TECHNISCHE UNIVERSITÄT
CHEMNITZ

Neurocomputing

Basics in mathematics

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https://tu-chemnitz.de/informatik/KI/edu/neurocomputing

Outline

1. Linear algebra
2. Calculus
3. Probability theory
4. Statistics
5. Information theory

1 - Linear algebra

Mathematical objects

- **Scalars** x are 0-dimensional values. They can either take real values ($x \in \mathfrak{R}$, e.g. $x = 1.4573$, floats in CS) or natural values ($x \in \mathbb{N}$, e.g. $x = 3$, integers in CS).
- **Vectors** $\mathbf{x}$ are 1-dimensional arrays of length d.
- The bold notation $\mathbf{x}$ will be used in this course, but you may also be accustomed to the arrow notation $\vec{x}$ used on the blackboard. When using real numbers, the **vector space** with d dimensions is noted $\mathfrak{R}^d$, so we can note $\mathbf{x} \in \mathfrak{R}^d$.
- Vectors are typically represented vertically to outline their d elements $x_1, x_2, \ldots, x_d$:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}$$

Mathematical objects

- **Matrices** A are 2-dimensional arrays of size (or shape) $m \times n$ (m rows, n columns, $A \in \mathfrak{R}^{m \times n}$).
- They are represented by a capital letter to distinguish them from scalars (classically also in bold $\mathbf{A}$ but not here). The element a_{ij} of a matrix A is the element on the i-th row and j-th column.

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

- **Tensors** $\mathcal{A}$ are arrays with more than two dimensions. We will not really do math on these objects, but they are useful internally (hence the name of the `tensorflow` library).

Vectors

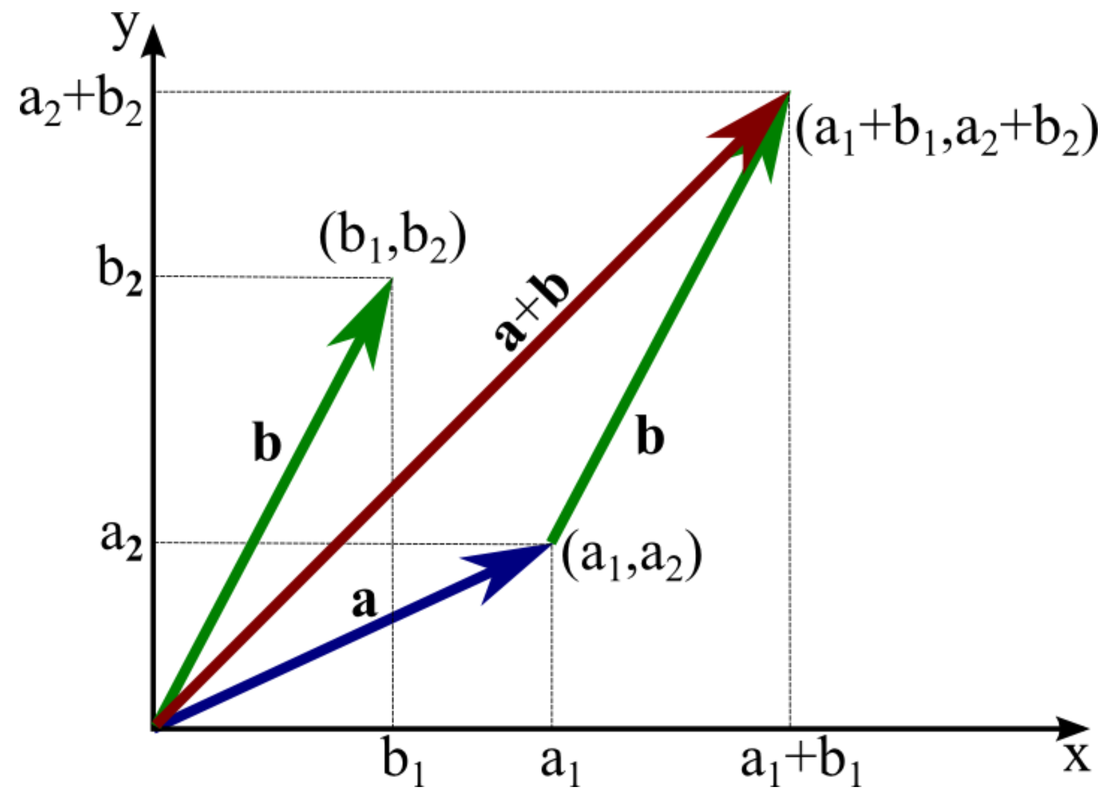
- A vector can be thought of as the **coordinates of a point** in an Euclidean space (such the 2D space), relative to the origin.
- A vector space relies on two fundamental operations, which are that:

- Vectors can be added:

$$\mathbf{x} + \mathbf{y} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix} + \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_d \end{bmatrix} = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_d + y_d \end{bmatrix}$$

- Vectors can be multiplied by a scalar:

$$a\,\mathbf{x} = a \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix} = \begin{bmatrix} a\,x_1 \\ a\,x_2 \\ \vdots \\ a\,x_d \end{bmatrix}$$



Source: https://mathinsight.org/image/vector_2d_add

Properties of vector spaces

- These two operations generate a lot of nice properties (see https://en.wikipedia.org/wiki/Vector_space for a full list), including:
  - associativity:

$$\mathbf{x} + (\mathbf{y} + \mathbf{z}) = (\mathbf{x} + \mathbf{y}) + \mathbf{z}$$

  - commutativity:

$$\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$$

  - the existence of a zero vector

$$\mathbf{x} + \mathbf{0} = \mathbf{x}$$

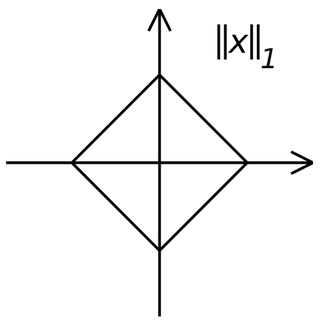
  - inversion:

$$\mathbf{x} + (-\mathbf{x}) = \mathbf{0}$$

  - distributivity:

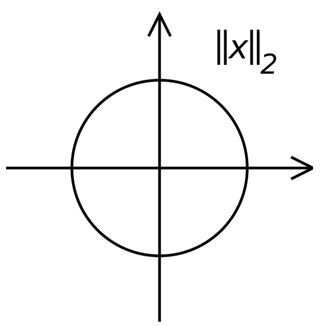
$$a\,(\mathbf{x} + \mathbf{y}) = a\,\mathbf{x} + a\,\mathbf{y}$$

Norm of a vector



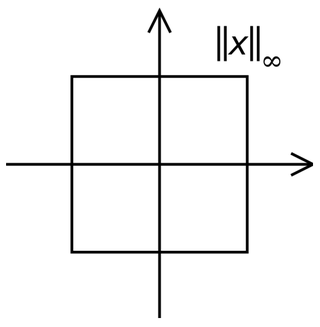
- Vectors have a **norm** (or length) $||\mathbf{x}||$. The most intuitive one (if you know the Pythagoras theorem) is the **Euclidean norm** or L^2-norm, which sums the square of each element:

$$||\mathbf{x}||_2 = \sqrt{x_1^2 + x_2^2 + \ldots + x_d^2}$$



- Other norms exist, distinguished by the subscript. The L^1 **-norm** (also called the Manhattan norm) sums the absolute value of each element:

$$||\mathbf{x}||_1 = |x_1| + |x_2| + \ldots + |x_d|$$



- The **p-norm** generalizes the Euclidean norm to other powers p:

$$||\mathbf{x}||_p = (|x_1|^p + |x_2|^p + \ldots + |x_d|^p)^{\frac{1}{p}}$$

- The **infinity norm** (or maximum norm) L^∞ returns the maximum element of the vector:

$$||\mathbf{x}||_\infty = \max(|x_1|, |x_2|, \ldots, |x_d|)$$

Source:
https://en.wikipedia.org/wiki/Norm_(mathematics)

Dot product

- One important operation for vectors is the **dot product** (also called scalar product or inner product) between two vectors:

$$\langle \mathbf{x} \cdot \mathbf{y} \rangle = \langle \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_d \end{bmatrix} \rangle = x_1\, y_1 + x_2\, y_2 + \ldots + x_d\, y_d$$

- The dot product basically sums one by one the product of the elements of each vector. The angular brackets are sometimes omitted ($\mathbf{x} \cdot \mathbf{y}$) but we will use them in this course for clarity.
- One can notice immediately that the dot product is **symmetric**:

$$\langle \mathbf{x} \cdot \mathbf{y} \rangle = \langle \mathbf{y} \cdot \mathbf{x} \rangle$$

and **linear**:

$$\langle (a\,\mathbf{x} + b\,\mathbf{y}) \cdot \mathbf{z} \rangle = a\,\langle \mathbf{x} \cdot \mathbf{z} \rangle + b\,\langle \mathbf{y} \cdot \mathbf{z} \rangle$$

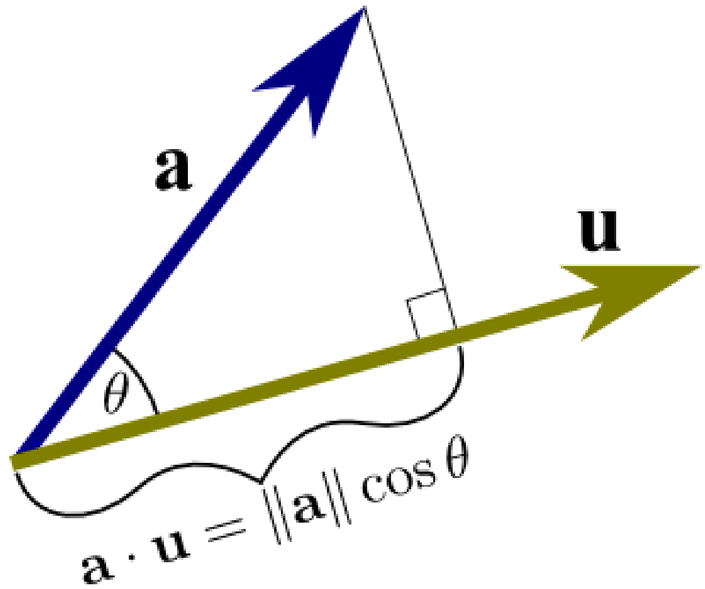
Dot product

- The dot product is an indirect measurement of the **angle** θ between two vectors:

$$\langle \mathbf{x} \cdot \mathbf{y} \rangle = ||\mathbf{x}||_2 \, ||\mathbf{y}||_2 \, \cos(\theta)$$

- If you normalize the two vectors by dividing them by their norm (which is a scalar), we indeed have the cosine of the angle between them
- The higher the normalized dot product, the more the two vectors point towards the same direction (**cosine distance** between two vectors).

$$\langle \frac{\mathbf{x}}{||\mathbf{x}||_2} \cdot \frac{\mathbf{y}}{||\mathbf{y}||_2} \rangle = \cos(\theta)$$



Source: https://mathinsight.org/image/dot_product_projection_unit_vector

Matrices

- Matrices are derived from vectors, so most of the previous properties will be true. Let's consider this 4x3 matrix:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \end{bmatrix}$$

- Each column of the matrix is a vector with 4 elements:

$$\mathbf{a}_1 = \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \end{bmatrix} \qquad \mathbf{a}_2 = \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \\ a_{42} \end{bmatrix} \qquad \mathbf{a}_3 = \begin{bmatrix} a_{13} \\ a_{23} \\ a_{33} \\ a_{43} \end{bmatrix}$$

- A $m \times n$ matrix is therefore a collection of n vectors of size m put side by side column-wise:

$$A = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \mathbf{a}_3 \end{bmatrix}$$

Properties of matrix spaces

- All properties of the vector spaces (associativity, commutativity, distributivity) also apply to matrices, as additions and multiplications with a scalar are defined.

$$\alpha A + \beta B = \begin{bmatrix} \alpha a_{11} + \beta b_{11} & \alpha a_{12} + \beta b_{12} & \alpha a_{13} + \beta b_{13} \\ \alpha a_{21} + \beta b_{21} & \alpha a_{22} + \beta b_{22} & \alpha a_{23} + \beta b_{23} \\ \alpha a_{31} + \beta b_{31} & \alpha a_{32} + \beta b_{32} & \alpha a_{33} + \beta b_{33} \\ \alpha a_{41} + \beta b_{41} & \alpha a_{42} + \beta b_{42} & \alpha a_{43} + \beta b_{43} \end{bmatrix}$$

Note: Beware, you can only add matrices of the same dimensions $m \times n$. You cannot add a 2×3 matrix to a 5×4 one.

Transposition

- The **transpose** A^T of a $m \times n$ matrix A is a $n \times m$ matrix, where the row and column indices are swapped:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}, \qquad A^T = \begin{bmatrix} a_{11} & a_{21} & \cdots & a_{m1} \\ a_{12} & a_{22} & \cdots & a_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{mn} \end{bmatrix}$$

- This is also true for vectors, which become horizontal after transposition:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}, \qquad \mathbf{x}^T = \begin{bmatrix} x_1 & x_2 & \dots & x_d \end{bmatrix}$$

Matrix multiplication

- If A is a $m \times n$ matrix and B a $n \times p$ matrix:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}, \quad B = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1p} \\ b_{21} & b_{22} & \cdots & b_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{np} \end{bmatrix}$$

we can multiply them to obtain a $m \times p$ matrix:

$$C = A \times B = \begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1p} \\ c_{21} & c_{22} & \cdots & c_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ c_{m1} & c_{m2} & \cdots & c_{mp} \end{bmatrix}$$

where each element c_{ij} is the dot product of the ith row of A and jth column of B:

$$c_{ij} = \langle A_{i,:} \cdot B_{:,j} \rangle = a_{i1}b_{1j} + a_{i2}b_{2j} + \cdots + a_{in}b_{nj} = \sum_{k=1}^{n} a_{ik}b_{kj}$$

Note: n, the number of columns of A and rows of B, must be the same!

