Lecture Notes

MATHEMATICS FOR MACHINE LEARNING

This version: November 5, 2025

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

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MISSING

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NB: in this chapter, we follow (?, ?).

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

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

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

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

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:

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

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

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

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

$$\tag{2.10}$$

[TODO: Generate figure]

2.1 Terminology

We denote an optimisation problem as follows:

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

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:

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

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

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

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

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:

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

■

Example: Explore some functions

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

2.4 First order methods

In general, finding a minimum by setting $\nabla f(x) = 0$ and solving for x is not possible. For that reason, we will consider iterative methods based on gradients.

The idea here is to go *downhill* following the gradient towards the minimum (ignoring the curvature information for now).

We will specify a starting point x_0 and calculate

$$x_{t+1} = x_t + \eta_t d_t, \tag{2.35}$$

where η_t is a *step size* and d_t is a *descent direction*, such as $-\nabla f$. Here, the subindex $\cdot_t$ represents the iteration number (starting from iteration $t = 0$). We iterate until convergence, that is, until the elements in the sequence $x_t, x_{t+1}, x_{t+2}, \ldots$ become constant (or very similar). If convergence is achieved, we will assume the minimum has been found.

Note that there are several *descent directions*, that is, directions d_t such that

$$L(x_t + \eta_t d_t) \leq L(x_t). \tag{2.36}$$

In fact, as long as $d_t^\top \nabla f \leq 0$, d_t is a descent direction. Clearly, choosing $d_t = -\nabla f(x_t)$ is the *steepest descent direction*.

2.4.1 Role of the step size

The step size η_t is also known as *learning rate*. Furthermore, we refer to the set $\{\eta_1, \eta_2, \ldots\}$ as the learning rate schedule.

We will usually consider a constant learning rate, that is, $\eta_t = \eta$, $\forall t \in \mathbb{N}$. Though this is the simplest choice, there are some concerns to this choice: if η is too large, the iteration may fail to converge; whereas if it is too small, it may not converge at all.

Example: convergence for a parabola

[TODO: Plot the level sets of a parabola (or another convex function). Show how the steepest descent converges/diverges for different learning rates]

The learning rate is usually tuned with heuristics. Since we will usually implement

$$x_{t+1} = x_t + \eta \nabla f(x_t), \tag{2.37}$$

we will usually set $\eta < ||\nabla f||^{-1}$, as this will result in a stable autoregressive system for the sequence x_t.

2.4.2 Momentum

In higher dimensions, we want to move faster in some directions and slow in other directions, depending on the value of the gradient in each coordinate. This can be achieved by:

$$m_t = \beta m_{t-1} + \nabla f(x_{t-1}) \tag{2.38}$$

$$x_t = x_{t-1} - \nabla_t m_t, \tag{2.39}$$

where m_t is a smoothed version of the gradient, and $\beta \in [0, 1]$ is a design (memory) parameter. This way, previous values of the gradient have effect on future updates: if a particular coordinate of the gradient is consistently large, then that coordinate will receive updated of a higher magnitude. This is particularly useful when the evaluation of the gradient is noisy.

2.4.3 Newton method

Newton's method is

$$x_{t+1} = x_t - \eta_t H_t^{-1} \nabla f(x_t), \tag{2.40}$$

where recall that $H_t = \nabla^2 f(x_t)$ denotes the Hessian of f at x_t. This update follows from considering the second order approximation of the loss function arond the current point, that is:

$$L(x) \simeq L(x_t) + (\nabla f(x_t))^\top (x - x_t) + \frac{1}{2}(x - x_t)^\top H_t (x - x_t), \tag{2.41}$$

the minimum of which is given by

$$x_\star = x_t - H_t^{-1} \nabla L(x_t), \tag{2.42}$$

where the learning rate can also be used.

Example: convergence for a parabola (2)

[TODO: Same a previous example, but with momentum and/or Newton]

2.5 Stochastic gradient descent

We now consider stochastic optimisation, where

$$L(x) = \mathbb{E}_{q(z)} L(x, z), \tag{2.43}$$

that is, when the loss function is random and we aim to minimise its expected value.

For instance, in linear regression we have $L(\theta) = \mathbb{E}_{q(y|x)}(y - \theta^\top x)$.

