Lecture Notes

MATHEMATICS FOR MACHINE LEARNING

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Latest version: `github.com/felipe-tobar/Maths-for-ML`

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NB: in this chapter, we follow (Murphy, 2022).

Optimisation is central to ML, since models are *trained* by minimising a loss function (or optimising a reward function). In general, model design involves the definition of a training objective, that is, a function that denotes how good a model is. This training objective is a function of the training data and a model, the latter usually represented by its parameters. The best model is is the chosen by optimising this function.

Example: Linear regression (LR)

In the LR setting, we aim to determine the function

$$\begin{aligned} f \colon \mathbb{R}^M &\to \mathbb{R} \\ x &\mapsto f(x) = a^\top x + b, \quad a \in \mathbb{R}^M, b \in \mathbb{R} \end{aligned} \tag{2.1}$$

conditional to a set of observations

$$\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N \subset \mathbb{R}^M \times \mathbb{R}. \tag{2.2}$$

Using least squares, the function f is chosen via minimisation of the sum of the square differences between observations $\{y_i\}_{i=1}^N$ and predictions $\{f(x_i)\}_{i=1}^N$. That is, we aim to minimise he loss:

$$J(\mathcal{D}, f) = \sum_{i=1}^N (y_i - f(x_i))^2 = \sum_{i=1}^N (y_i - a^\top x_i - b)^2. \tag{2.3}$$

[TODO: Generate figure: Check fig 1 ML lecture notes]

Example: Logistic regression

Here, we aim to determine the function

$$\begin{aligned} f \colon \mathbb{R}^M &\to \mathbb{R} \\ x &\mapsto f(x) = \frac{1}{1 + e^{-\theta^\top x + b}}, \quad \theta \in \mathbb{R}^M, b \in \mathbb{R} \end{aligned} \tag{2.4}$$

conditional to the observations

$$\mathcal{D} = \{(x_i, c_i)\}_{i=1}^N \subset \mathbb{R}^M \times \{0, 1\}. \tag{2.5}$$

The standard loss function for the classification problem is the cross entropy, given by:

$$J(\mathcal{D}, f) = -\frac{1}{N} \sum_{i=1}^N (c_i \log f(x_i) + (1 - c_i) \log(1 - f(x_i))) \tag{2.6}$$

$$= \frac{1}{N} \sum_{i=1}^N \left(\log(1 + e^{-\theta^\top x + b}) - y_i(-\theta^\top x + b) \right) \tag{2.7}$$

[TODO: Generate figure]

Example: Clustering (K-means)

Given a set of observations

$$\mathcal{D} = \{x_i\}_{i=1}^N \subset \mathbb{R}^M, \tag{2.8}$$

we aim to find cluster centres (or prototypes) $\mu_1, \mu_2, \dots, \mu_K$ and *assignment variables* $\{r_{ik}\}_{i,k=1}^{N,K}$, to minimise the following loss

$$J(\mathcal{D}, f) = \sum_{i=1}^{N} \sum_{k=1}^{K} r_{ik} ||x_i - \mu_k||^2 \tag{2.9}$$

$$\tag{2.10}$$

[TODO: Generate figure]

2.1 Terminology

We denote an optimisation problem as follows:

$$\min_{x \in \mathcal{X}} f(x) \quad \text{s.t.} \quad g_i(x) \leq 0,\ h_j(x) = 0,\ i = 1, \dots, I,\ j = 1, \dots, J. \tag{2.11}$$

We describe the components of this statement in detail:

- **Objective function:** The function $f : \mathcal{X} \to \mathbb{R}$ is the quantity to be minimised, with respect to x.
- **Optimisation variable:** Minimising f requires fining the value of x such that $f(x)$ is minimum. This is also written as

$$x_\star = \arg\min_{x \in \mathcal{X}} f(x) \quad \text{s.t.} \quad g_i(x) \leq 0,\ h_j(x) = 0. \tag{2.12}$$

- **Restrictions:** These are denoted by the functions g_i and h_i above, which describe the requirements for the optimiser in the form of equalities and inequalities, respectively.
- **Feasible region:** This is the subset of the domain that complies with the restrictions, that is

$$C = \{x \in \mathcal{X}, \quad \text{s.t.} \quad g_i(x) \leq 0,\ h_j(x) = 0,\ i = 1, \dots, I,\ j = 1, \dots, J\} \tag{2.13}$$