Matrix multiplication

- The element c_{ij} of $C = A \times B$ is the dot product between the ith row of A and the jth column of B.

$$c_{11} = a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} + a_{14}b_{41}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \\ b_{41} & b_{42} & b_{43} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \end{bmatrix}$$

2 x 4 4 x 3 2 x 3

$$c_{22} = a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32} + a_{24}b_{42}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \\ b_{41} & b_{42} & b_{43} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \end{bmatrix}$$

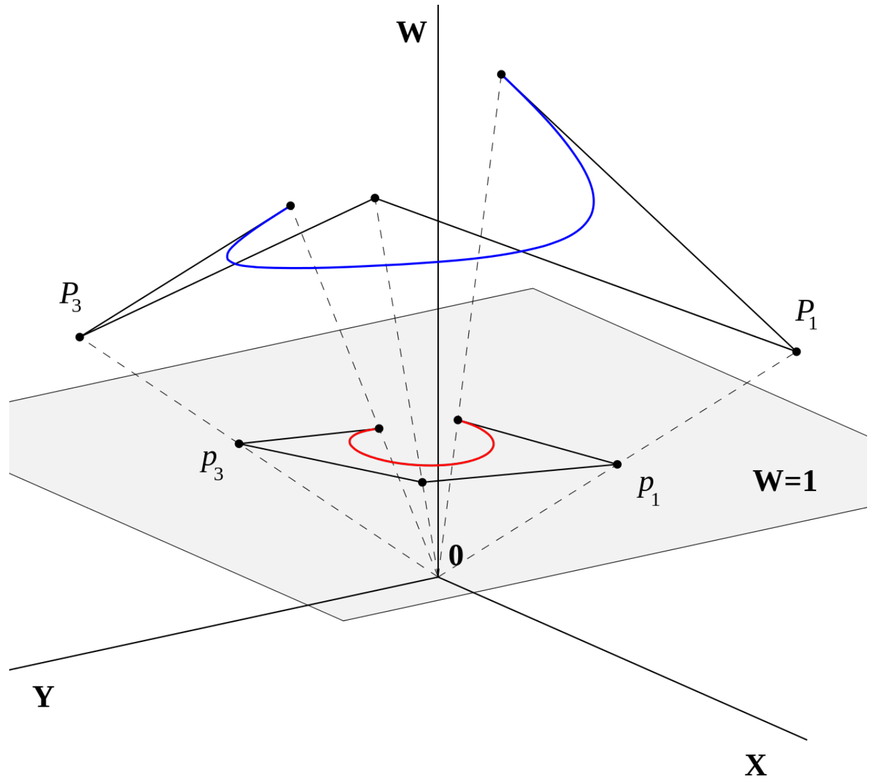
Source:
https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Book%3A_Mathematical_Methods_in_Chemistry_(Levitus)/15%3A_

Matrix-vector multiplication

- Thinking of vectors as $n \times 1$ matrices, we can multiply a matrix $m \times n$ with a vector:

$$\mathbf{y} = A \times \mathbf{x} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

- The result $\mathbf{y}$ is a vector of size m.
- In that sense, a matrix A can transform a vector of size n into a vector of size m:
  - A represents a **projection** from $\mathfrak{R}^n$ to $\mathfrak{R}^m$.



Source:
https://en.wikipedia.org/wiki/Homogeneous_coordinate

Dot product

- Note that the **dot product** between two vectors of size n is the matrix multiplication between the transpose of the first vector and the second one:

$$\mathbf{x}^T \times \mathbf{y} = \begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix} \times \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = x_1\, y_1 + x_2\, y_2 + \dots + x_n\, y_n = \langle \mathbf{x} \cdot \mathbf{y} \rangle$$

Matrix inversion

- Square matrices of size $n \times n$ can be inverted.
- The **inverse** A^{-1} of a matrix A is defined by:

$$A \times A^{-1} = A^{-1} \times A = I$$

where I is the identity matrix (a matrix with ones on the diagonal and 0 otherwise).

- Matrix inversion allows to solve linear systems of equations. Given the problem:

$$\begin{cases} a_{11}\, x_1 + a_{12}\, x_2 + \ldots + a_{1n}\, x_n = b_1 \\ a_{21}\, x_1 + a_{22}\, x_2 + \ldots + a_{2n}\, x_n = b_2 \\ \ldots \\ a_{n1}\, x_1 + a_{n2}\, x_2 + \ldots + a_{nn}\, x_n = b_n \end{cases}$$

which is equivalent to:

$$A \times \mathbf{x} = \mathbf{b}$$

- We can multiply both sides to the left with A^{-1} (if it exists) and obtain:

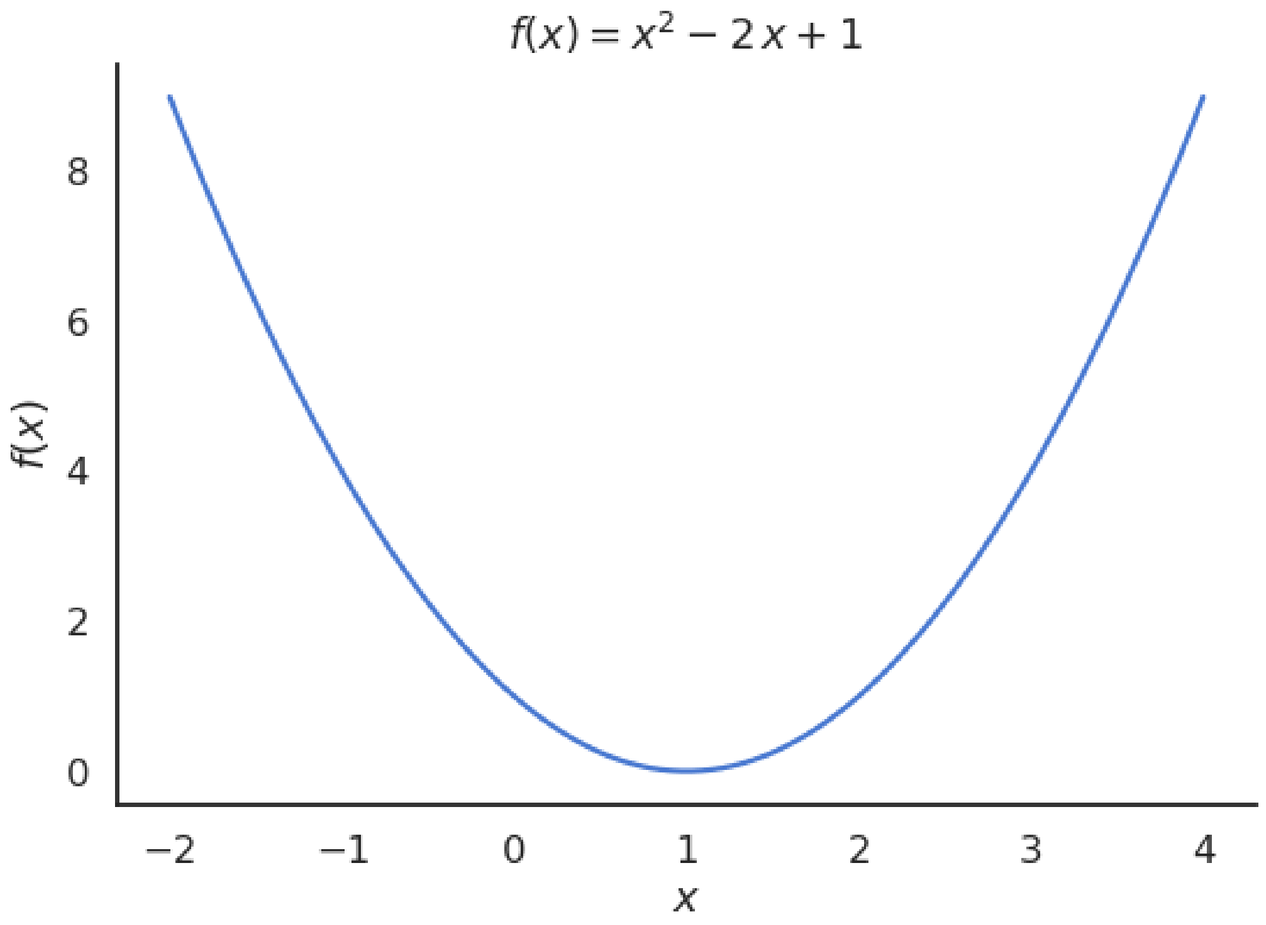
$$\mathbf{x} = A^{-1} \times \mathbf{b}$$

2 - Calculus

Univariate functions

- A **univariate function** f associates to any real number $x \in \mathfrak{R}$ (or a subset of $\mathfrak{R}$ called the support of the function) another (unique) real number $f(x)$:

$$\begin{aligned} f: \quad & \mathfrak{R} \to \mathfrak{R} \\ & x \mapsto f(x), \end{aligned}$$



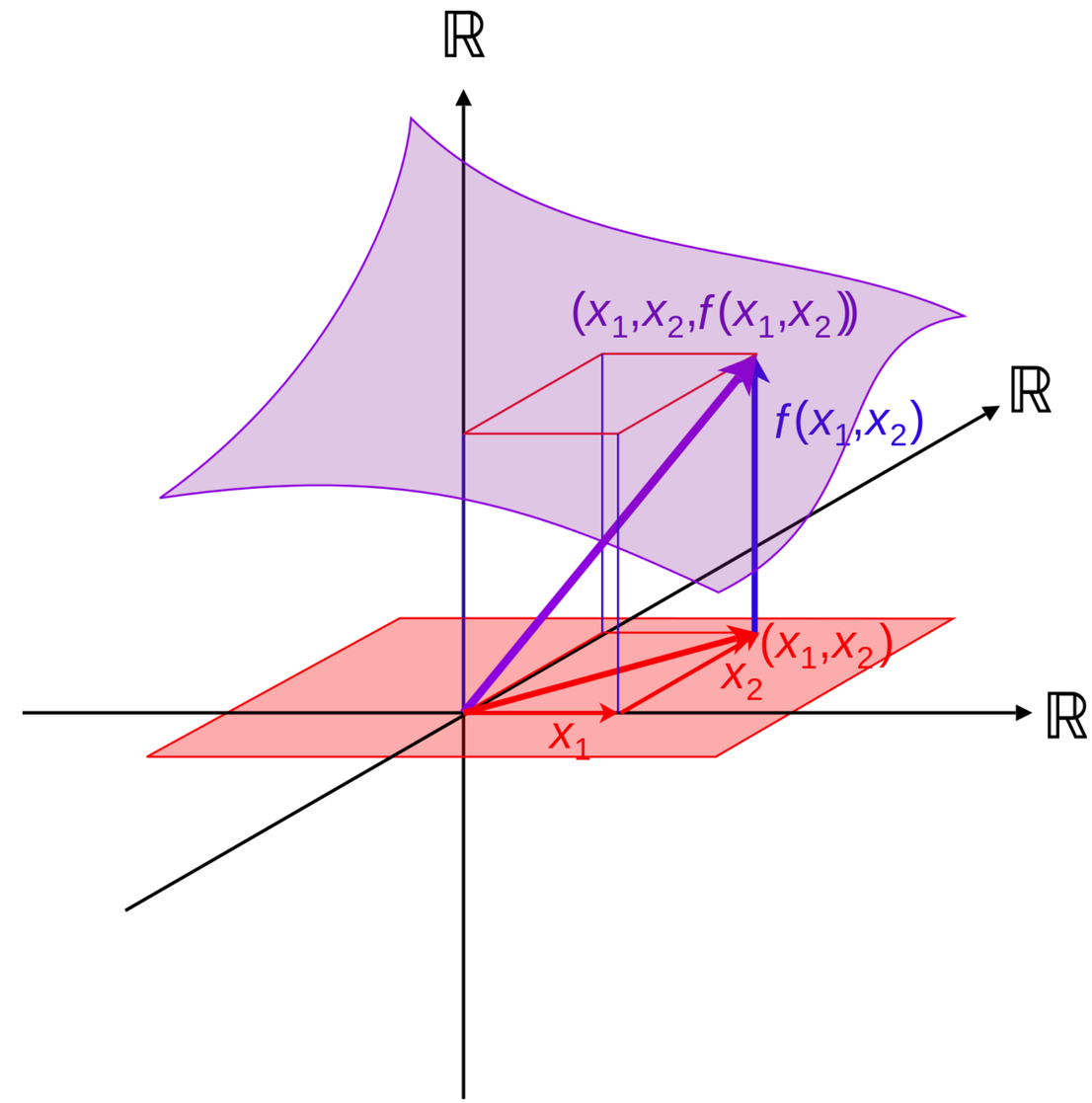
Multivariate functions

- A **multivariate function** f associates to any vector $\mathbf{x} \in \mathfrak{R}^n$ (or a subset) a real number $f(\mathbf{x})$:

$$f: \quad \mathfrak{R}^n \to \mathfrak{R}$$
$$\mathbf{x} \mapsto f(\mathbf{x}),$$

- The variables of the function are the elements of the vector.
- For low-dimensional vector spaces, it is possible to represent each element explicitly, for example:

$$f: \quad \mathfrak{R}^3 \to \mathfrak{R}$$
$$x, y, z \mapsto f(x, y, z),$$

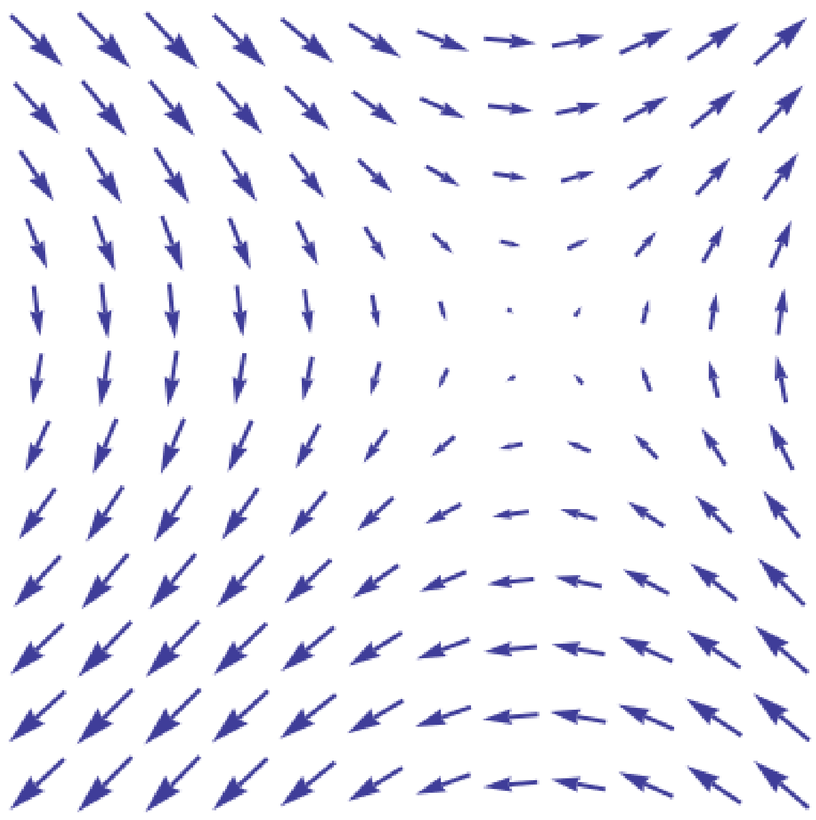


Source: https://en.wikipedia.org/wiki/Function_of_several_real_variables

Vector fields

- **Vector fields** associate to any vector $\mathbf{x} \in \mathfrak{R}^n$ (or a subset) another vector (possibly of different size):

$$\begin{aligned} \vec{f}: \quad & \mathfrak{R}^n \rightarrow \mathfrak{R}^m \\ & \mathbf{x} \mapsto \vec{f}(\mathbf{x}), \end{aligned}$$



