Advanced ML — Lecture 1: Preliminaries

Charalampos Giannakis

Linear Algebra

Let $A \in \mathbb{R}^{m\times n}$ be a matrix with entries A_{ij} where i indexes rows and j indexes columns.

Properties of matrices

- $AA^{-1} = A^{-1}A = I$
- $(AB)^T = B^T A^T$
- $(AB)^{-1} = B^{-1}A^{-1}$
- $(A^\top)^{-1} = (A^{-1})^\top$
- $(A^\top)^\top = A$
- $(A+B)^\top = A^\top + B^\top$
- Consequence $(A+BC)^T = A^T + C^T B^T$
- Symmetric matrix: $A^\top = A$
- Positive definite: $x^\top A x > 0$ for all non-zero x and A symmetric
- All vectors in this course will be column vectors
- Recall, if $A \in \mathbb{R}^{m\times n}$ is a matrix and $x \in \mathbb{R}^n$ a vector, then the i-th element of Ax is given by $(Ax)_i = \sum_{j=1}^n a_{ij}x_j$

Vector Calculus

Let $a \in \mathbb{R}^n$ and $b \in \mathbb{R}^n$ be a vector, and $x \in \mathbb{R}$ a scalar.

- $\left(\frac{\partial \mathbf{a}}{\partial x}\right)_i = \left(\frac{\partial}{\partial x}(a_1,\dots,a_n)\right)_i = \left(\frac{\partial a_1}{x},\dots,\frac{\partial a_n}{x}\right)_i = \frac{\partial a_i}{\partial x}$
- $\left(\frac{\partial x}{\partial \mathbf{a}}\right)_i = \left(\frac{\partial x}{\partial(a_1,\dots,a_n)}\right)_i = \left(\frac{\partial x}{\partial a_1},\dots,\frac{\partial x}{\partial a_n}\right)_i = \frac{\partial x}{\partial a_i}$ scalar-vector derivative
- $\left(\frac{\partial \mathbf{a}}{\partial \mathbf{b}}\right)_{ij} = \left(\frac{\partial(a_1,\dots,a_m)}{\partial(b_1,\dots,b_n)}\right)_{ij} = \underbrace{\begin{bmatrix} \frac{\partial a_1}{\partial b_1} & \cdots & \frac{\partial a_1}{\partial b_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial a_m}{\partial b_1} & \cdots & \frac{\partial a_m}{\partial b_n} \end{bmatrix}_{ij}}_{\text{Jacobian matrix}} = \frac{\partial a_i}{\partial b_j}$ vector-vector derivative.

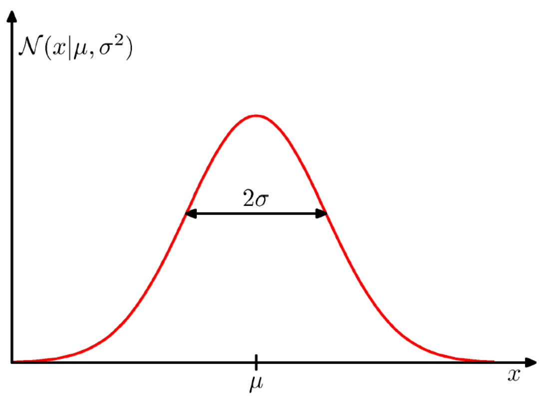
- Example: let $a \in \mathbb{R}^n$ and $x \in \mathbb{R}^n$. What is $\frac{\partial}{\partial x}(x^\top a)$?
- Solution: this is a scalar–vector derivative, thus $\left(\frac{\partial}{\partial x}(x^\top a)\right)_i = \frac{\partial}{\partial x_i}(x^\top a) = \frac{\partial}{\partial x_i}\left(\sum_{j=1}^n a_j x_j\right) = a_i$
- Thus $\frac{\partial}{\partial x}(x^\top a) = a^\top, \qquad \frac{\partial}{\partial x}(a^\top x) = a^\top$
- Another example. Let $b \in \mathbb{R}^m$, $A \in \mathbb{R}^{m\times n}$, and $x \in \mathbb{R}^n$
  What is $\frac{\partial}{\partial x}(b^\top Ax)$?
- Solution: this is a scalar–vector derivative, thus
  $\left(\frac{\partial}{\partial x}(b^\top Ax)\right)_i = \frac{\partial}{\partial x_i}(b^\top Ax) = \frac{\partial}{\partial x_i}\left(\sum_{k=1}^n \sum_{j=1}^m b_j a_{jk} x_k\right) = \sum_{j=1}^m b_j a_{ji} = \sum_{j=1}^m a_{ij}^\top b_j = (A^\top b)_i$
- Hence, $\frac{\partial}{\partial x}(b^\top Ax) = b^\top A$
- $\frac{\partial x}{\partial x} = I$
- $\frac{\partial (Ax)}{\partial x} = A$
- $\frac{\partial (x^\top A)}{\partial x} = A^\top$
- $\frac{\partial (x^\top Ax)}{\partial x} = x^\top(A + A^\top)$, and $2x^\top A$ if A is symmetric
- $\frac{\partial^2 (x^\top Ax)}{\partial x\, \partial x^\top} = A + A^\top$, and $2A$ if A is symmetric
- Proof: $\left(\frac{\partial x}{\partial x}\right)_{ij} = \frac{\partial x_i}{\partial x_j} = \begin{cases} 0, & \text{if } i \neq j, \\ 1, & \text{if } i = j \end{cases}$
- $\frac{\partial (Ax)}{\partial x} = A$
- Proof: $\left(\frac{\partial (Ax)}{\partial x}\right)_{ij} = \frac{\partial (Ax)_i}{\partial x_j} = \frac{\partial}{\partial x_j}\sum_{k=1}^n a_{ik} x_k = a_{ij}$
- $\dfrac{\partial (x^\top Ax)}{\partial x} = x^\top(A + A^\top)$
- Proof: $\left(\frac{\partial (x^\top Ax)}{\partial x}\right)_i = \frac{\partial}{\partial x_i}\left(\sum_{k=1}^n \sum_{l=1}^n a_{kl}\, x_l\, x_k\right) = \sum_{k=1}^n \sum_{l=1}^n a_{kl}\, \frac{\partial}{\partial x_i}(x_l x_k) =$
  $= \sum_{k=1}^n a_{ki}\, x_k \;+\; \sum_{l=1}^n a_{il}\, x_l = (A^\top x)_i \;+\; (Ax)_i$ Hence, $\dfrac{\partial (x^\top Ax)}{\partial x} = x^\top(A + A^\top)$
- If $a, b, x \in \mathbb{R}^n$, then $\dfrac{\partial}{\partial x}\,(a^\top x x^\top b) = x^\top(ab^\top + ba^\top)$
- Proof: $\frac{\partial}{\partial x_i}(a^\top x x^\top b) = \frac{\partial}{\partial x_i}\left(\sum_{k=1}^n a_k x_k \sum_{l=1}^n x_l b_l\right) = b_i \sum_{k=1}^n a_k x_k + a_i \sum_{l=1}^n x_l b_l = b_i a^\top x + a_i b^\top x = (b_i a^\top + a_i b^\top)x$