- **Local / global optima.** Values for the optimisation variable that solve the optimisation problem wither locally or globally. More formally:

$$x_\star \text{ is a local optima} \iff \exists \lambda > 0 \quad \text{s.t.} \quad x_\star = \arg\min_{x \in \mathcal{X} \ \text{s.t.} \ ||x - x_\star|| \leq \lambda} f(x). \tag{2.14}$$

$$x_\star \text{ is a global optima} \iff x_\star = \arg\min_{x \in \mathcal{X}} f(x). \tag{2.15}$$

Interplay between constrains and local/global optima

[TODO: generate figure, how different restrictions change the number and type of optima]

Example: XXX

[TODO: Show a few parametric functions and indicate their (closed-form) minima]

2.2 Continuous unconstrained optimisation

We will ignore constrains in this section, and we will focus on problems of the form

$$\theta \in \arg\min_{\theta \in \Theta} L(\theta). \tag{2.16}$$

We emphasise that if $\theta_\star$ satisfies the above, then

$$\forall \theta \in \Theta,\ L(\theta_\star) \leq L(\theta), \tag{2.17}$$

meaning that it is a **global** optimum. However, as this might be very hard to find, we are also interested in local optima, that is, $\theta_\star$ such that

$$\exists\, \delta > 0\ \ \forall\, \theta \in \Theta\ \text{ s.t. } \|\theta - \theta_\star\| < \delta \ \Rightarrow\ L(\theta_\star) \leq L(\theta). \tag{2.18}$$

We now review the optimality conditions.

Assumption 2.1. The loss function L is twice differentiable.

Denoting $g(\theta) = \nabla_\theta L(\theta)$ and $H(\theta) = \nabla^2_\theta L(\theta)$, we can state the following optimality conditions.

- **First order necessary condition:** If $\theta_\star$ is a local minimum, then
  - $\nabla_\theta L(\theta_\star) = 0$
- **Second order necessary condition:** If $\theta_\star$ is a local minimum, then
  - $\nabla_\theta L(\theta_\star) = 0$
  - $\nabla^2_\theta L(\theta_\star)$ is positive semidefinite
- **Second order sufficient condition:** If $\theta_\star$ is a local minimum if and only if
  - $\nabla_\theta L(\theta_\star) = 0$
  - $\nabla^2_\theta L(\theta_\star)$ is positive definite

Example: different stationary points

Let us consider the function

$$\begin{aligned} f \colon \mathbb{R}^2 &\to \mathbb{R} \\ x &\mapsto f(x) = (p-1)x^2 + (p+1)y^2, \quad p \in \mathbb{R} \end{aligned} \tag{2.19}$$

Observe that

$$\nabla f = \begin{bmatrix} 2(p-1)x \\ 2(p+1)y \end{bmatrix}, \tag{2.20}$$

meaning that the only stationary points is $(x, y) = (0, 0)$. Furthermore,

$$\nabla^2 f = \begin{bmatrix} 2(p-1) & 0 \\ 0 & 2(p+1) \end{bmatrix}, \tag{2.21}$$

where we have 3 possible cases:

- $p > 1$: The stationary point is a minimum
- $-1 < p < 1$: The stationary point is a *saddle point*
- $p < -1$: The stationary point is a maximum

[TODO: generate figure for all three cases, discuss case $|p| = 1$]

2.3 Convex optimisation

This setting is defined by having a convex objective function and a convex feasible region. Critically, in the setting of convex optimisation a local minimum (according to the first/second order conditions presented above) is a global minimum. We next formally provide the relevant definitions.

Definition 2.1 (Convex set)**.** $\mathcal{S}$ is a convex set if $\forall x, x' \in \mathcal{S}$, we have:

$$\lambda x + (1-\lambda)x' \in \mathcal{S}, \quad \forall\, \lambda \in [0, 1]. \tag{2.22}$$

[TODO: Generate figures for convex and non-convex sets]

Definition 2.2 (Epigraph of a function)**.** The epigraph of a function $f : \mathcal{X} \to \mathbb{R}$ is the set defined by the region above the graph of the function, that is,

$$\text{epi}(f) = \{\, (x, t) \in \mathcal{X} \times \mathbb{R} \mid f(x) \leq t \,\}. \tag{2.23}$$

Definition 2.3 (Convex function)**.** f is a convex function if its epigraph is convex. Equivalently, f is convex is it is supported on a convex set and $\forall x, x' \in \mathcal{X}$

$$f\big(\lambda x + (1-\lambda)x'\big) \;\leq\; \lambda f(x) + (1-\lambda) f(x'), \quad \forall\, \lambda \in [0, 1]. \tag{2.24}$$

Furthermore, is the inequality is strict, we say that the function is **strictly convex**.