Source: https://en.wikipedia.org/wiki/Vector_field

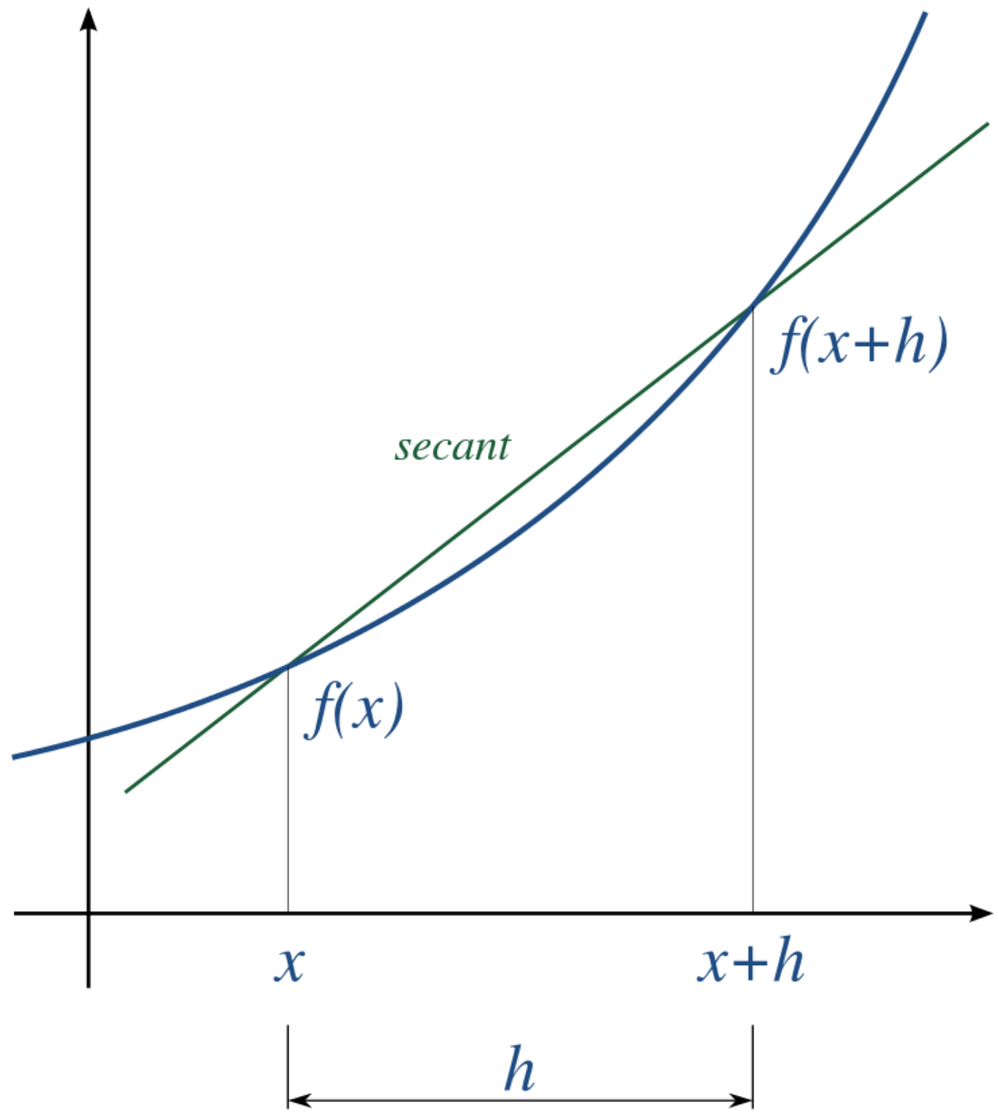
Note: The matrix-vector multiplication $\mathbf{y} = A \times \mathbf{x}$ is a linear vector field, mapping any vector $\mathbf{x}$ into another vector $\mathbf{y}$.

Differentiation

- Differential calculus deals with the **derivative** of a function, a process called differentiation.
- The derivative $f'(x)$ or $\frac{df(x)}{dx}$ of a univariate function $f(x)$ is defined as the local *slope* of the tangent to the function for a given value of x:

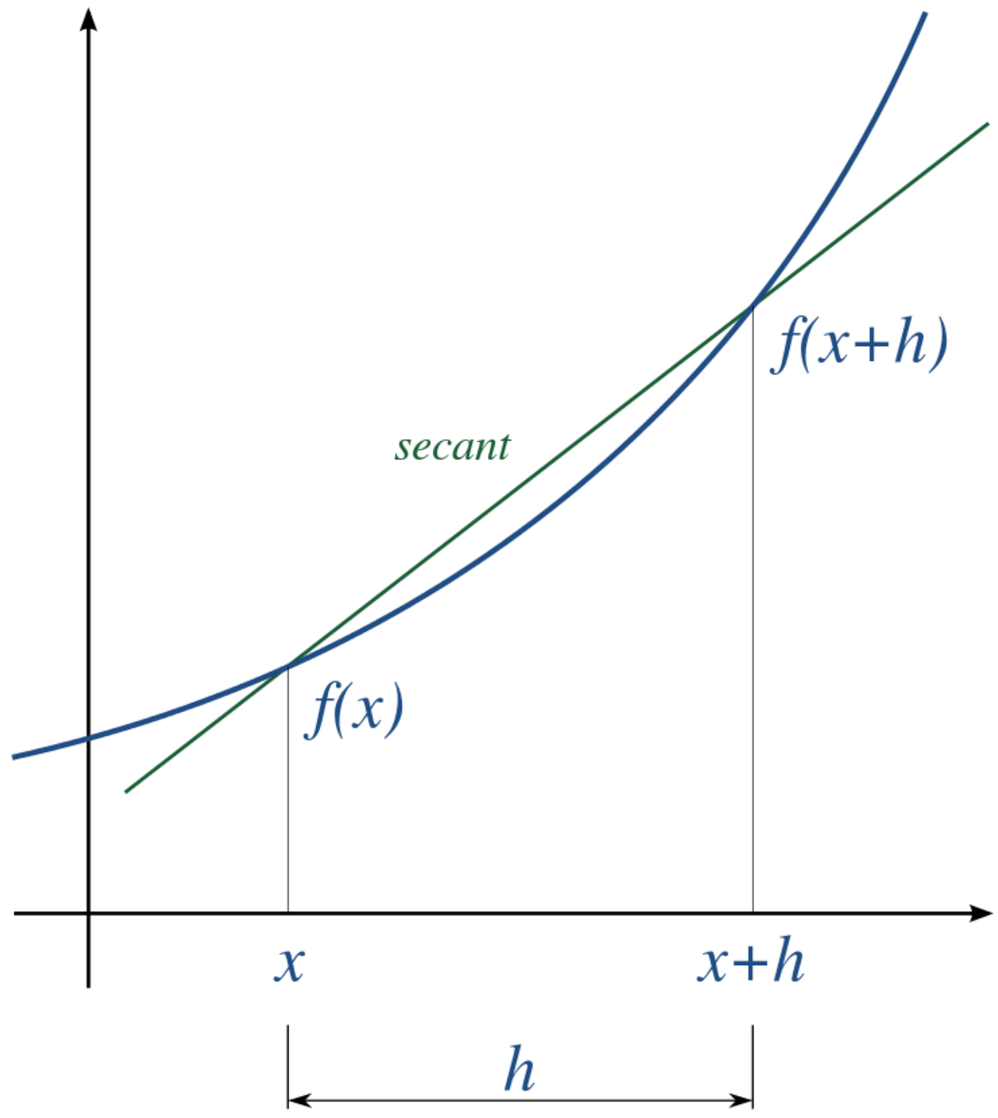
$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- The line passing through the points $(x, f(x))$ and $(x+h, f(x+h))$ becomes tangent to the function when h becomes very small.



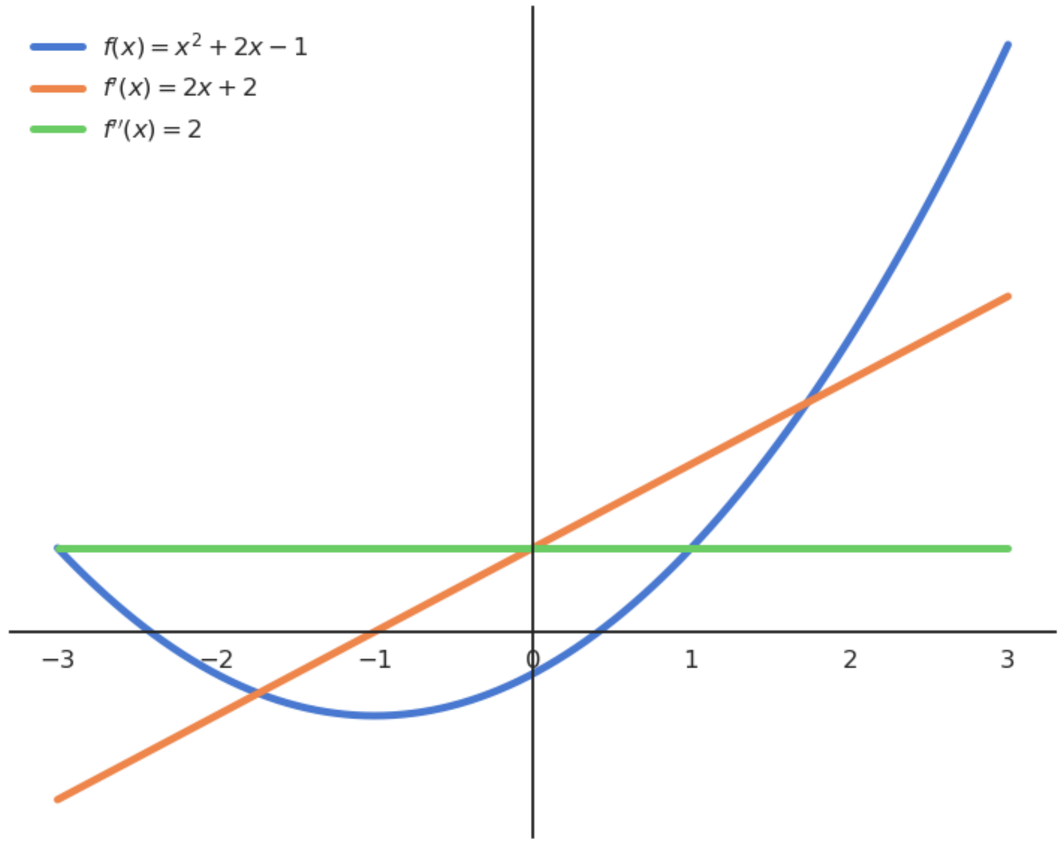
Differentiation

- The sign of the derivative tells you how the function behaves locally:
    - If the derivative is positive, increasing a little bit x increases the function $f(x)$, so the function is **locally increasing**.
    - If the derivative is negative, increasing a little bit x decreases the function $f(x)$, so the function is **locally decreasing**.
- It basically allows you to measure the local influence of x on $f(x)$: if I change a little bit the value x, what happens to $f(x)$? This will be very useful in machine learning.



Extrema

- A special case is when the derivative is equal to 0 in x. x is then called an **extremum** (or optimum) of the function, i.e. it can be a maximum or minimum.
- You can tell whether an extremum is a maximum or a minimum by looking at its second-order derivative:
  - If $f''(x) > 0$, the extremum is a **minimum**.
  - If $f''(x) < 0$, the extremum is a **maximum**.
  - If $f''(x) = 0$, the extremum is a **saddle point**.



Gradients

- The derivative of a **multivariate function** $f(\mathbf{x})$ is a vector of partial derivatives called the **gradient of the function** $\nabla_{\mathbf{x}} f(\mathbf{x})$:

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \\ \cdots \\ \frac{\partial f(\mathbf{x})}{\partial x_n} \end{bmatrix}$$

- The subscript to the ∇ operator denotes *with respect to* (w.r.t) which variable the differentiation is done.

Partial derivatives

- A **partial derivative** w.r.t. to particular variable (or element of the vector) is simply achieved by differentiating the function while considering all other variables to be **constant**. For example the function:

$$f(x, y) = x^2 + 3\,x\,y + 4\,x\,y^2 - 1$$

can be partially differentiated w.r.t. x and y as:

$$\begin{cases} \dfrac{\partial f(x, y)}{\partial x} = 2\,x + 3\,y + 4\,y^2 \\ \dfrac{\partial f(x, y)}{\partial y} = 3\,x + 8\,x\,y \end{cases}$$

Jacobian

- The gradient can be generalized to **vector fields**, where the **Jacobian** or **Jacobi matrix** is a matrix containing all partial derivatives.

$$J = \begin{bmatrix} \dfrac{\partial \mathbf{f}}{\partial x_1} & \cdots & \dfrac{\partial \mathbf{f}}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} & \cdots & \dfrac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_m}{\partial x_1} & \cdots & \dfrac{\partial f_m}{\partial x_n} \end{bmatrix}$$

Analytical properties

- Differentiation is linear, which means that if we define the function:

$$h(x) = a\,f(x) + b\,g(x)$$

its derivative is:

$$h'(x) = a\,f'(x) + b\,g'(x)$$

- A product of functions can also be differentiated analytically (product rule):

$$(f(x) \times g(x))' = f'(x) \times g(x) + f(x) \times g'(x)$$

Example:

$$f(x) = x^2\,e^x$$

$$f'(x) = 2\,x\,e^x + x^2 \cdot e^x$$

Chain rule

- A very important concept for neural networks is the **chain rule**, which tells how to differentiate **function compositions** (functions of a function) of the form:

$$(f \circ g)(x) = f(g(x))$$

- The derivative of $f \circ g$ is:

$$(f \circ g)'(x) = (f' \circ g)(x) \times g'(x)$$

- The chain rule may be more understandable using Leibniz's notation:

$$\frac{d(f \circ g)(x)}{dx} = \frac{df(g(x))}{dg(x)} \times \frac{dg(x)}{dx}$$

- By posing $y = g(x)$ as an intermediary variable, it becomes:

$$\frac{df(y)}{dx} = \frac{df(y)}{dy} \times \frac{dy}{dx}$$

Chain rule

- The function :

$$h(x) = \frac{1}{2\,x + 1}$$

is the function composition of $g(x) = 2\,x + 1$ and $f(x) = \frac{1}{x}$, whose derivatives are known:

$$g'(x) = 2$$

$$f'(x) = -\frac{1}{x^2}$$

- Its derivative according to the **chain rule** is:

$$h'(x) = f'(g(x)) \times g'(x) = -\frac{1}{(2\,x + 1)^2} \times 2$$

Chain rule

- The chain rule also applies to partial derivatives:

$$\frac{\partial f \circ g(x,y)}{\partial x} = \frac{\partial f \circ g(x,y)}{\partial g(x,y)} \times \frac{\partial g(x,y)}{\partial x}$$

and gradients:

$$\nabla_{\mathbf{x}} f \circ g(\mathbf{x}) = \nabla_{g(\mathbf{x})} f \circ g(\mathbf{x}) \times \nabla_{\mathbf{x}}\, g(\mathbf{x})$$

