

Machine Learning

Appendix

Yannick Le Cacheux

CentraleSupélec - Université Paris Saclay

September 2024

Table of Contents

- 1 Notations
- 2 Probability reminders
- 3 Linear algebra reminders
- 4 Matrix calculus

Outline

- 1 Notations
- 2 Probability reminders
- 3 Linear algebra reminders
- 4 Matrix calculus

Notations

In general, in this class:

- A lowercase, non bold letter is a scalar:

$$x \in \mathbb{R}$$

- A lowercase, bold letter is a vector:

$$\mathbf{x} \in \mathbb{R}^N$$

- An uppercase, bold letter is a matrix:

$$\mathbf{X} \in \mathbb{R}^{M \times N}$$

Outline

- 1 Notations
- 2 Probability reminders**
- 3 Linear algebra reminders
- 4 Matrix calculus

Expectation and (co)variance

$$\text{cov}[X, Y] = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$$

$$\mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y]$$

$\mathbb{E}[XY] = \mathbb{E}[X]\mathbb{E}[Y]$ if and only if X and Y are independent, *i.e.*

$$\mathbb{E}[XY] = \mathbb{E}[X]\mathbb{E}[Y] \iff X \perp\!\!\!\perp Y$$

If $X = Y$ then

$$\text{cov}[X, X] = \text{var}[X] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$$

Outline

- 1 Notations
- 2 Probability reminders
- 3 Linear algebra reminders**
- 4 Matrix calculus

Linear algebra

The projection $\text{Proj}_{\mathbf{b}}(\mathbf{a})$ of vector \mathbf{a} onto vector \mathbf{b} :

- Has amplitude

$$\|\mathbf{a}\|\cos(\theta)$$

where θ is the angle between \mathbf{a} and \mathbf{b}

- Has direction

$$\frac{\mathbf{b}}{\|\mathbf{b}\|}$$

(unit vector in the direction of \mathbf{b})

- The dot product between \mathbf{a} and \mathbf{b} is

$$\mathbf{a}^\top \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \cos(\theta)$$

- Consequently,

$$\text{Proj}_{\mathbf{b}}(\mathbf{a}) = \frac{\mathbf{a}^\top \mathbf{b}}{\|\mathbf{b}\|^2} \cdot \mathbf{b}$$

Outline

- 1 Notations
- 2 Probability reminders
- 3 Linear algebra reminders
- 4 Matrix calculus**

Matrix calculus

We can define:

- Derivatives of scalars with respect to vectors (*i.e.* gradients):

$$\text{For } a \in \mathbb{R}, \mathbf{x} \in \mathbb{R}^N, \quad \frac{\partial a}{\partial \mathbf{x}} \in \mathbb{R}^N \quad \text{and} \quad \boxed{\left(\frac{\partial a}{\partial \mathbf{x}} \right)_i = \frac{\partial a}{\partial x_i}}$$

- But also derivatives of vectors with respect to scalars:

$$\text{For } \mathbf{a} \in \mathbb{R}^N, x \in \mathbb{R}, \quad \frac{\partial \mathbf{a}}{\partial x} \in \mathbb{R}^N \quad \text{and} \quad \boxed{\left(\frac{\partial \mathbf{a}}{\partial x} \right)_i = \frac{\partial a_i}{\partial x}}$$

- Or derivatives of vectors w.r.t. vectors:

$$\text{For } \mathbf{a} \in \mathbb{R}^M, \mathbf{b} \in \mathbb{R}^N, \quad \frac{\partial \mathbf{a}}{\partial \mathbf{b}} \in \mathbb{R}^{M \times N} \quad \text{and} \quad \boxed{\left(\frac{\partial \mathbf{a}}{\partial \mathbf{b}} \right)_{ij} = \frac{\partial a_i}{\partial b_j}}$$

- etc

Matrix calculus

We can then prove:

- If \mathbf{a} is constant with respect to \mathbf{x} ($\mathbf{a} \neq \mathbf{a}(\mathbf{x})$):

$$\frac{\partial}{\partial \mathbf{x}}(\mathbf{x}^\top \mathbf{a}) = \frac{\partial}{\partial \mathbf{x}}(\mathbf{a}^\top \mathbf{x}) = \mathbf{a} \quad (1)$$

- For matrices $\mathbf{A}(x)$ and $\mathbf{B}(x)$ that depend on x :

$$\frac{\partial}{\partial x}(\mathbf{A}\mathbf{B}) = \frac{\partial \mathbf{A}}{\partial x} \mathbf{B} + \mathbf{A} \frac{\partial \mathbf{B}}{\partial x} \quad (2)$$

Exercise¹: prove that for $\mathbf{A}(x)$:

$$\frac{\partial \mathbf{A}^{-1}}{\partial x} = -\mathbf{A}^{-1} \frac{\partial \mathbf{A}}{\partial x} \mathbf{A}^{-1}$$

¹Hint: use the fact that $\mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$ and equation (2)

Matrix calculus

- For any 3 matrices **A**, **B** and **C** that do not depend on a 4th matrix **X**, and defined such that the equation below makes sense, we can prove:

Lemma

$$\frac{\partial \|\mathbf{A}\mathbf{X}\mathbf{B} + \mathbf{C}\|_2^2}{\partial \mathbf{X}} = 2\mathbf{A}^\top (\mathbf{A}\mathbf{X}\mathbf{B} + \mathbf{C})\mathbf{B}^\top$$

- This is a generic result whose special cases we will often be useful in this course.

Outline

- 1 Notations
- 2 Probability reminders
- 3 Linear algebra reminders
- 4 Matrix calculus

Constrained optimization

Coming soon