Example: Convex functions (in 1D)

The following are convex function from $\mathbb{R}$ to $\mathbb{R}$:

- $f(x) = x^2$
- $f(x) = e^{ax}$, $a \in \mathbb{R}$
- $f(x) = -\log x$
- $f(x) = x^a$, $a > 1$, $x > 0$
- $f(x) = |x|^a$, $a \geq 1$
- $f(x) = x \log x$, $x > 0$

[TODO: Generate figures, indicate epigraph (for convex and non-convex functions]

We now review some important results in convex optimisation

Proposition 2.1. Consider $f : \mathcal{X} \subset \mathbb{R} \to \mathbb{R}$ differentiable. We have that if $f'(x) \geq 0 \, \forall x \in \mathbb{R}$, f is non-decreasing

Proof. By the fundamental theorem of calculus, we have that for $a, b \in \mathbb{R}, a < b$,

$$f(b) - f(a) = \int_a^b f'(x)dx, \tag{2.25}$$

since $f'(x) \geq 0, \forall x \in [a, b]$, we have $\int_a^b f'(x)dx \geq 0$, therefore $f(b) \geq f(a)$, which means that f is non-decreasing. ■

Proposition 2.2. Consider $f : \mathcal{X} \subset \mathbb{R}^d \to \mathbb{R}$ differentiable. The direction of maximum growth of f at x_0 is along its gradient $\nabla f(x_0)$

Proof. Let us consider $x' = x_0 + \rho u$, where $u \in \mathcal{X}, ||u|| = 1$, and $\rho > 0$ is a small constant. We find the maximum growth direction by maximising $f(x') - f(x_0)$ with respect to u. We consider the Taylor expansion

$$f(x') = f(x_0) + \nabla f(x_0)\rho u + \mathcal{O}(\rho^2), \tag{2.26}$$

and thus conclude that $f(x') - f(x_0) \simeq \nabla f(x_0)\rho u$, meaning that the maximum growth can be achieved by choosing u parallel to $\nabla f(x_0)$. That is, $\nabla f(x_0)$ is the direction of maximum growth for f at x_0. ■

Teorema 2.1. *Suppose $f : \mathcal{X} \subset \mathbb{R}^d \to \mathbb{R}$ twice differentiable, then f is convex if and only if ∇^2 is positive semi definite.*

Proof. We consider $d = 1$. Using the FTC,

$$f'(b) - f'(a) = \int_a^b f''(x)dx \geq 0, \tag{2.27}$$

which implies that f' is non-decreasing. Therefore (using FTC again),

$$f(b) - f(a) = \int_a^b f'(x)dx \geq (b - a)f'(a), \tag{2.28}$$

equivalently,

$$f(b) \geq f(a)'(b - a)f'(a), \tag{2.29}$$

meaning that the function f *is always above its tangent.* Evaluating (2.29) for (a, z) and (b, z), where $z = (1 - t)a + tb$, we have

$$f(z) \geq f(a) + (z - a)f'(a) \tag{2.30}$$

$$f(z) \geq f(b) + (z - b)f'(b). \tag{2.31}$$

Then, multiplying the above equations by $(1 - t)$ and t respectively and summing them, we obtain:

$$\begin{aligned} f(z) &\geq (1 - t)f(a) + tf(b) + (1 - t)(tb - ta)f'(a) + t[(1 - t)a - (1 - t)b]f'(b) && (2.32) \\ &= (1 - t)f(a) + tf(b) + (1 - t)t(b - a)[f'(a) - f'(b)] && (2.33) \\ &\geq (1 - t)f(a) + tf(b) && (2.34) \end{aligned}$$

■

Example: Explore some functions

[TODO: Choose some functions, compute the derivative and Hessian, analyse them]

2.4 First order methods

2.4.1 Role of the step size

2.4.2 Momentum

2.5 Stochastic gradient descent

References

Murphy, K. P. (2022). *Probabilistic machine learning: An introduction.* MIT Press. Retrieved from `probml.ai`