Integrals

- The opposite operation of differentation is **integration**. Given a function $f(x)$, we search a function $F(x)$ whose *derivative* is $f(x)$:

$$F'(x) = f(x)$$

- The **integral** of f is noted:

$$F(x) = \int f(x)\,dx$$

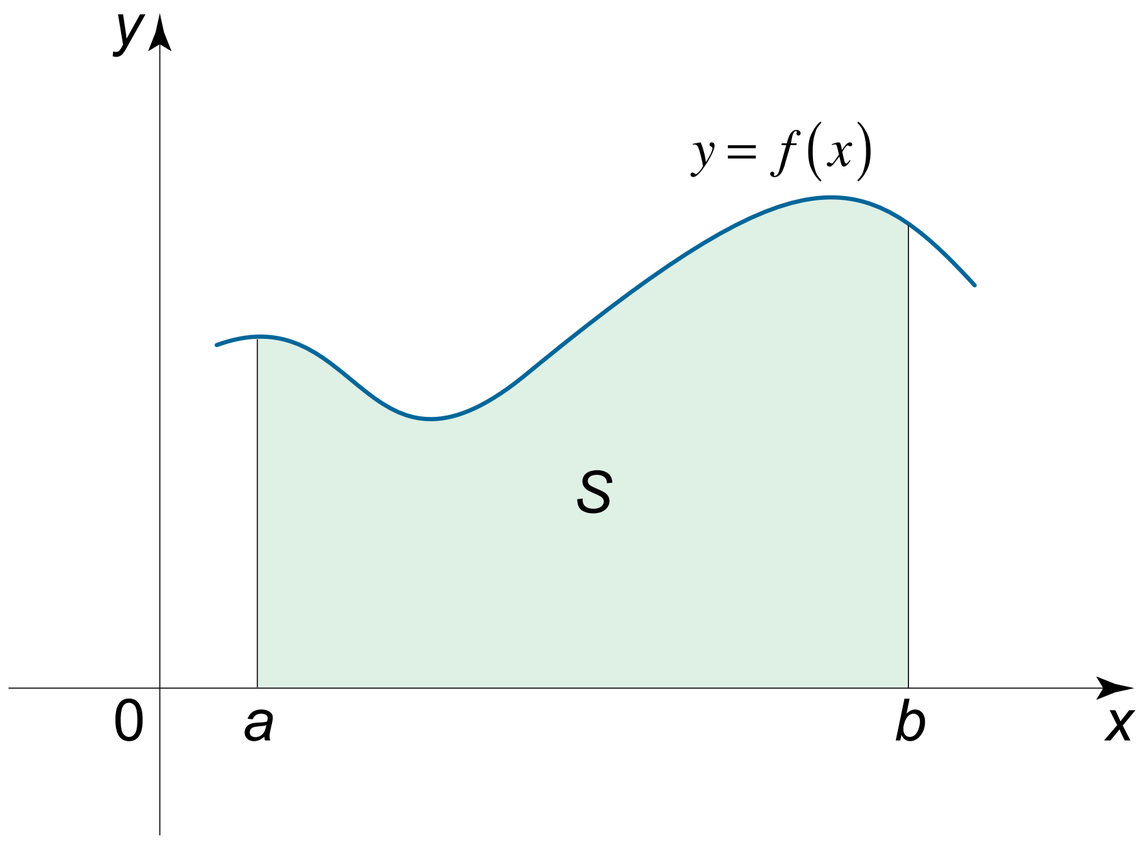
dx being an infinitesimal interval (similar to h in the definition of the derivative).

- There are tons of formal definitions of integrals (Riemann, Lebesgue, Darboux…) and we will not get into details here as we will not use integrals a lot.

Integrals

- The most important to understand for now is maybe that the integral of a function is the **area under the curve**.
- The area under the curve of a function f on the interval $[a, b]$ is:

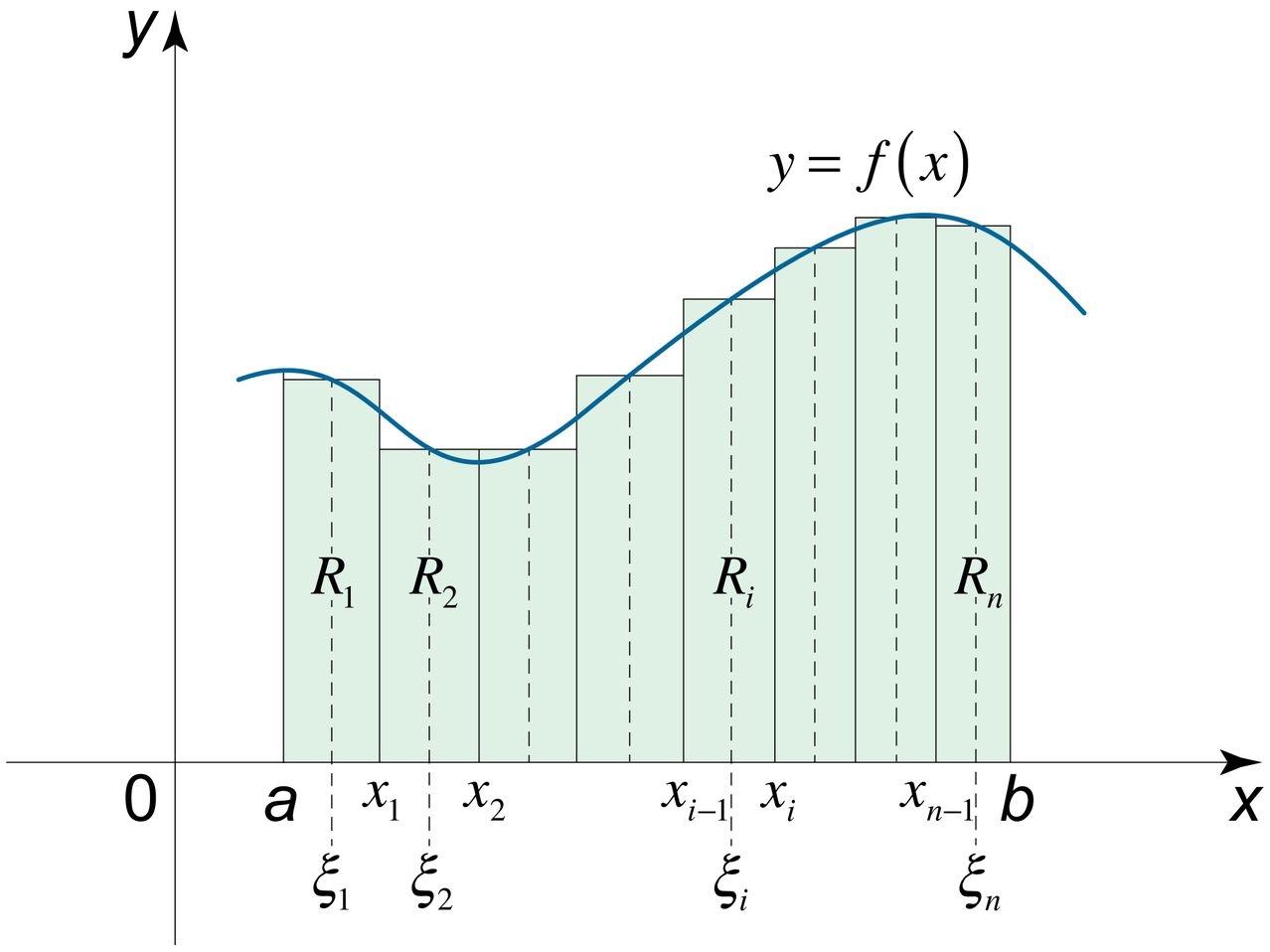
$$S = \int_a^b f(x)\,dx$$



Source: https://www.math24.net/riemann-sums-definite-integral/

Integrals

- One way to approximate this surface is to split the interval $[a, b]$ into n intervals of width dx with the points $x_1, x_2, \ldots, x_n$.
- This defines n rectangles of width dx and height $f(x_i)$, so their surface is $f(x_i)\,dx$.
- The area under the curve can then be approximated by the sum of the surfaces of all these rectangles.



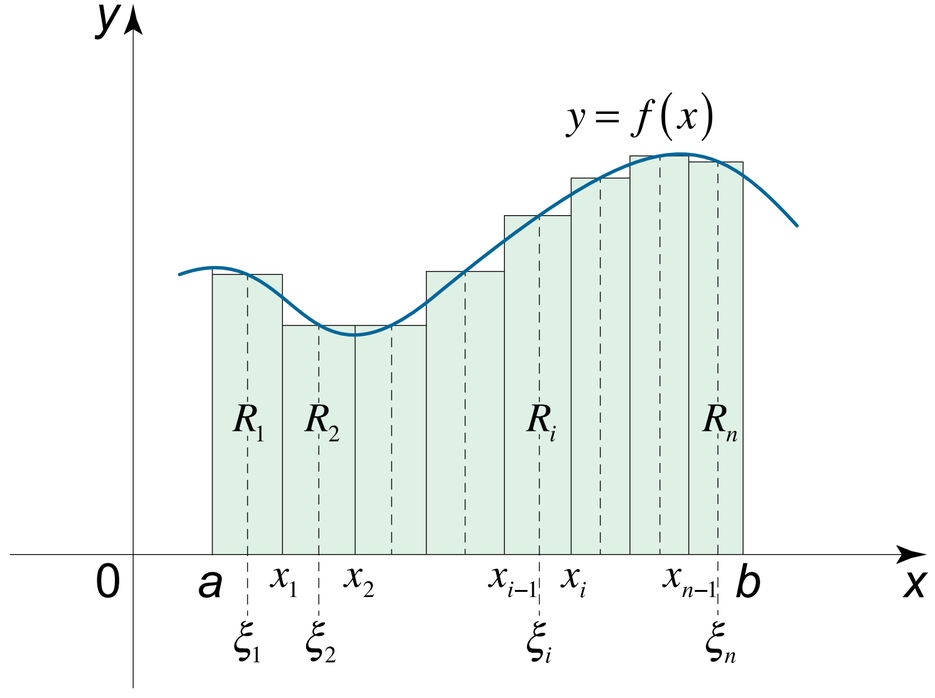
Source: https://www.math24.net/riemann-sums-definite-integral/

Integrals

- When $n \to \infty$, or equivalently $dx \to 0$, the sum of these rectangular areas (called the Riemann sum) becomes exactly the area under the curve. This is the definition of the definite integral:

$$\int_a^b f(x)\,dx = \lim_{dx \to 0} \sum_{i=1}^{n} f(x_i)\,dx$$

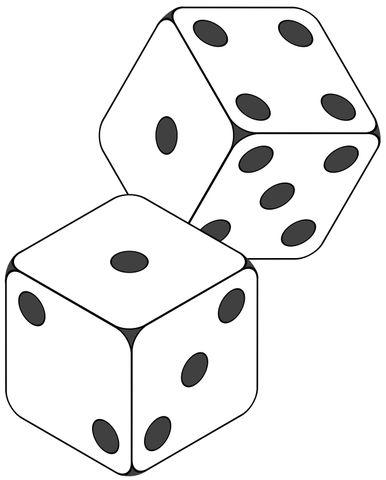
- Very roughly speaking, the integral can be considered as the equivalent of a sum for continuous functions.



Source: https://www.math24.net/riemann-sums-definite-integral/

3 - Probability theory

Discrete probability distributions



Credit: https://commons.wikimedia.org/wiki/File:2-Dice-Icon.svg

- Let's note X a **discrete random variable** with n realizations (or outcomes) $x_1, \ldots, x_n$.
- The **probability** that X takes the value x_i is defined by the *relative frequency of occurrence*, i.e. the proportion of samples having the value x_i, when the total number N of samples tends to infinity:

$$P(X = x_i) = \frac{\text{Number of favorable cases}}{\text{Total number of samples}}$$

- The set of probabilities $\{P(X = x_i)\}_{i=1}^{n}$ define the **probability distribution** for the random variable (or probability mass function, pmf).
- By definition, we have $0 \leq P(X = x_i) \leq 1$ and the probabilities **have** to respect:

$$\sum_{i=1}^{n} P(X = x_i) = 1$$

Mathematical expectation and variance

- An important metric for a random variable is its **mathematical expectation** or expected value, i.e. its “mean” realization weighted by the probabilities:

$$\mathbb{E}[X] = \sum_{i=1}^{n} P(X = x_i)\, x_i$$

- The expectation does not even need to be a valid realization:

$$\mathbb{E}[\text{Coin}] = \frac{1}{2}\,0 + \frac{1}{2}\,1 = 0.5$$

$$\mathbb{E}[\text{Dice}] = \frac{1}{6}\,(1 + 2 + 3 + 4 + 5 + 6) = 3.5$$

- We can also compute the mathematical expectation of **functions of** a random variable:

$$\mathbb{E}[f(X)] = \sum_{i=1}^{n} P(X = x_i) f(x_i)$$

Mathematical expectation and variance

- The **variance** of a random variable is the squared deviation around the mean:

$$\mathrm{Var}(X) = \mathbb{E}[(X - \mathbb{E}[X])^2] = \sum_{i=1}^{n} P(X = x_i)\,(x_i - \mathbb{E}[X])^2$$

