Master Program in *Data Science and Business Informatics*

Statistics for Data Science

Lesson 11 - Distances between distributions

Salvatore Ruggieri

Department of Computer Science
University of Pisa, Italy
salvatore.ruggieri@unipi.it

Distances and Metrics

A numerical measurement of how far apart two objects are.

Distances and Metrics

A distance over a set $\mathcal{A}$ is a function $d : \mathcal{A} \times \mathcal{A} \to \mathbb{R}$ such that:

- $d(x, y) \geq 0$ *non-negativity*
- $d(x, y) = 0$ iff $x = y$ *identity of indiscernibles*
- $d(x, y) = d(y, x)$ *symmetry*

Moreover, d is called a metric if in addition:

- $d(x, z) \leq d(x, y) + d(y, z)$ *triangle inequality*

Examples over $\mathcal{A} = \mathbb{R}^n$:

- Manhattan or L_1 distance $d_1(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_1 = \sum_{i=1}^n |\mathbf{x}_i - \mathbf{y}_i|$
- Euclidian or L_2 distance $d_2(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_2 = \sqrt{\sum_{i=1}^n (\mathbf{x}_i - \mathbf{y}_i)^2}$
- Chebyshev or L_∞ distance $d_\infty(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_\infty = \max_{i=1}^n |\mathbf{x}_i - \mathbf{y}_i|$

We aim at defining distances and metrics over probability distributions, i.e., when $\mathcal{A} = \{F \mid F : \mathbb{R} \to [0, 1] \text{ is a CDF}\}$

Distances over probability distributions

A numerical measurement of how far apart two probability distributions are.

- ML/DM models are supposed to be applied on the same distribution as the training set:
  - How far is the test data distribution from the one of the training data? *[Transfer learning*
  - Is the data changing over time, thus my model is inadequate? *[Dataset shift]*
- ML/DM algorithms are supposed to choose the best hypothesis:
  - What is the split in a DT which best distinguish the distribution of classes?
  - Is my model separating positive and negatives as much as possible?
  - Is my clustering separating groups with different distributions?
- Data preprocessing looks at feature distribution:
  - Are these two features conveying the same information?
  - Can this feature be predictive to the class feature?
- ... and many other applications in Data Science

Total variation distance and KS distance

Let X, Y be random variables:

- Total Variation (TV) distance (discrete and continuous case):

$$d_{TV}(X,Y) = \frac{1}{2}\sum_i |p_X(a_i) - p_Y(a_i)| \qquad d_{TV}(X,Y) = \frac{1}{2}\int |f_X(x) - f_Y(x)|dx$$

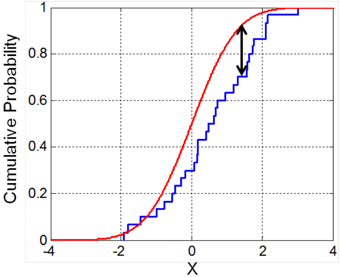
  - d_{TV} is a metric with $d_{TV}(X,Y) \in [0,1]$

- Kolmogorov-Smirnov (KS) distance:

$$d_{KS}(X,Y) = \sup_x |F_X(x) - F_Y(x)|$$

  - d_{KS} is a metric with $d_{KS}(X,Y) \in [0,1]$

- d_{TV} and d_{KS} have no closed forms in general
- d_{KS} can be estimated from samples of the distributions



See R script

Entropy $H(X)$ of a random variable X

- The **Shannon's information entropy** is the average level of "information" (or "surprise", "uncertainty", "unpredictability") inherent to the variable's possible outcomes
  - Information is inversely proportional to probability $\frac{1}{p(a_i)}$
    - Highly likely/unlikely events carry less/more new information
  - Information content $ic()$ of two independent events should sum up $\log \frac{1}{p(a_i)}$
    - $ic(p(A \cap B)) = ic(p(A)) + ic(p(B)) = ic(p(A)p(B))$
    - $ic(p(\Omega)) = ic(1) = 0$
    - $ic(p(A)) \geq 0$
- $H(X) = E[-\log p(X)]$ (*discrete*) $\qquad H(X) = E[-\log f(X)]$ (*continuous*)

$$H(X) = -\sum_i p(a_i) \log p(a_i) \qquad H(X) = -\int_{-\infty}^{\infty} f(x) \log f(x) dx$$