In practice we are unable to compute this expectation since we don't know the law $q(z)$. However, since we usually have samples of q, we can do a sample approximation og the expectation. In fact, we will consider

$$L(\theta) = \frac{1}{N} \sum_{i=1}^{n} L(x, z_i). \tag{2.44}$$

In the linear regression example, this would be $L(\theta) = \frac{1}{N} \sum_{i=1}^{n} (y_i - \theta^\top x_i)^2$.

The gradient is then also approximated using a batch of, say, B samples. That is,

$$\nabla L(\theta) \simeq \frac{1}{N} \sum_{i=1}^{B} \nabla L(x, z_i) \tag{2.45}$$

Example: random loss function for linear regression

[TODO: Plot a q function: its theoretical value and sample approximations using a finite set of datapoints]

Recall that in general we will consider parameter updates of the form

$$\theta_{t+1} = \theta_t - M_t^{-1} g_t \tag{2.46}$$

where M_t is an estimate of the norm of the gradient g_t, as this ensures convergence (or prevents divergence). We next explore some different choices of this estimate.

2.5.1 Adagrad

This considers the following iterative rule (d denotes the coordinate):

$$\theta_{t+1,d} = \theta_{t,d} - \eta_t \frac{1}{\sqrt{s_{t,d} + \epsilon}} g_{t,d}, \tag{2.47}$$

where $s_{t,d} = \sum_{i=1}^{t} g_{i,d}^2$. This can also be expressed in vector format as

$$\Delta\theta_t = -\eta_t \frac{1}{s_t} g_t. \tag{2.48}$$

The aim of this update rule is that control the magnitude of the step size for each coordinate of the parameter independently, based on a rolling estimate using previous gradient evaluations. Notice that the computation of $s_{t,d}$ assigns the same importance to all gradient evaluations in time.

2.5.2 RMSProp

Adagrad might fail to represent the current gradient magnitude by not emphasising current evaluations of the gradient. This can be solved by replacing the sum in the computation of $s_{t,d}$ by a moving average. That is,

$$s_{t+1,d} = \beta s_{t,d} + (1 - \beta) g_{t,d}^2, \tag{2.49}$$

where the *forgetting factor* β is usually chosen closer to 0.9. Then, the update rule also follows

$$\Delta\theta_t = -\eta_t \frac{1}{s_t} g_t. \tag{2.50}$$

2.5.3 Adam

The de facto optimiser in deep learning is Adam (Adaptive Moment Estimation), which combines RMSProp and momentum. Adam's update follows:

$$m_t = \beta_m m_{t-1} + (1 - \beta_m) g_t \tag{2.51}$$

$$s_t = \beta_s s_{t-1} + (1 - \beta_s) g_t^2. \tag{2.52}$$

Then,

$$\theta_t = \theta_{t-1} - \eta_t \frac{m_t}{\sqrt{s_t} + \epsilon} \tag{2.53}$$

Example: different optimisers

[TODO: If possible, show different optimisers in a toy example]

3 Probability

3.1 Introduction

NB: in this chapter, we follow (?, ?).

The field of probability studies, from a quantitative perspective, how *likely* an event is. Conceptually, and perhaps historically, there are two main interpretations of probability. The first one is **frequentist probability**, which relates to frequency of occurrence, and then applies only to event that can be repeated an infinite number of times, such as throwing a dice or flopping a coin. As a consequence, this standpoint fails to assign a probability to events that are impossible to repeat, such as the average temperature of the Earth's surface reaching an all-time maximum in the year 2025. A second interpretation is that of **Bayesian probability**, which represents uncertainty about the occurrence of an event. This uncertainty might come from different sources, such unknown features in the experiments (epistemological uncertainty) or random components (aleatoric uncertainty). In this case, events need not be repeatable be be assigned with a probability.

A basic knowledge of probability theory, definitions and results in fundamental in ML. This is because in ML we design, train and deploy mathematical models that i) aim to capture/quantify uncertainty, and ii) deal with noise-corrupted training data. Therefore, a rigorous account of uncertainty is central to real-world ML applications.

3.1.1 Definitions

To start studying probability, we will focus on the outcome ω of a hypothetical experiment, e.g., throwing a dice, where ω can take values $\{1, 2, 3, 4, 5, 6\}$. In this context, we can define:

Definition 3.1 (Sample space)**.** The set containing all the possible outcomes ω of an experiment is called sample space and is denoted by Ω.