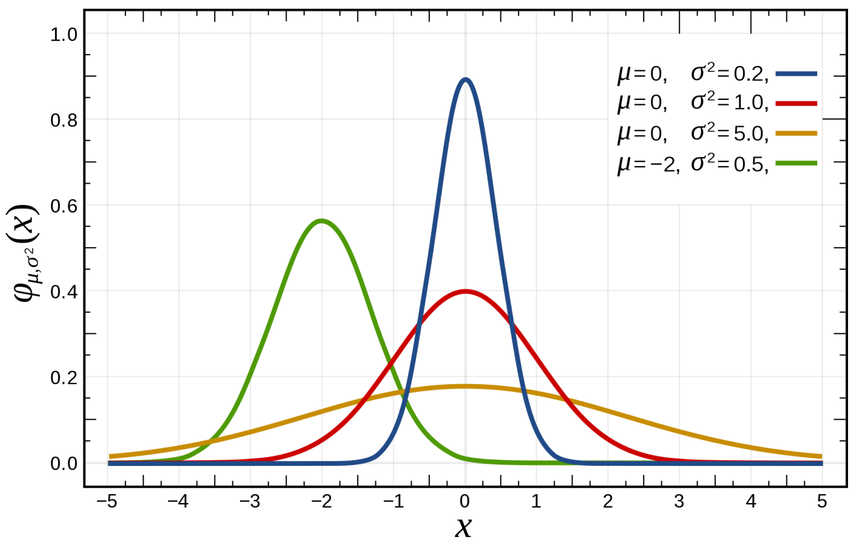
- Variance of a coin:

$$\mathrm{Var}(\mathrm{Coin}) = \frac{1}{2}\,(0 - 0.5)^2 + \frac{1}{2}\,(1 - 0.5)^2 = 0.25$$

- Variance of a dice:

$$\mathrm{Var}(\mathrm{Dice}) = \frac{1}{6}\,((1 - 3.5)^2 + (2 - 3.5)^2 + (3 - 3.5)^2 + (4 - 3.5)^2 + (5 - 3.5)^2 + (6 - 3.5)^2) = \frac{105}{36}$$

Continuous probability distributions



Source: https://en.wikipedia.org/wiki/Normal_distribution

- **Continuous random variables** can take an infinity of continuous values, e.g. $\mathfrak{R}$ or some subset.
- The closed set of values they can take is called the **support** $\mathcal{D}_X$ of the probability distribution.
- The probability distribution is described by a **probability density function** (pdf) $f(x)$.
- The pdf of a distribution must be positive ($f(x) \geq 0 \, \forall x \in \mathcal{D}_X$) and its integral must be equal to 1:

$$\int_{x \in \mathcal{D}_X} f(x) \, dx = 1$$

- The pdf does not give the probability of taking a particular value x (it is 0), but allows to get the probability that a value lies in a specific interval:

$$P(a \leq X \leq b) = \int_a^b f(x) \, dx$$

- One can however think of the pdf as the **likelihood** that a value x comes from that distribution.

Expectation and variance of continuous distributions

- The mathematical expectation is now defined by an integral instead of a sum:

$$\mathbb{E}[X] = \int_{x \in \mathcal{D}_X} f(x)\, x\, dx$$

the variance:

$$\mathrm{Var}(X) = \int_{x \in \mathcal{D}_X} f(x)\, (x - \mathbb{E}[X])^2\, dx$$

or a function of the random variable:

$$\mathbb{E}[g(X)] = \int_{x \in \mathcal{D}_X} f(x)\, g(x)\, dx$$

- Note that the expectation operator is **linear**:

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

Some parameterized probability distributions

- Probability distributions can in principle have any form: $f(x)$ is unknown.
- However, specific parameterized distributions can be very useful: their pmf/pdf is fully determined by a couple of parameters.
- The **Bernouilli** distribution is a binary (discrete, 0 or 1) distribution with a parameter p specifying the probability to obtain the outcome 1:

$$P(X = 1) = p \text{ and } P(X = 0) = 1 - p$$

$$P(X = x) = p^x \, (1 - p)^{1-x}$$

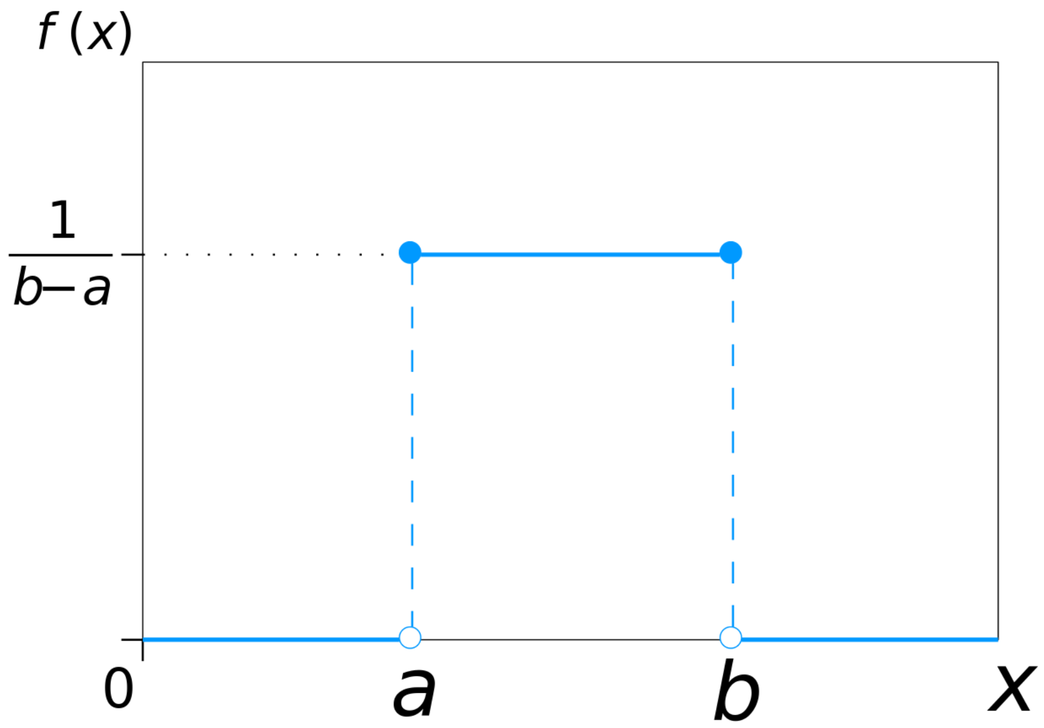
$$\mathbb{E}[X] = p$$

- The **Multinouilli** or **categorical** distribution is a discrete distribution with k realizations. Each realization x_i is associated with a parameter $p_i > 0$ representing its probability. We have $\sum_i p_i = 1$.

$$P(X = x_i) = p_i$$

- Knowing p or the p_i tells us everything about the discrete distributions.

The uniform distribution



Credit: https://en.wikipedia.org/wiki/Uniform_distribution_(continuous)

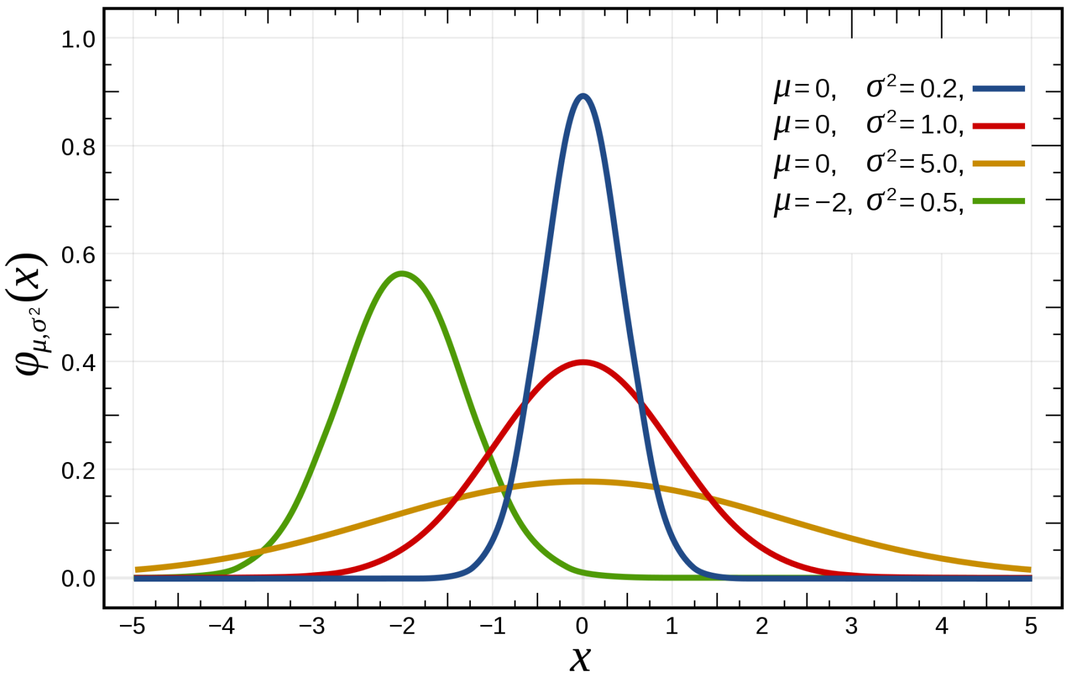
- The **uniform distribution** has an equal and constant probability of returning values between a and b, never outside this range.
- It is parameterized by two parameters:
  - the start of the range a.
  - the end of the range b.
- Its support is $[a, b]$.

- The pdf of the uniform distribution $\mathcal{U}(a, b)$ is defined on $[a, b]$ as:

$$f(x; a, b) = \frac{1}{b - a}$$

- Knowing a and b completely defines the distribution.

The normal or Gaussian distribution



Credit: https://en.wikipedia.org/wiki/Normal_distribution

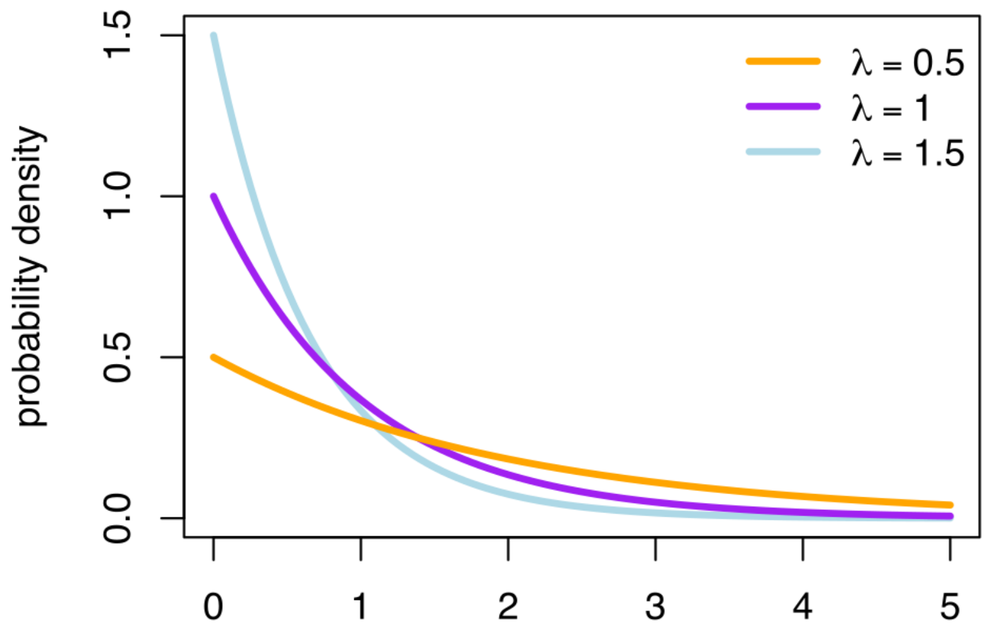
- For continuous distributions, the **normal distribution** is the most frequently encountered one.
- It is parameterized by two parameters:
  - the mean μ.
  - the variance σ^2 (or standard deviation σ).
- Its support is $\mathfrak{R}$.

- The pdf of the normal distribution $\mathcal{N}(\mu, \sigma)$ is defined on $\mathfrak{R}$ as:

$$f(x; \mu, \sigma) = \frac{1}{\sqrt{2\,\pi\,\sigma^2}}\, e^{-\dfrac{(x-\mu)^2}{2\,\sigma^2}}$$

- Knowing μ and σ completely defines the distribution.

The exponential distribution



Credit: https://en.wikipedia.org/wiki/Exponential_distribution

- The **exponential distribution** is the probability distribution of the time between events in a Poisson point process, i.e., a process in which events occur continuously and independently at a constant average rate.
- It is parameterized by one parameter:
  - the rate λ.
- Its support is $\mathfrak{R}^+$ $(x > 0)$.

- The pdf of the exponential distribution is defined on $\mathfrak{R}^+$ as:

$$f(x; \lambda) = \lambda\, e^{-\lambda\, x}$$

- Knowing λ completely defines the distribution.

Joint probabilities

- Let's now suppose that we have two random variables X and Y with different probability distributions $P(X)$ and $P(Y)$.
- The **joint probability** $P(X, Y)$ denotes the probability of observing the realizations x **and** y at the same time:

$$P(X = x, Y = y)$$

- If the random variables are **independent**, we have:

$$P(X = x, Y = y) = P(X = x)\,P(Y = y)$$

- If you know the joint probability, you can compute the **marginal probability distribution** of each variable:

$$P(X = x) = \sum_{y} P(X = x, Y = y)$$

- The same is true for continuous probability distributions:

$$f(x) = \int f(x, y)\,dy$$

Conditional probabilities

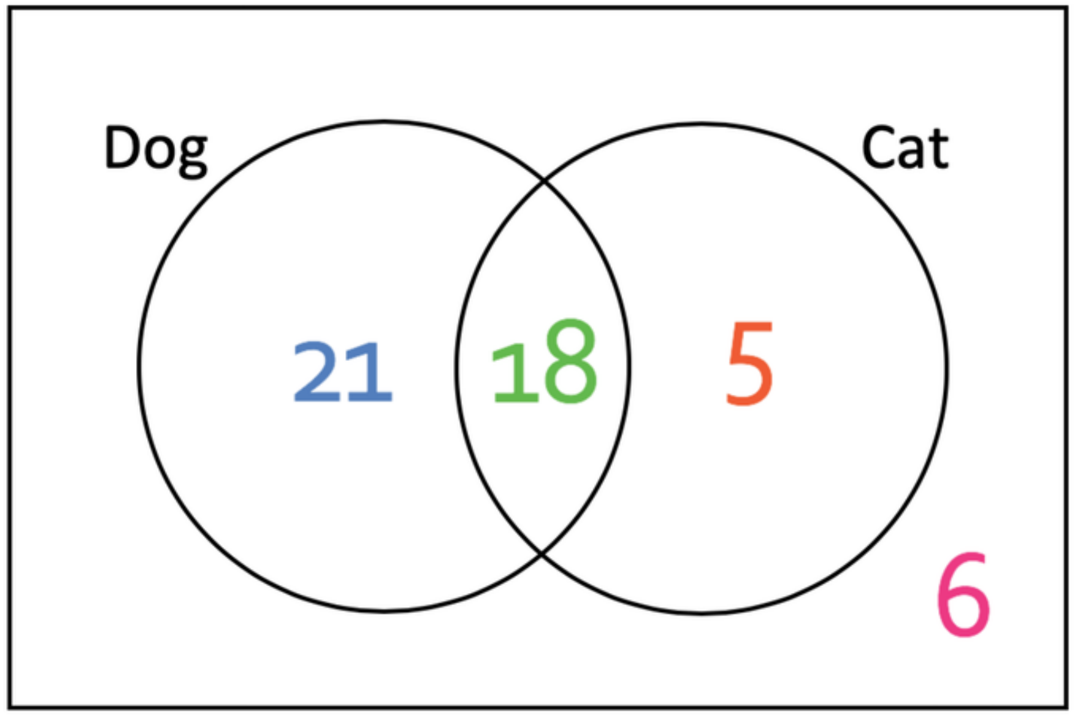
- Some useful information between two random variables is the **conditional probability**.
- $P(X = x|Y = y)$ is the conditional probability that $X = x$, **given** that $Y = y$ is observed.
- $Y = y$ is not random anymore: it is a **fact** (at least theoretically).
- You wonder what happens to the probability distribution of X now that you know the value of Y.
- Conditional probabilities are linked to the joint probability by:

$$P(X = x|Y = y) = \frac{P(X = x, Y = y)}{P(Y = y)}$$

- If X and Y are **independent**, we have $P(X = x|Y = y) = P(X = x)$ (knowing Y does not change anything to the probability distribution of X).
- We can use the same notation for the complete probability distributions:

$$P(X|Y) = \frac{P(X, Y)}{P(Y)}$$

Joint and conditional probabilities: using a Venn diagram



Credit: https://www.elevise.co.uk/g-e-m-h-5-u.html

- You ask 50 people whether they like cats or dogs:
  - 18 like both cats and dogs.
  - 21 like only dogs.
  - 5 like only cats.
  - 6 like none of them.
- We consider loving cats and dogs as random variables (and that our sample size is big enough to use probabilities…)
- We have $P(\text{dog}) = \frac{18+21}{50}$ and $P(\text{cat}) = \frac{18+5}{50}$.
- Among the 23 who love cats, which proportion also loves dogs?