  - For X discrete, $H(X) \geq 0$ since $-\log p(X) = \log {}^1/_{p(X)} \geq 0$
    - zero reached when $p(a_1) = 1$ and $p(a_i) = 0$ for $i \neq 1$
  - For $X \sim Ber(p)$, $H(X) = -p \log p - (1-p) \log (1-p)$ *[binary entropy function]*
    - for $X \sim Ber(0.5)$: $H(X) = -2 \cdot {}^1/_2 \log {}^1/_2 = 1$ *[unit of entropy is called a* ***bit****]*

Entropy bounds

Corollary of Jensen's inequality [T, Ex. 8.11].

For a concave function g, namely $g''(x) \leq 0$: $g(E[X]) \geq E[g(X)]$

- $\log(x)$ is concave since $\log''(x) = -1/x^2 \leq 0$
- Let X be discrete with finite domain of n elements
  - By corollary above:

$$H(X) = E[\log \frac{1}{p(X)}] \leq \log E[\frac{1}{p(X)}]$$

  - By change of variable:

$$E[\frac{1}{p(X)}] = \sum_i \frac{p(a_i)}{p(a_i)} = n$$

  and then maximum entropy is:

$$H(X) \leq \log n$$

  - E.g., $X \sim Ber(p)$, maximum entropy (uncertainty) for equiprobable events $p = 1/2$

See R script

Cross entropy

- X, Y discrete random variables with p.m.f. p_X and p_Y:
- Cross entropy of X w.r.t. Y: $H(X;Y) = E_X[-\log p(Y)]$

$$H(X;Y) = -\sum_i p_X(a_i) \log p_Y(a_i)$$

$$\text{with } p_X(a_i) \log p_Y(a_i) = \begin{cases} 0 & \text{if } p_X(a_i) = 0 \\ -\infty & \text{if } p_X(a_i) > 0 \wedge p_Y(a_i) = 0 \end{cases}$$

- $H(X;Y)$ is the "information" or "uncertainty" or "loss" when using Y to encode X
- The closer p_X and p_Y, the lower is $H(X;Y)$
- The lower bound is for $Y = X$, for which $H(X;Y) = H(X)$

Kullback-Leibler divergence

KL divergence

For X, Y discrete random variables with p.m.f. p_X and p_Y:

$$D_{KL}(X \parallel Y) = \sum_i p_X(a_i) \log \frac{p_X(a_i)}{p_Y(a_i)} = H(X;Y) - H(X)$$

- Measure how distribution of Y (model) can reconstruct the distribution of X (data)
  - Also called: *relative entropy* or *information gain* of X w.r.t. Y
- Properties
  - $D_{KL}(X \parallel Y) \geq 0$ [**Gibbs' inequality**]
  - $D_{KL}(X \parallel Y) = 0$ iff $F_X = F_Y$
  - $D_{KL}(X \parallel Y) \neq D_{KL}(Y \parallel X)$ *[not a distance!]*
- For X, Y continuous: $D_{KL}(X \parallel Y) = \int_{-\infty}^{\infty} f_X(x) \log \frac{f_X(x)}{f_Y(x)} dx$

See R script

Joint entropy

- X, Y discrete random variables with p.m.f. p_X and p_Y:
- Joint p.m.f. p_{XY}. Joint entropy of (X, Y):

$$H((X,Y)) = -\sum_{i,j} p_{XY}(a_i, a_j) \log p_{XY}(a_i, a_j)$$

- If $X \perp\!\!\!\perp Y$, then:

$$H((X,Y)) = -\sum_{i,j} p_X(a_i) p_Y(a_j)(\log p_X(a_i) + \log p_Y(a_j)) =$$

$$= -(\sum_i p_X(a_i))(\sum_j p_Y(a_j) \log p_Y(a_j)) - (\sum_j p_Y(a_j))(\sum_i p_X(a_i) \log p_X(a_i)) = H(X) + H(Y)$$

