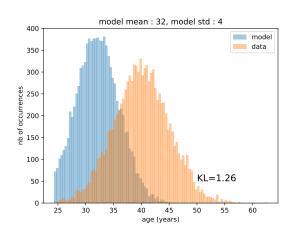
# Machine learning II, unsupervised learning and agents: density estimation



KL divergence

Kernel density estimation

## Density estimation

Objective : compute a probability distribution that represents the data well.

The Maximum Likelihood method is one example method.

We observe a dataset  $D_n = (x_1, ..., x_n)$ .

We first need to choose a **model** (which is the distribution) of the dataset, p.

Then, we must optimize the parameters of this model, noted  $\theta$ .

The likelihood (vraisemblance) of the model is

$$L(\theta) = p(x_1, \dots, x_n | \theta)$$
 (1)

The likelihood (vraisemblance) of the model is

$$L(\theta) = p(x_1, \dots, x_n | \theta)$$
 (2)

If  $(x_1, \ldots, x_n)$  are conditionally independant, then it writes :

$$L(\theta) = \prod_{i=1}^{n} p(x_i | \theta)$$
 (3)

The likelihood (vraisemblance) of the model is

$$L(\theta) = \prod_{i=1}^{n} p(x_i | \theta)$$
 (4)

This is the function that we want to maximize.

#### Remark on max-likelihood

Most of the time it's written this way : "minimise  $-logL(\theta)$ " Because the log transforms the product into a sum, which is easier to differentiate.

$$-logL(\theta) = -\sum_{i=1}^{n} \log(p(x_i|\theta))$$
 (5)

Exercice 1: We observe the data (1,0). We assume that these data come from a random variable that follows a Bernoulli distribution of parameter p. What is the likelihood of these observations as a function of p?

Exercice 1: We observe the data (1,0). We assume that these data come from a random variable that follows a Bernoulli distribution of parameter p. What is the likelihood of these observations as a function of p?

$$L = P(1|p)P(0|p) \tag{6}$$

Exercice 1: We observe the data (1,0). We assume that these data come from a random variable that follows a Bernoulli distribution of parameter p. What is the likelihood of these observations as a function of p?

$$L = P(1|p)P(0|p) \tag{7}$$

For which value of p is this likelihood maximum?

Exercice 2: We observe the data (2.5, 3.5). We assume that these data come from a normal law of parameters  $\mu$  and  $\sigma$ . What is the likelihood of  $(\mu, \sigma)$ ?

Exercice 2: We observe the data (2.5, 3.5). We assume that these data come from a normal law of parameters  $\mu$  and  $\sigma$ .

$$L = p(2.5|\mu,\sigma)p(3.5|\mu,\sigma) \tag{8}$$

Exercice 2: We observe the data (2.5, 3.5). We assume that these data come from a normal law of parameters  $\mu$  and  $\sigma$ .

$$L = p(2.5|\mu,\sigma)p(3.5|\mu,\sigma)$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(\frac{2.5-\mu}{\sigma})^2} \times \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(\frac{3.5-\mu}{\sigma})^2}$$
(9)

Exercice 2: We observe the data (2.5, 3.5). We assume that these data come from a normal law of parameters  $\mu$  and  $\sigma$ .

$$L = p(2.5|\mu,\sigma)p(3.5|\mu,\sigma)$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2}(\frac{2.5-\mu}{\sigma})^2} \times \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2}(\frac{3.5-\mu}{\sigma})^2}$$
(10)

We wan show that the likelihood is maximum for :

$$\hat{\mu} = \frac{2.5+3.5}{2}$$

$$\hat{\sigma^2} = \frac{(2.5 - \hat{\mu})^2 + (3.5 - \hat{\mu})^2}{2}$$

## Kullbach-Leibler Divergence

The KL divergence is a measure of the discrepancy between two distributions.

# Expected value (espérance)

▶ For a discrete random variable X that takes the values  $x_i$  with probability  $p_i$ :

$$E(X) = \sum_{i=1}^{n} p_i x_i \tag{11}$$

▶ For a continuous random variable X with density p(x):

$$E(X) = \int x p(x) dx \tag{12}$$

## Kullbach-Leibler Divergence

- ► The samples  $(x_1, ..., x_n)$  are described by an empirical distribution.
- The Kullbach-Leibler divergence is a tool to compare distributions.
- It is not a distance: it is not symmetric, no triangular inequality.

## Kullbach-Leibler Divergence

$$\mathcal{D}[p||q] = \mathbb{E}_{\sim p}[\log(\frac{p}{q})] \tag{13}$$

For discrete variables

$$\mathcal{D}[p||q] = \sum_{i} p(i) \log \frac{p(i)}{q(i)}$$
 (14)

for continuous variables

$$\mathcal{D}[p||q] = \int_{X} p(x) \log \frac{p(x)}{q(x)} dx \tag{15}$$

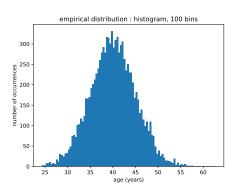
#### Exercice 2: Fitting a distribution

- cd kl divergence
- A two dimensional dataset is contained in empirical\_distribution.csv. It represents the age distribution of some groupe of people. We want to study this age distribution.
- ▶ load it in **fit\_empirical.py**. We will use the functions provided in the file in order to find the best model, meaning here the model M, such that  $KL(M||\tilde{P})$  is smallest, with  $\tilde{P}$  the empirical distribution of the data.

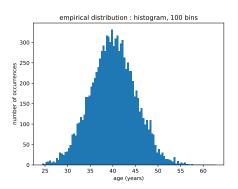
#### Exercice 2: Fitting a distribution

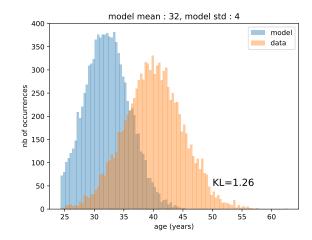
- ▶ First step : choice of the model
- ▶ Plot the histogram of the data : what model seems to be relevant?

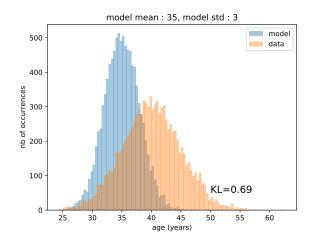
- ▶ First step : choice of the model
- ► Plot the histogram of the data : what model seems to be relevant?



- ▶ We will use normal laws. We want to fint the normal law that is the closest to the empirical data
- We measure the proximity between the model and the empirical data with the KL divergence.







## Kernel density estimation

```
https:
//seaborn.pydata.org/generated/seaborn.kdeplot.html
```