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.*
  - *Arnold J. Insel, Lawrence E. Spence, Stephen H. Friedberg: Linear Algebra, 4th Edition. Prentice Hall. 2013.*
  - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra, 12th Edition. 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:

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

The second derivative:

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

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

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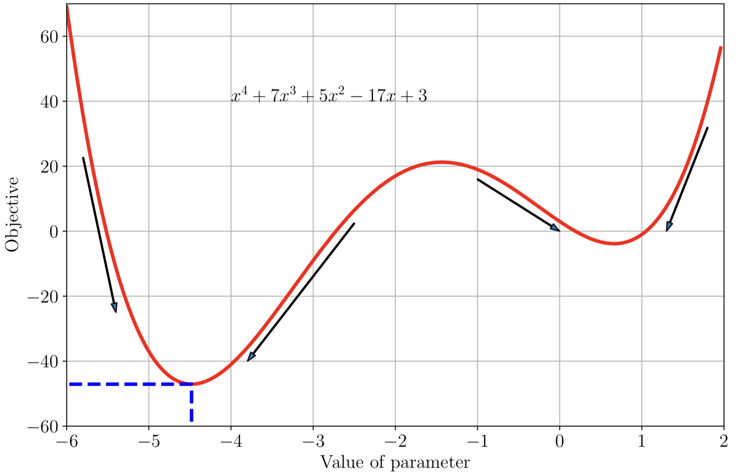
By checking whether $\frac{\mathrm{d}^2\ell(x)}{\mathrm{d}x^2}$ is positive or negative at the stationary point(s), we know $x = -1.4$ is a (local) maximum.

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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  - Maximization objective $\Longrightarrow$ follows the (positive) gradient $\Longrightarrow$ "gradient ascent".

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    - Minimization objective $\Longrightarrow$ follows the negative gradient $\Longrightarrow$ "gradient descent".
    - Maximization objective $\Longrightarrow$ follows the (positive) gradient $\Longrightarrow$ "gradient ascent".
- For optimization in higher dimensions, it is almost impossible to visualize the idea of gradients, descent directions and optimal values.

Outline

The Problem

Solving for the minimum of a real-valued function

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

where $f : \mathbb{R}^d \to \mathbb{R}$ 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: $f(\mathbf{x}_0) \geq f(\mathbf{x}_1) \geq \cdots$ 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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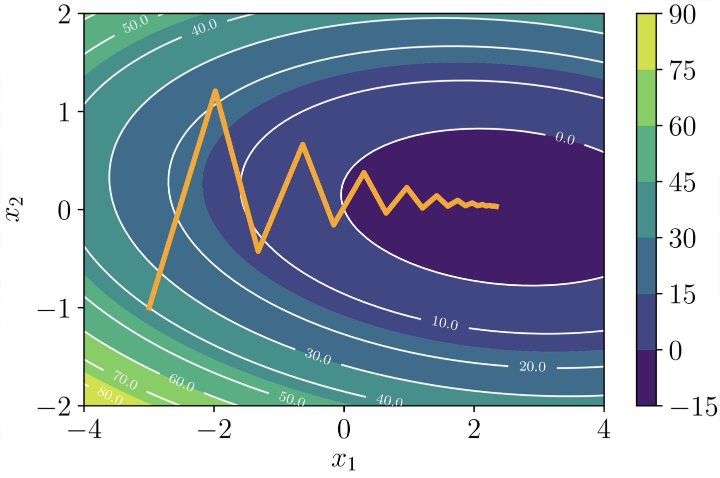
Running gradient descent and starting at $\mathbf{x}_0 = [-3, \ -1]^\top$, what's $\mathbf{x}_1$? And what's $\mathbf{x}_2$?

Example (2/2)


2
1
0
−1
−2
x_2
−4
−2
0
2
4
x_1
50.0
40.0
0.0
10.0
30.0
20.0
70.0
60.0
80.0
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40.0
90
75
60
45
30
15
0
−15

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$$\frac{\mathrm{d}f}{\mathrm{d}t} = \mathbf{0}.$$

But

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

On the Step-size

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

On the Step-size

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

Another Example: Solving a Linear Equation System

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Consider $\boldsymbol{A}\mathbf{x} = \mathbf{b}$.

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

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

  where $\|\cdot\|$ is the ℓ_2-norm.

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Okay, this is just an example and somehow not a good idea because there is an analytic solution. (Solving $\nabla_{\mathbf{x}}\ell(\mathbf{x}) = \mathbf{0}$)

Outline

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 $\alpha \in [0, 1]$):

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

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\end{aligned}
$$

Outline

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.

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Updating $\boldsymbol{\theta}$:

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

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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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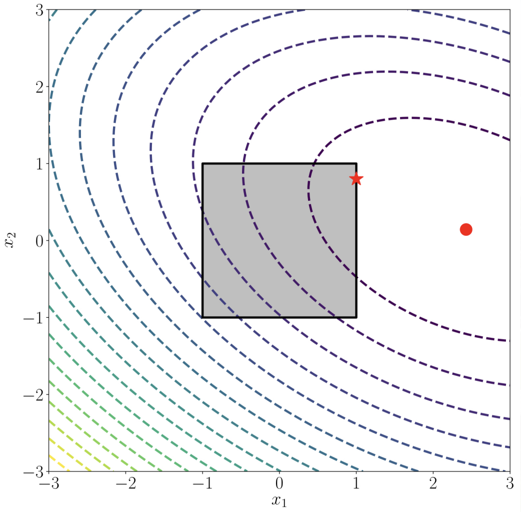
Constrained Optimization



Constrained Optimization

The objective function:

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

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 $\boldsymbol{\lambda}_i \geq 0$, 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

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

The dual problem

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

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

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

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For any function φ 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

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

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

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

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- Recall the original problem:

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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.

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

- $\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda})$ is a lower bound of $J(\mathbf{x})$.
  $\therefore\ J(\mathbf{x}) = \max_{\boldsymbol{\lambda} \geq \mathbf{0}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda})$.
- Recall the original problem:
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  Hence,
  $$\min_{\mathbf{x} \in \mathbb{R}^d} \max_{\boldsymbol{\lambda} \geq \mathbf{0}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) \geq \max_{\boldsymbol{\lambda} \geq \mathbf{0}} \min_{\mathbf{x} \in \mathbb{R}^d} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}).$$

Computation Issues

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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).

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- What's about "equality" constraints?

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

Discussions