Normal Distribution

The **univariate normal distribution** describes a random variable X with mean μ and variance σ^2. Its probability density function is given by:

$p(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$.

This distribution is the foundation for much of probability and statistics, as it captures many naturally occurring phenomena due to the central limit theorem.
The bell-shaped curve shows how values close to the mean are more likely, with probabilities tapering off symmetrically on both sides.



Moments of the univariate normal

Let $X \sim \mathcal{N}(\mu, \sigma^2)$ with pdf $p(x) = \mathcal{N}(x \mid \mu, \sigma^2)$. Its first two moments and variance are

- $\mathbb{E}[X] = \mu$
- $\mathbb{E}[X^2] = \mu^2 + \sigma^2$
- $\mathrm{Var}[X] = \mathbb{E}[X^2] - \mathbb{E}[X]^2 = \sigma^2$

Mean.

$$\mathbb{E}[X] = \int_{-\infty}^{\infty} x\, p(x)\, dx = \int_{-\infty}^{\infty} x \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)\, dx.$$

Change variables $y = \dfrac{x-\mu}{\sigma}$ (so $x = \mu + \sigma y$ and $dx = \sigma\, dy$):

$$\mathbb{E}[X] = \int_{-\infty}^{\infty} (\mu + \sigma y)\, \phi(y)\, dy = \mu \underbrace{\int_{-\infty}^{\infty} \phi(y)\, dy}_{=1} + \sigma \underbrace{\int_{-\infty}^{\infty} y\, \phi(y)\, dy}_{=0} = \mu.$$

Here

$$\phi(y) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{y^2}{2}\right),$$

which is the standard normal density.
Thus,

$$\int_{-\infty}^{\infty} \phi(y)\,dy = 1 \quad \text{and} \quad \int_{-\infty}^{\infty} y\phi(y)\,dy = 0$$

since $\phi(y)$ is even and $y\phi(y)$ is an odd function.

Second moment.

$$\mathbb{E}[X^2] = \int_{-\infty}^{\infty} x^2\,p(x)\,dx = \int_{-\infty}^{\infty} (\mu+\sigma y)^2\,\phi(y)\,dy = \mu^2 \underbrace{\int \phi}_{=1} + 2\mu\sigma \underbrace{\int y\phi}_{=0} + \sigma^2 \int_{-\infty}^{\infty} y^2\phi(y)\,dy.$$

It remains to show $\int_{-\infty}^{\infty} y^2\phi(y)\,dy = 1.$

Auxiliary integral $\int y^2\phi(y)\,dy$.