Definition 3.2 (Event space)**.** The set $\mathcal{A}$, referred to as event space, contains all possible subset of the sample space Ω. Therefore, each element $A \in \mathcal{A}$ represents a possible results of the experiment.

Definition 3.3 (Probability)**.** The function

$$\mathbb{P} : \mathcal{A} \to [0, 1] \tag{3.1}$$

$$x \mapsto \mathbb{P}(x) \tag{3.2}$$

denotes the probability of the result of the experiment falling inside the elements of $\mathcal{A}$, that is, $\mathbb{P}(A) = \mathbb{P}(\omega \in A)$. The function $\mathbb{P}$ needs to fulfil some standard properties such as $\mathbb{P}(\Omega) = 1, \mathbb{P}(\emptyset) = 0$, and $\mathbb{P}(A^c) = 1 - \mathbb{P}(A)$.

$\mathcal{A}$ vs Ω

Why is the probability defined over $\mathcal{A}$ and not over Ω? Discuss via some examples

Examples

[TODO: Consider basic examples (dice, coin, uniform, rain), and present the sample space, event space, and probability]

We refer to the triplet $(\Omega, \mathcal{A}, \mathbb{P})$ as **probability space**.

3.1.2 Basic properties

The joint probability of events A and B is denoted by

$$\mathbb{P}(A \wedge B) = \mathbb{P}(A \cap B) = \mathbb{P}(A, B), \tag{3.3}$$

note that if $\omega \in A$ and $\omega \in B$, then, $\omega \in A \cap B$.

The conditional probability of the event A occurring, given that the event B occurred is denoted by

$$\mathbb{P}(A|B) = \frac{\mathbb{P}(A, B)}{\mathbb{P}(B)}, \tag{3.4}$$

which is only valid when $\mathbb{P}(B) > 0$.

Additionally, we say that events A and B are **independent** iff $\mathbb{P}(A, B) = \mathbb{P}(A)\mathbb{P}(B)$. Observe that this implies that

$$\mathbb{P}(A|B) = \frac{\mathbb{P}(A, B)}{\mathbb{P}(B)} = \frac{\mathbb{P}(A)\mathbb{P}(B)}{\mathbb{P}(B)} = \mathbb{P}(A), \tag{3.5}$$

meaning that when A and B are independent, the latter provides no **information** for A.

Lastly, the probability of intersection, i.e., the probability of the events $\omega \in A$ or $\omega \in B$ is given by

$$\mathbb{P}(A \vee B) = \mathbb{P}(A) + \mathbb{P}(B) - \mathbb{P}(A \wedge B). \tag{3.6}$$

3.2 Random variables

In general, other than basic toy examples, we do not refer to the underlying experiment and its sample/event spaces. We instead consider *quantities of interest* that result from the outcome of the experiment. Therefore, let us consider a map from the sample space to a target space $\mathcal{T}$, e.g., $\mathcal{T} = \mathbb{R}$, $\mathcal{T} = \mathbb{N}$ or $\mathcal{T} = \{1, 2, 3, \ldots, N\}$.

Definition 3.4 (Random variable)**.** A function

$$X : \Omega \to \mathcal{T} \tag{3.7}$$

$$\omega \mapsto X(\omega) \tag{3.8}$$

is referred to as random variable. In general, we will denote the function as X and its value as x, ignoring the explicit dependence on ω.

Observación 3.1. From now on, we will consider the outcome of the experiment (living in the sample space) as the value of the RV, this aims to have a more streamlined setup avoiding the need of a map from Ω to $\mathcal{T}$. Accordingly, the event space $\mathcal{A}$ and the probability $\mathbb{P}$ correspond to the outcomes (values) of X, we will usually denote the sample space by $\mathcal{X}$.

3.2.1 Discrete RVs

If the sample space is finite or countably infinite, we will say that the RVis discrete. In this case, we denote the probability of the event $X = x$ by $\mathbb{P}(X = x)$. We define de following.