Mutual information

Mutual information

For X, Y discrete random variables with p.m.f. p_X and p_Y and joint p.m.f. p_{XY}:

$$I(X,Y) = D_{KL}(p_{XY} \parallel p_X p_Y) = \sum_{i,j} p_{XY}(a_i, a_j) \log \frac{p_{XY}(a_i, a_j)}{p_X(a_i) p_Y(a_j)} = H(X) + H(Y) - H((X,Y))$$

- MI measures how dependent two distributions are
  - Measure how product of marginals can reconstruct the joint distribution
- Properties
  - $I(X,Y) = I(Y,X)$, and $I(X,Y) \geq 0$
  - $I(X,Y) = 0$ iff $X \perp\!\!\!\perp Y$
  - $NMI = \frac{I(X,Y)}{\min\{H(X),H(Y)\}} \in [0,1]$ *[Normalized mutual information]*
- For X, Y continuous: $I(X,Y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_{XY}(x,y) \log \frac{f_{XY}(x,y)}{f_X(x) f_Y(y)} dxdy$

See R script

The data processing inequality

- Let X be unknown, and assume to observe a noisy version Y of it
- Let $Z = f(Y)$ be a data processing to improve the "quality" of Y
- Z does not increase the information about X, i.e.: *[Data processing inequality]*

$$I(X, Y) \geq I(X, Z)$$

- If $I(X, Y) = I(X, Z)$ and Z is a summary of Y, we call it a *sufficient statistics*
  - Let $X \sim Ber(\theta)$ and $Y = (Y_1, \dots, Y_n) \sim Ber(\theta)^n$ modelling i.i.d. observations
  - $Z = \sum_{i=1}^{n} Y_i \sim Binom(n, \theta)$ is a sufficient statistics
  - **Proof (sketch):** use $D_{KL}(p_{XY} \parallel p_X p_Y)$ and:

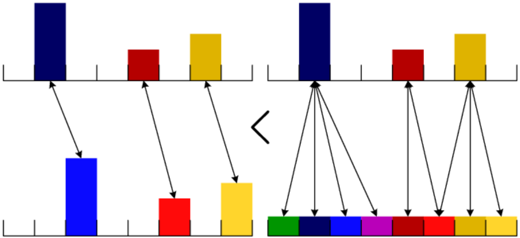
$$p(Y_1 = y1, \dots, Y_n = y_n) = \prod_i \theta^{y_i}(1-\theta)^{(1-y_i)} = \theta^{\sum_i y_i}(1-\theta)^{n-\sum_i y_i} = p(Z = \sum_i y_i)$$

Earth mover's distance / Wasserstein metric

- The minimum cost to transform one distribution to another
- Cost $=$ amount of mass to move $\times$ distance to move it
- X, Y discrete random variables:

$$EMD(X, Y) = \frac{\sum_{i,j} F_{i,j} \cdot |a_i - a_j|}{\sum_{i,j} F_{i,j}}$$

where F is the flow which minimizes the numerator (total cost) subject to **some constraints**.



Earth mover's distance / Wasserstein metric

- The minimum cost to transform one distribution to another
- Solution of the transportation problem for X, Y multivariate (version from **Ramdas et al. 2015**):

$$EMD(X,Y) = \int_0^1 \|F_X^{-1}(p) - F_Y^{-1}(p)\| \, dp$$

For X, Y univariate, this simplifies to:

$$EMD(X,Y) = \sum_i |F_X(a_i) - F_Y(a_i)| \qquad EMD(X,Y) = \int_{-\infty}^{\infty} |F_X(x) - F_Y(x)| dx$$

- For empirical distributions from **ordered** samples $x_1, \dots, x_n$ and $y_1, \dots, y_n$:

$$EMD(X,Y) = \frac{1}{n} \sum_i |x_i - y_i|$$

See R script

Reference book chapter for this lesson

Kevin P. Murphy (2022)
Probabilistic Machine Learning: An Introduction
Chapter 6: Information Theory
online book