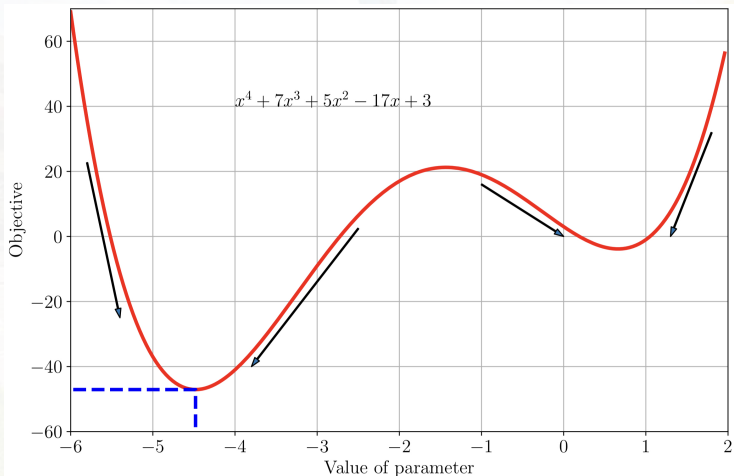
$$\frac{d^2\ell(x)}{dx^2} = 12x^2 + 42x + 10.$$

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

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.



Heads Up

- 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”.

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- For “maximization” objectives, we shall follow the (positive) gradients.
 - 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)

Example

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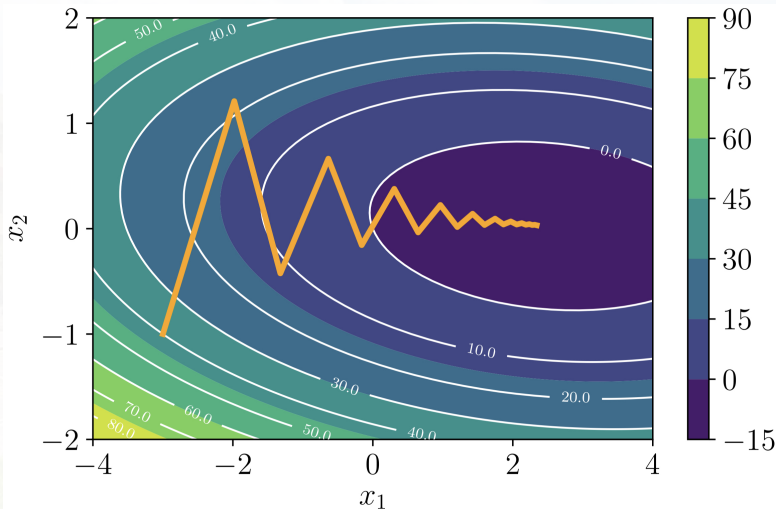
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Running gradient descent and starting at $\mathbf{x}_0 = [-3, -1]^\top$, what's \mathbf{x}_1 ?
And what's \mathbf{x}_2 ?

Example (2/2)



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 - A **contour** of f : $f(\gamma(t)) = C$ for some constant $C \in \mathbb{R}$.

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

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

- Adaptive gradient descent: rescale the step-size γ at each iteration.

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- Adaptive gradient descent: rescale the step-size γ 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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Consider $\mathbf{Ax} = \mathbf{b}$.

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- We want to find the solution *approximately* by minimizing the squared error

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

where $\|\cdot\|$ is the ℓ_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 $\alpha \in [0, 1]$):

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

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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

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

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

Stochastic Gradient Descent (3/5)

Updating θ :

$$\theta_{t+1} \leftarrow \theta_t - \gamma_t (\nabla L(\theta_t))^T$$

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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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- Reasons:
 - We only require the gradient to be an unbiased estimate of the true gradient.

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

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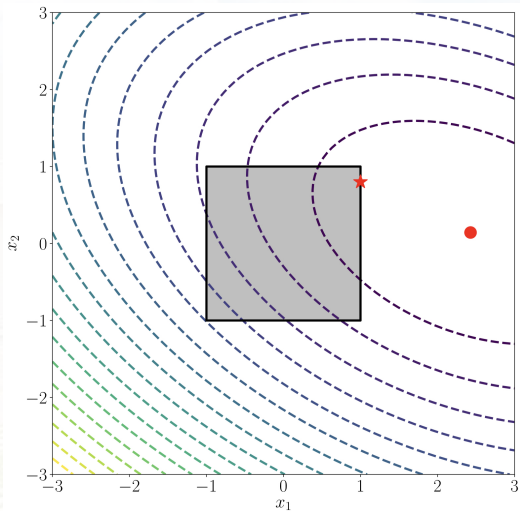
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- Benefits for mini-batch:
 - Quick to estimate.
 - Noisy estimate allows us to get out of some bad local optima.
 - Good for generalization.

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

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

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

The dual problem

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

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($\boldsymbol{\lambda} \geq \mathbf{0} \Leftrightarrow \lambda_i \geq 0$ 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 φ with two arguments \mathbf{x}, \mathbf{y} ,

$$\max_{\mathbf{y}} \min_{\mathbf{x}} \varphi(\mathbf{x}, \mathbf{y}) \leq \min_{\mathbf{x}} \max_{\mathbf{y}} \varphi(\mathbf{x}, \mathbf{y}).$$

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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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- Recall the original problem:

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

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

v.s.

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \boldsymbol{\lambda}^\top \mathbf{g}(\mathbf{x}).$$

- $\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda})$ is a lower bound of $J(\mathbf{x})$.
 $\therefore J(\mathbf{x}) = \max_{\boldsymbol{\lambda} \geq 0} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda})$.

- Recall the original problem:

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

Hence,

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

Computation Issues

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

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- $\mathcal{D}(\boldsymbol{\lambda}) = \min_{\mathbf{x} \in \mathbb{R}^d} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda})$: pointwise minimum of affine functions of $\boldsymbol{\lambda}$.
 - The outer problem of maximization over $\boldsymbol{\lambda}$ can be efficiently computed.
($\mathcal{D}(\boldsymbol{\lambda})$ is concave so finding the maximum is easy).

Remark

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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