Definition 3.5 (Probability mass function (pmf))**.** For a discrete RV $X \in \mathcal{X}$ the function

$$p_X : \mathcal{X} \to [0, 1] \tag{3.9}$$

$$x \mapsto p_X(x) = \mathbb{P}(X = x) \tag{3.10}$$

denotes the probability of the event in which the RV X takes the value $x \in \mathcal{X}$. Evidently,

$$\sum_{x \in \mathcal{X}} p_X(x) = 1. \tag{3.11}$$

Discrete RV

[TODO: Give an example, e.g., a dice, picking items and/or a infinite state space one]

3.2.2 Continuous RVs

If $\mathcal{X} = \mathbb{R}^d$, with $d > 1$, or any other infinitely uncountable space, we say that the RV is continuous. Observe that in this case we cannot defined a pmf as in Def. 3.5. This is because since there is an uncountable number of symbols in the sample space $\mathcal{X}$, we cannot assign each of them with a probability strictly greater than zero and still a total probability mass equal to one. Therefore, we make use of the event space and assign probabilities to intervals rather tan particular values.

Definition 3.6 (Cumulative distribution function (cdf))**.** For a continuous RV $X \in \mathcal{X}$, we can define the probability of X to be less or equal that a given value $x \in \mathcal{X}$ by

$$P_X : \mathcal{X} \to [0, 1] \tag{3.12}$$

$$x \mapsto P_X(x) = \mathbb{P}(X \leq x). \tag{3.13}$$

Observe that this also allows to denote the probability of X lying in a bounded interval, that is,

$$\mathbb{P}(a \leq X \leq b) = P_X(b) - P_X(a). \tag{3.14}$$

The cdf is monotonically non-decreasing by construction, and, when $\mathcal{X} = \mathbb{R}$, we have

$$\lim_{x \to -\inf} P_X(x) = 0 \tag{3.15}$$

$$\lim_{x \to \inf} P_X(x) = 1. \tag{3.16}$$

The idea to assign probabilities to intervals, suggest that there exists a density of probability, that is, an amount of probability mass per unit of length. This is formalised via the following definition.

Definition 3.7 (Probability density function (pdf))**.** For a continuous RV $X \in \mathcal{X}$, the probability density function of X is given by the function

$$p_X : \mathcal{X} \to \mathbb{R} \tag{3.17}$$

$$x \mapsto p_X(x) = \frac{d}{dx} P_X(x). \tag{3.18}$$

This is possible when P_X is differentiable.

Knowing the pdf, we can express:

$$\mathbb{P}(a \leq X \leq b) = \int_a^b p_X(x)dx = P_X(b) - P_X(a), \tag{3.19}$$

which is a direct particular case of the fundamental theorem of Calculus.

Also, for Δx small, we have

$$\mathbb{P}(x \leq X \leq x + \Delta x) = \int_x^{x+\Delta x} p_X(x)dx \simeq p(x)\Delta x. \tag{3.20}$$

Lastly, if the cdf is **strictly monotonically increasing**, its inverse exists and it is known as the **quantile function**. The use quantiles is useful when assessing the value of the RV wrt the range of possible values.

Examples

[TODO: Show the Gaussian distribution and present cdf, pdf and quantile]

3.2.3 Properties and identities

Probability can be thought of as an extension of logical reasoning. The following properties are consistent with such extension. Let us first consider, in the same was as we did when we defined event probabilities, the following.

Both for discrete (pmf) and discrete (pdf) RVs, we can denote $p(x, y)$ the joint pdf/pmf for RVs $X \in \mathcal{X}$ and $Y \in \mathcal{Y}$. This can be seen as the probability of the *intersection* event, where $X = x$ and $Y = y$.

Furthermore, we can write

$$p_X(x) = \sum_{y \in \mathcal{Y}} p(x, y) \quad \text{(discrete)} \tag{3.21}$$

$$p_X(x) = \int_{\mathcal{Y}} p(x, y) dy \quad \text{(continuous)}. \tag{3.22}$$

In the ML community, this is known as **sum rule**, since it allows us to express the density $p(y)$ from a joint density by summing over all possible values.

A related expression is the so called **law of total probability**, which reads

$$p_X(x) = \sum_{y \in \mathcal{Y}} p(x|y)p(y) \quad \text{(discrete)} \tag{3.23}$$

$$p_X(x) = \int_{\mathcal{Y}} p(x|y)p(y) dy \quad \text{(continuous)}. \tag{3.24}$$

This operation is usually called **marginalisation**, or **disintegration** (of y).

References

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