Lecture Notes

# MATHEMATICS FOR MACHINE LEARNING

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

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# 1 Introduction

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# 2 Optimisation

**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.

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**Example: Linear regression (LR)**

In the LR setting, we aim to determine the function

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

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:

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

[FT: Camilo, por favor generar figura aqui. Mira la fig 1 del apunte del curso de AM]

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**Example: Logistic regression**

Here, we aim to determine the function

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

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:

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

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

**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) $\mu_1, \mu_2, \ldots, \mu_K$ and *assignment variables* $\{r_{ik}\}_{i,k=1}^{N,K}$, to minimise the following loss

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

$$\tag{2.10}$$

## 2.1 Terminology

We denote an optimisation problem as follows:

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

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

- **Local / global optima.** Values for the optimisation variable that solve the optimisation problem wither locally or globally. More formally:
$$x_\star \text{ is a local optima} \iff \exists \lambda > 0 \;\text{ s.t. }\; x_\star = \arg\min_{x \in \mathcal{X} \;\text{ s.t. }\; ||x - x_\star|| \leq \lambda} f(x). \tag{2.14}$$
$$x_\star \text{ is a global optima} \iff x_\star = \arg\min_{x \in \mathcal{X}} f(x). \tag{2.15}$$

**Interplay between constrains and local/global optima**

# 3 Continuous unconstrained optimisation

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

$$\theta \in \arg\min_{\theta \in \Theta} L(\theta). \tag{3.1}$$

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

$$\forall \theta \in \Theta, \ L(\theta_\star) \leq L(\theta), \tag{3.2}$$

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

$$\exists \delta > 0 \ \forall \theta \in \Theta \ \text{s.t.} \ \|\theta - \theta_\star\| < \delta \ \Rightarrow \ L(\theta_\star) \leq L(\theta). \tag{3.3}$$

## 3.1 Optimality Conditions

**Assumption 3.1.** The loss function $L$ is twice differentiable.

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

# References

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