- The joint probability of loving both cats and dogs is $P(\text{cat}, \text{dog}) = \frac{18}{50}$.
- The conditional probability of loving dogs given one loves cats is:

$$P(\text{dog}|\text{cat}) = \frac{P(\text{cat}, \text{dog})}{P(\text{cat})} = \frac{\frac{18}{50}}{\frac{23}{50}} = \frac{18}{23}$$

Bayes' rule

- Noticing that the definition of conditional probabilities is symmetric:

$$P(X, Y) = P(X|Y)\,P(Y) = P(Y|X)\,P(X)$$

we can obtain the **Bayes' rule**:

$$P(Y|X) = \frac{P(X|Y)\,P(Y)}{P(X)}$$

- It is very useful when you already know $P(X|Y)$ and want to obtain $P(Y|X)$ (**Bayesian inference**).
  - $P(Y|X)$ is called the **posterior probability**.
  - $P(X|Y)$ is called the **likelihood**.
  - $P(Y)$ is called the **prior probability** (belief).
  - $P(X)$ is called the **model evidence** or **marginal likelihood**.

Bayes' rule : example

- Let's consider a disease D (binary random variable) and a medical test T (also binary). The disease affects 10% of the general population:

$$P(D = 1) = 0.1 \qquad P(D = 0) = 0.9$$

- When a patient has the disease, the test is positive 80% of the time:

$$P(T = 1|D = 1) = 0.8 \qquad P(T = 0|D = 1) = 0.2$$

- When a patient does not have the disease, the test is still positive 10% of the time:

$$P(T = 1|D = 0) = 0.1 \qquad P(T = 0|D = 0) = 0.9$$

- Given that the test is positive, what is the probability that the patient is ill?

Bayes' rule : example

$$P(D=1|T=1) = \frac{P(T=1|D=1)\,P(D=1)}{P(T=1)}$$

$$= \frac{P(T=1|D=1)\,P(D=1)}{P(T=1|D=1)\,P(D=1) + P(T=1|D=0)\,P(D=0)}$$

$$= \frac{0.8 \times 0.1}{0.8 \times 0.1 + 0.1 \times 0.9}$$

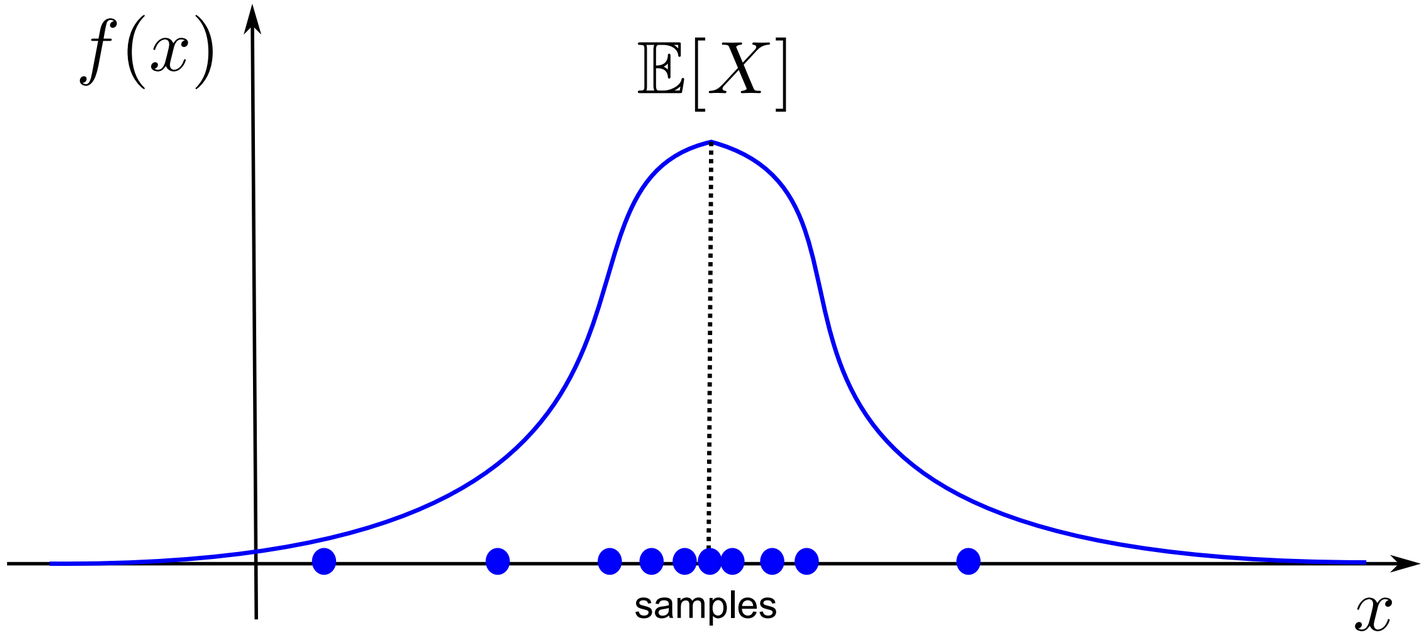
$$= 0.47$$

4 - Statistics

Random sampling / Monte Carlo sampling

- In ML, we will deal with random variables whose exact probability distribution is unknown, but we are interested in their expectation or variance anyway.
- **Random sampling** or **Monte Carlo sampling** (MC) consists of taking N samples x_i out of the distribution X (discrete or continuous) and computing the **sample average**:

$$\mathbb{E}[X] = \mathbb{E}_{x \sim X}[x] \approx \frac{1}{N} \sum_{i=1}^{N} x_i$$



- More samples will be obtained where $f(x)$ is high (x is probable), so the average of the sampled data will be close to the expected value of the distribution.

Random sampling / Monte Carlo sampling

Law of big numbers

> As the number of identically distributed, randomly generated variables increases, their sample mean (average) approaches their theoretical mean.

MC estimates are only correct when:

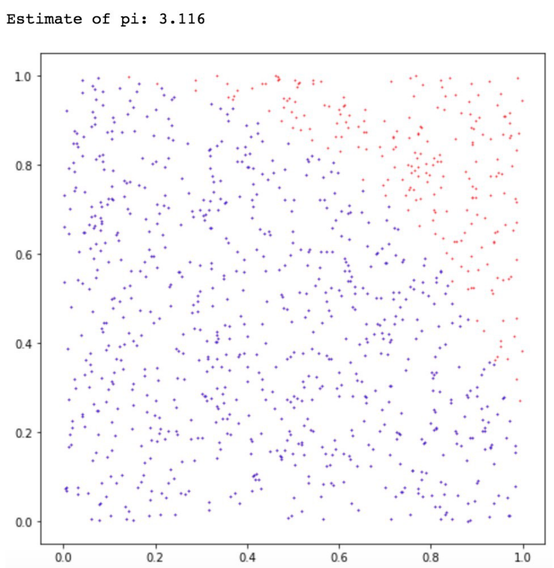
- the samples are **i.i.d** (independent and identically distributed):
  - independent: the samples must be unrelated with each other.
  - identically distributed: the samples must come from the same distribution X.
- the number of samples is large enough. Usually $N > 30$ for simple distributions.

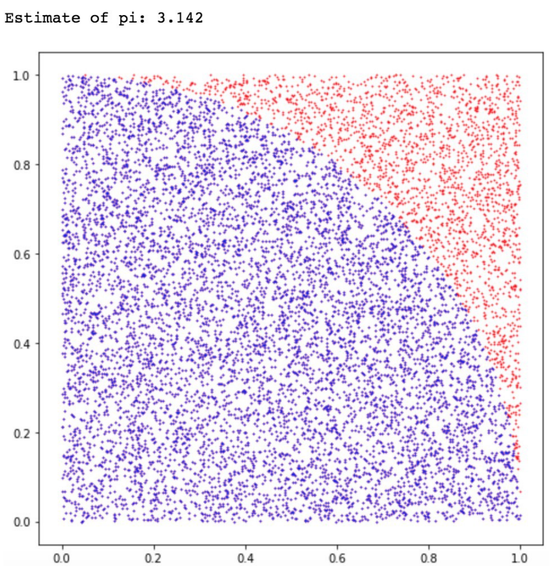
Random sampling / Monte Carlo sampling

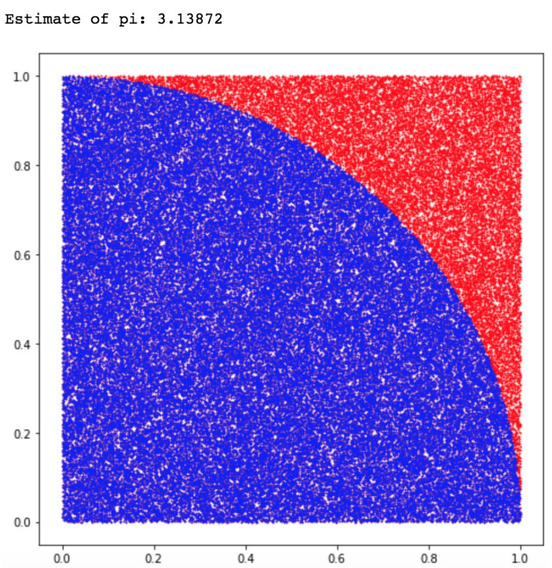
- One can estimate any function of the random variable with random sampling:

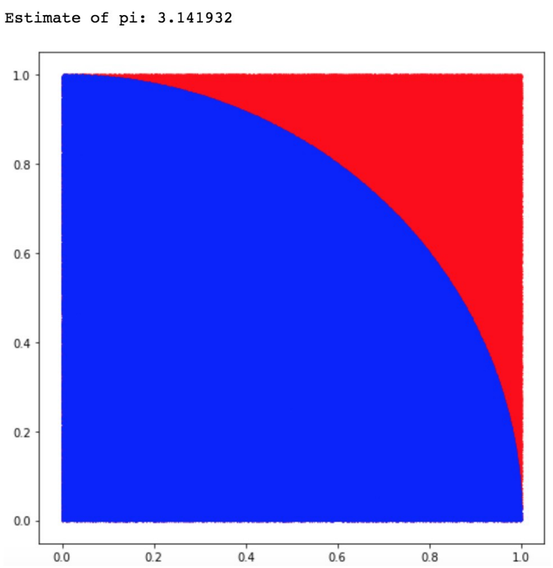
$$\mathbb{E}[f(X)] = \mathbb{E}_{x \sim X}[f(x)] \approx \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$

- Example of Monte Carlo sampling to estimate $\pi/4$:









Credit https://towardsdatascience.com/an-overview-of-monte-carlo-methods-675384eb1694

Central limit theorem

- Suppose we have an unknown distribution X with expected value $\mu = \mathbb{E}[X]$ and variance σ^2.
- We can take randomly N samples from X to compute the sample average:

$$S_N = \frac{1}{N} \sum_{i=1}^{N} x_i$$

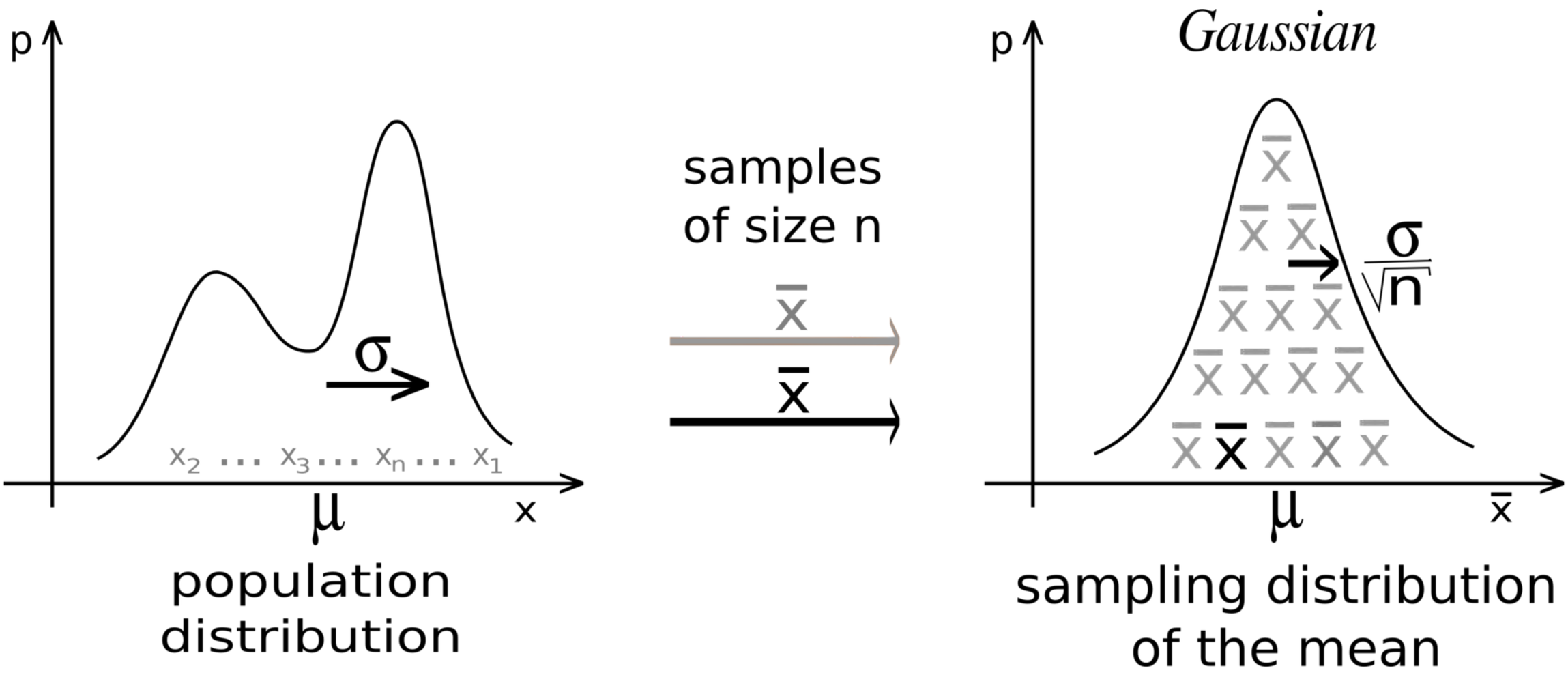
- The **Central Limit Theorem** (CLT) states that:

> The distribution of sample averages is normally distributed with mean μ and variance $\frac{\sigma^2}{N}$.

$$S_N \sim \mathcal{N}(\mu, \frac{\sigma}{\sqrt{N}})$$

Central limit theorem

- If we perform the sampling multiple times, even with few samples, the average of the sampling averages will be very close to the expected value.
- The more samples we get, the smaller the variance of the estimates.
- Although the distribution X can be anything, the sampling averages are normally distributed.



Credit: https://en.wikipedia.org/wiki/Central_limit_theorem

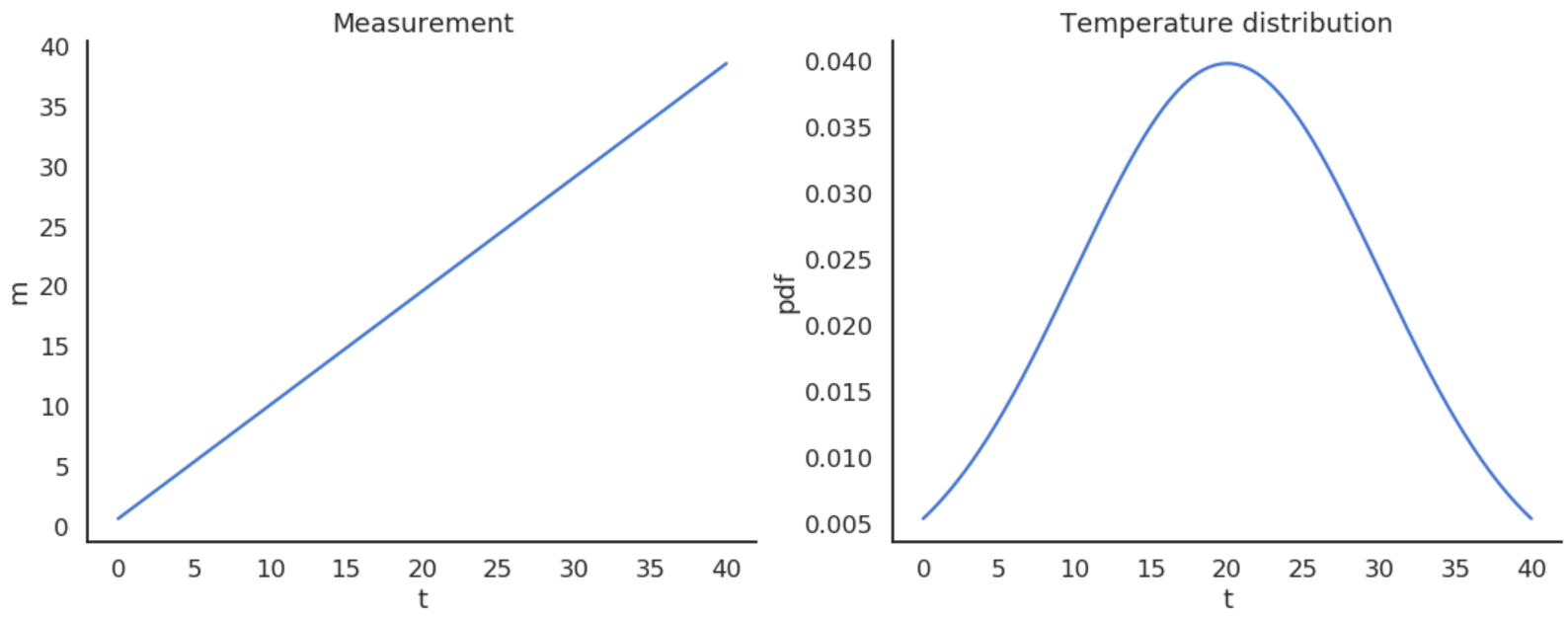
Estimators

- CLT shows that the sampling average is an **unbiased estimator** of the expected value of a distribution:

$$\mathbb{E}(S_N) = \mathbb{E}(X)$$

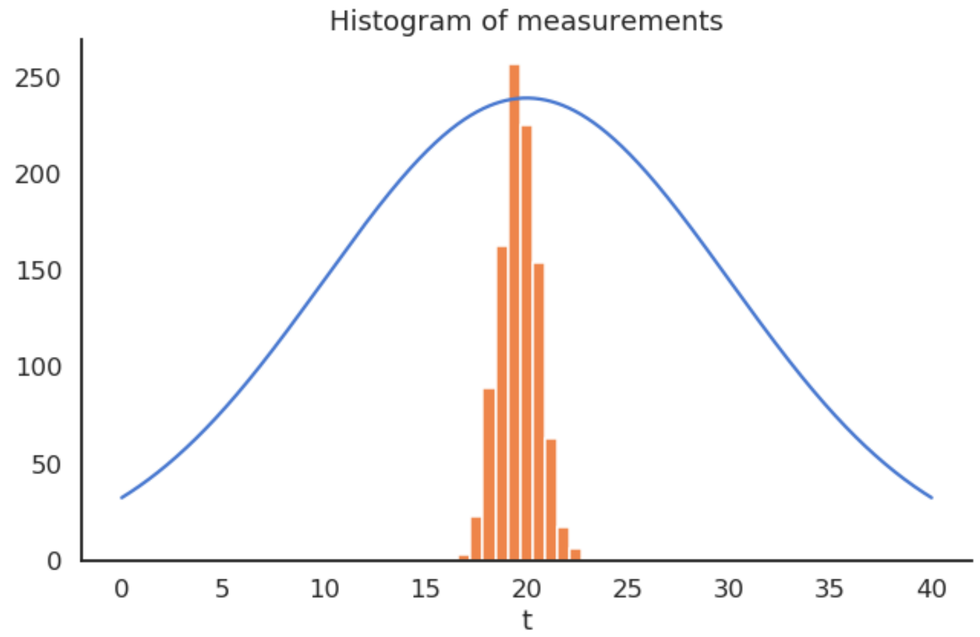
- An estimator is a random variable used to measure parameters of a distribution (e.g. its expectation). The problem is that estimators can generally be **biased**.
- Take the example of a thermometer M measuring the temperature T. T is a random variable (normally distributed with $\mu = 20$ and $\sigma = 10$) and the measurements M relate to the temperature with the relation:

$$M = 0.95\,T + 0.65$$



Estimators

- The thermometer is not perfect, but do random measurements allow us to estimate the expected value of the temperature?
- We could repeatedly take 100 random samples of the thermometer and see how the distribution of sample averages look like:



- But, as the expectation is linear, we actually have:

$$\mathbb{E}[M] = \mathbb{E}[0.95\,T + 0.65] = 0.95\,\mathbb{E}[T] + 0.65 = 19.65 \neq \mathbb{E}[T]$$

- The thermometer is a **biased estimator** of the temperature.

Estimators

- Let's note θ a parameter of a probability distribution X that we want to estimate (it does not have to be its mean).
- An **estimator** $\hat{\theta}$ is a random variable mapping the sample space of X to a set of sample estimates.
- The **bias** of an estimator is the mean error made by the estimator:

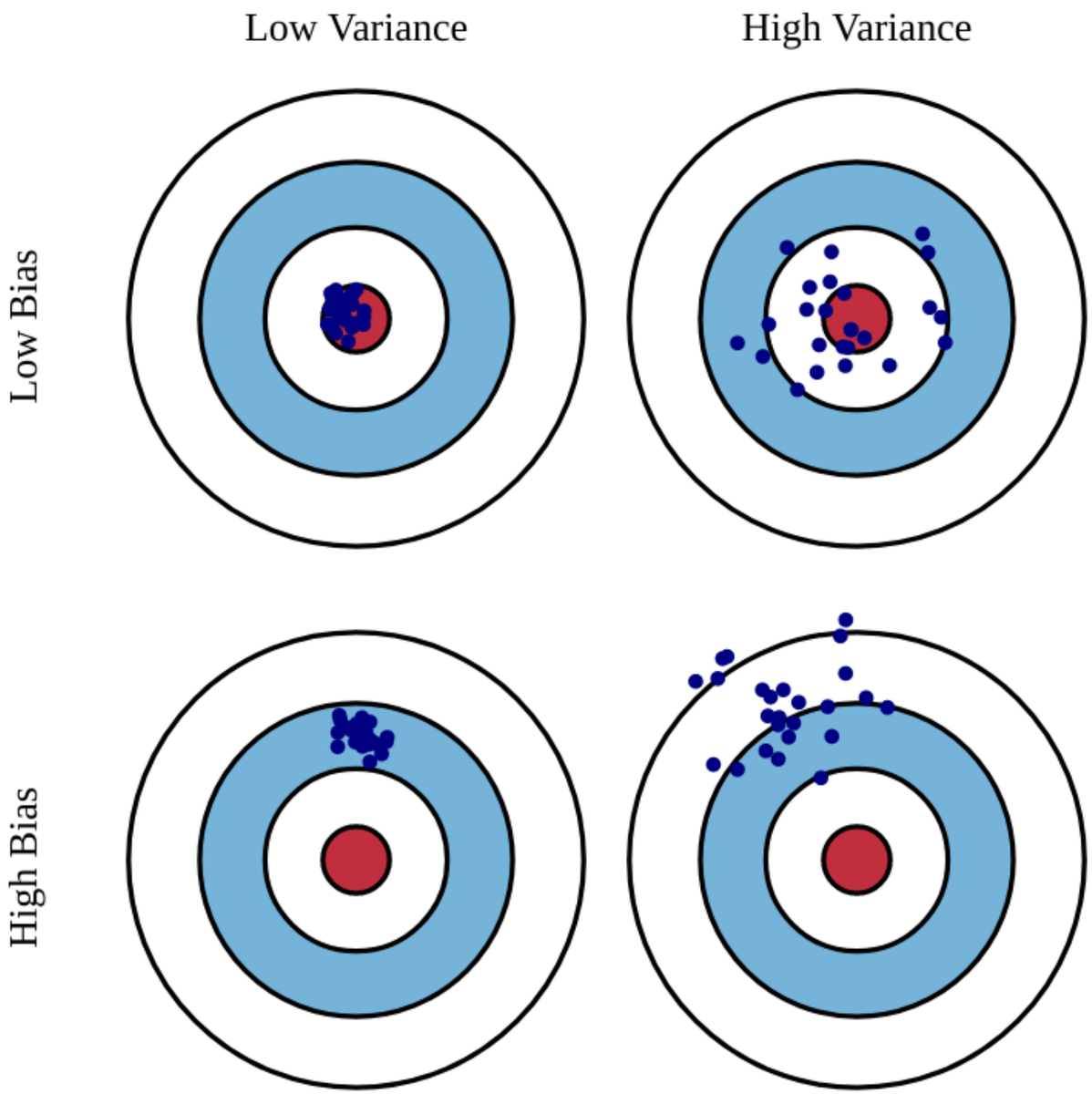
$$\mathcal{B}(\hat{\theta}) = \mathbb{E}[\hat{\theta} - \theta] = \mathbb{E}[\hat{\theta}] - \theta$$

- The **variance** of an estimator is the deviation of the samples around the expected value:

$$\mathrm{Var}(\hat{\theta}) = \mathbb{E}[(\hat{\theta} - \mathbb{E}[\hat{\theta}])^2]$$

- Ideally, we would like estimators with:
  - **low bias**: the estimations are correct on average (= equal to the true parameter).
  - **low variance**: we do not need many estimates to get a correct estimate (CLT: $\frac{\sigma}{\sqrt{N}}$)

Estimators: bias and variance

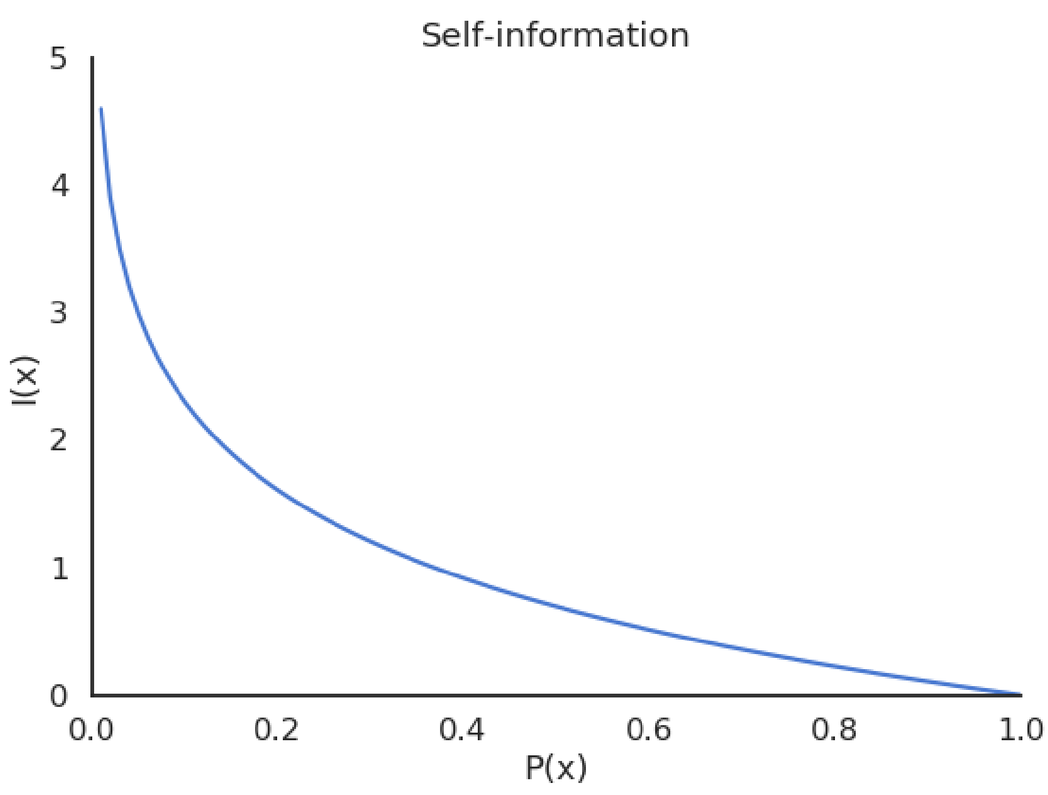


- Unfortunately, the perfect estimator does not exist.
- Estimators will have a bias and a variance:
  - **Bias**: the estimated values will be wrong, and the policy not optimal.
  - **Variance**: we will need a lot of samples (trial and error) to have correct estimates.
- One usually talks of a **bias/variance** trade-off: if you have a small bias, you will have a high variance, or vice versa.
- In machine learning, bias corresponds to underfitting, variance to overfitting.