Write it without the $1/\sqrt{2\pi}$ factor, then put the factor back:

$$\int_{-\infty}^{\infty} y^2\phi(y)\,dy = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} y^2 e^{-y^2/2}\,dy.$$

Integration by parts with $u = y$ and $dv = ye^{-y^2/2}dy$ gives $v = -e^{-y^2/2}$ and $du = dy$, hence

$$\int_{-\infty}^{\infty} y^2 e^{-y^2/2}\,dy = \Big[-ye^{-y^2/2}\Big]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} e^{-y^2/2}\,dy = 0 + \sqrt{2\pi}.$$

Therefore

$$\int_{-\infty}^{\infty} y^2\phi(y)\,dy = \frac{1}{\sqrt{2\pi}} \cdot \sqrt{2\pi} = 1.$$

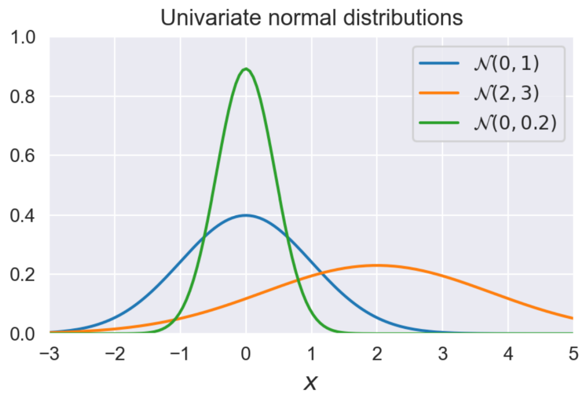
Putting this into the second-moment expression:

$$\mathbb{E}[X^2] = \mu^2 + \sigma^2.$$

Variance.

$$\mathrm{Var}[X] = \mathbb{E}[X^2] - \big(\mathbb{E}[X]\big)^2 = (\mu^2+\sigma^2) - \mu^2 = \sigma^2.$$

Illustration of univariate normal distributions



The figure shows three different univariate normal distributions, each with different mean and variance. We observe that:

- The **blue curve** $\mathcal{N}(0, 1)$ is the standard normal: centered at 0 with unit variance, giving a moderate spread.

- The **orange curve** $\mathcal{N}(2, 3)$ has a larger variance. Its peak is flatter, and the distribution is spread more widely, reflecting greater uncertainty. The mean is shifted to 2, so the entire distribution is displaced to the right.

- The **green curve** $\mathcal{N}(0, 0.2)$ has a much smaller variance. It is sharply peaked around 0, reflecting low variability.

This comparison highlights the distinct roles of the mean μ (shifting the center of the distribution) and the variance σ^2 (controlling the spread).

Multivariate Normal Distribution

The **multivariate normal distribution** generalizes the univariate normal distribution to D dimensions. Its probability density function is given by:

$$\mathcal{N}(x \mid \mu, \Sigma) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left\{-\tfrac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu)\right\},$$

where:

- μ is a D-dimensional **mean vector**, indicating the central location of the distribution.

- Σ is a $D \times D$ **covariance matrix**, which must be symmetric and positive definite. It encodes the variances of individual dimensions along the diagonal, and covariances between dimensions in the off-diagonal entries.

- $|\Sigma|$ denotes the **determinant of** Σ, which measures the volume scaling of the distribution.

Comment:
The covariance matrix Σ not only determines the spread of the distribution but also encodes correlations between variables. When Σ is diagonal, the variables are independent, and the distribution reduces to a product of independent univariate Gaussians. When off-diagonal terms are present, the shape becomes elliptical, reflecting correlations.

Bivariate Normal Examples

To visualize the role of the covariance matrix Σ, consider the case of a **bivariate normal distribution**.

- When the covariance matrix is diagonal with no correlation, the variables are independent:

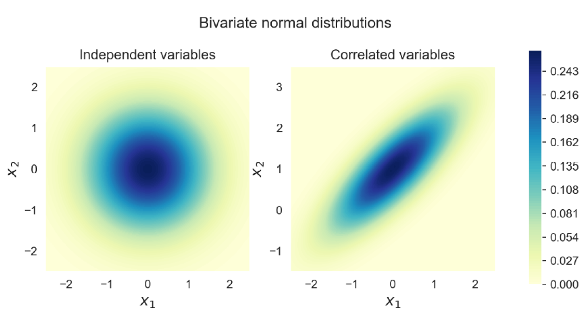
$$\mathcal{N}\left(\begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\right)$$

  The distribution is circular and symmetric, meaning x_1 and x_2 vary independently.

- When the covariance matrix has strong off-diagonal terms, the variables are correlated:

$$\mathcal{N}\left(\begin{bmatrix}0\\1\end{bmatrix}, \begin{bmatrix}1 & 0.8\\0.8 & 1\end{bmatrix}\right)$$

  Here, the contours of the distribution become **elliptical**, indicating a linear relationship between x_1 and x_2.



Comment:
This highlights how the covariance matrix Σ shapes the distribution.
- The **diagonal entries** control the spread (variance) of each variable.
- The **off-diagonal entries** introduce correlation, tilting and stretching the distribution along certain directions.