5 - Information theory

Information

- **Information theory** (Claude Shannon) asks how much information is contained in a probability distribution.
- Information is related to **surprise** or **uncertainty**: are the outcomes of a random variable surprising?
  - Almost certain outcomes ($P \sim 1$) are not surprising because they happen all the time.
  - Almost impossible outcomes ($P \sim 0$) are very surprising because they are very rare.



- A useful measurement of how surprising is an outcome x is the **self-information**:

$$I(x) = -\log P(X = x)$$

- Depending on which log is used, self-information has different units:
  - $\log_2$: bits or shannons.
  - $\log_e = \ln$: nats.
- But it is just a rescaling, the base never matters.

Entropy

- The **entropy** (or Shannon entropy) of a probability distribution is the expected value of the self-information of its outcomes:

$$H(X) = \mathbb{E}_{x \sim X}[I(x)] = \mathbb{E}_{x \sim X}[-\log P(X = x)]$$

- It measures the **uncertainty**, **randomness** or **information content** of the random variable.

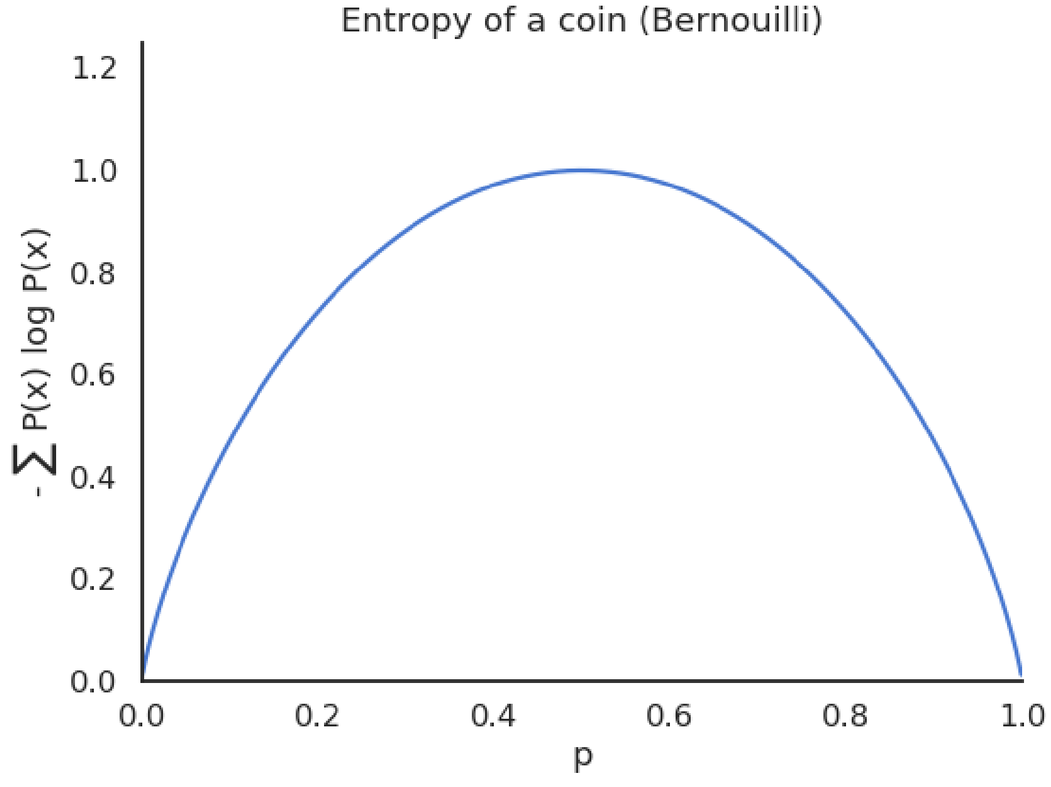
- In the discrete case:

$$H(X) = -\sum_{x} P(x)\ \log P(x)$$

- In the continuous case:

$$H(X) = -\int_{x} f(x)\ \log f(x)\, dx$$

- The entropy of a Bernouilli variable is maximal when both outcomes are **equiprobable**.
- If a variable is **deterministic**, its entropy is minimal and equal to zero.



Joint and conditional entropies

- The **joint entropy** of two random variables X and Y is defined by:

$$H(X, Y) = \mathbb{E}_{x\sim X, y\sim Y}[-\log P(X = x, Y = y)]$$

- The **conditional entropy** of two random variables X and Y is defined by:

$$H(X|Y) = \mathbb{E}_{x\sim X, y\sim Y}[-\log P(X = x|Y = y)] = \mathbb{E}_{x\sim X, y\sim Y}[-\log \frac{P(X = x, Y = y)}{P(Y = y)}]$$

- If the variables are **independent**, we have:

$$H(X, Y) = H(X) + H(Y) \qquad \text{or} \qquad H(X|Y) = H(X)$$

- Both are related by:

$$H(X|Y) = H(X, Y) - H(Y)$$

- The equivalent of Bayes' rule is:

$$H(Y|X) = H(X|Y) + H(Y) - H(X)$$

Mutual Information

- The most important information measurement between two variables is the **mutual information** MI (or information gain):

$$I(X, Y) = H(X) - H(X|Y) = H(Y) - H(Y|X)$$

- It measures how much information the variable X holds on Y:
  - If the two variables are **independent**, the MI is 0 : X is as random, whether you know Y or not.

$$I(X, Y) = 0$$

  - If the two variables are **dependent**, knowing Y gives you information on X, which becomes less random, i.e. less uncertain / surprising.

$$I(X, Y) > 0$$

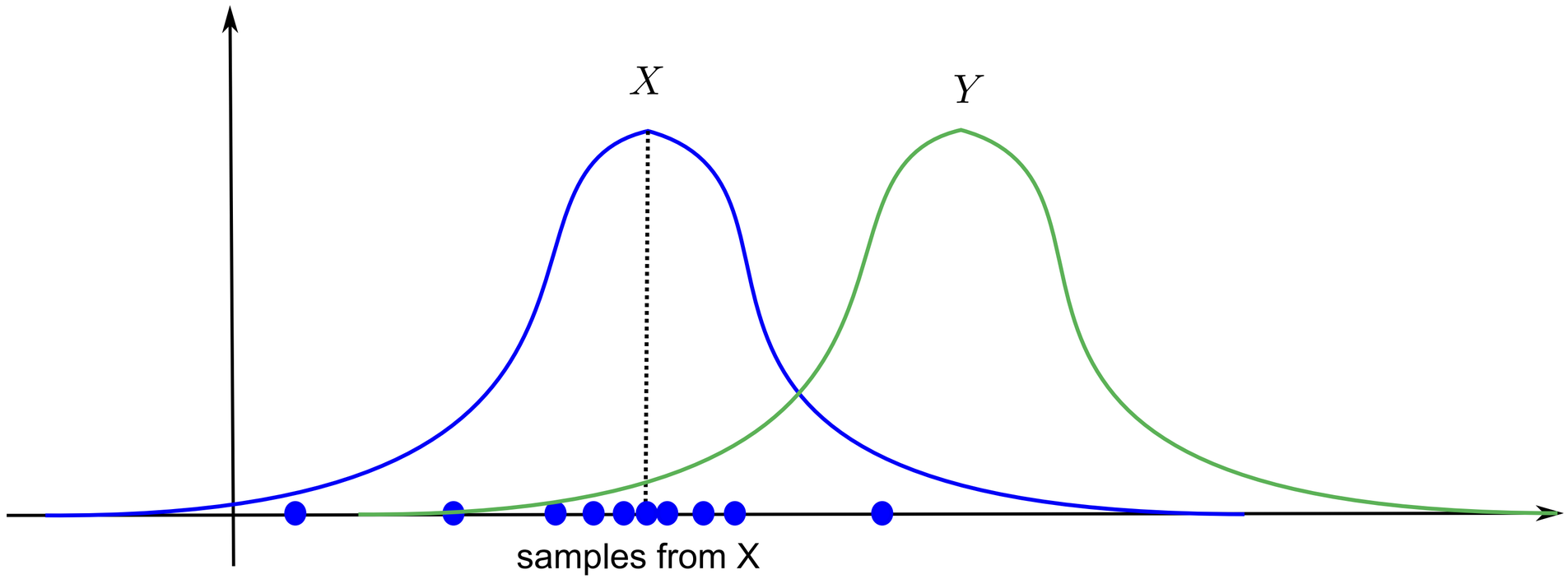
- If you can fully predict X when you know Y, it becomes deterministic ($H(X|Y) = 0$) so the mutual information is maximal ($I(X, Y) = H(X)$).

Cross-entropy

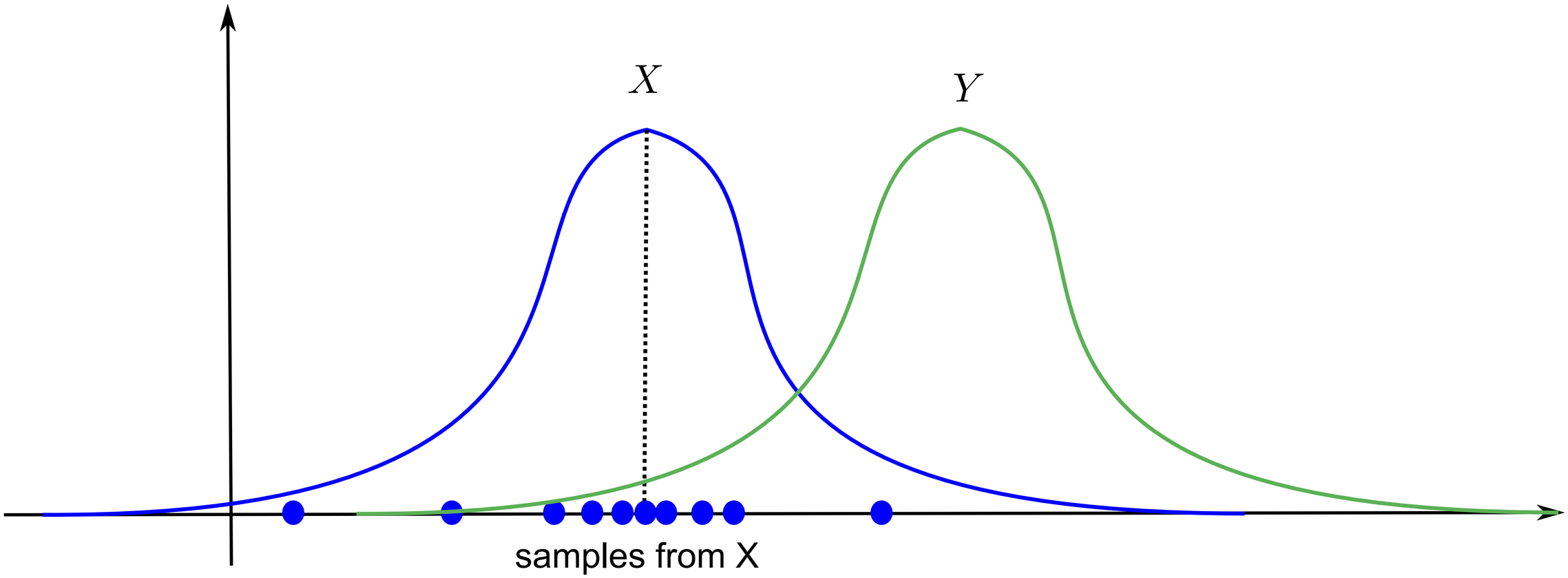
- The **cross-entropy** between two distributions X and Y is defined as:

$$H(X, Y) = \mathbb{E}_{x \sim X}[-\log P(Y = x)]$$

- Beware that the notation $H(X, Y)$ is the same as the joint entropy, but it is a different concept!
- The cross-entropy measures the **negative log-likelihood** that a sample x taken from the distribution X could also come from the distribution Y.
- More exactly, it measures how many bits of information one would need to distinguish the two distributions X and Y.



Cross-entropy



$$H(X, Y) = \mathbb{E}_{x \sim X}[-\log P(Y = x)]$$

- If the two distributions are the same *almost anywhere*, one cannot distinguish samples from the two distributions:
  - The cross-entropy is the same as the entropy of X.
- If the two distributions are completely different, one can tell whether a sample Z comes from X or Y:
  - The cross-entropy is higher than the entropy of X.

Kullback-Leibler divergence

- In practice, the **Kullback-Leibler divergence** $\mathrm{KL}(X||Y)$ is a better measurement of the similarity (statistical distance) between two probability distributions:

$$\mathrm{KL}(X||Y) = \mathbb{E}_{x\sim X}[-\log \frac{P(Y=x)}{P(X=x)}]$$

- It is linked to the cross-entropy by:

$$\mathrm{KL}(X||Y) = H(X,Y) - H(X)$$

- If the two distributions are the same *almost anywhere*:
  - The KL divergence is zero.
- If the two distributions are different:
  - The KL divergence is positive.
- Minimizing the KL between two distributions is the same as making the two distributions “equal”.
- Again, the KL is not a metric, as it is not symmetric.