## Machine Learning for EDS

## Tutorial week 2

## 2023/2024

Generically in the following exercises, consider  $\mathcal{X}$  to be a measurable space of features,  $\mathcal{Y}$  a measurable space of outputs, P a distribution over  $\mathcal{X} \times \mathcal{Y}$ ,  $(X,Y) \sim P$ , and  $\eta(X) = \mathbb{E}[Y|X]$ .

**Problem 1** Consider two 6-face dice: die 1 and die 2. On die 1, 3 faces are blue, and 3 faces are red. On die 2, 5 faces are blue, and the remaining one is red. First choose a die at random, say die 1 with probability  $p \in [0,1]$ . The selected die is rolled and the color appearing on the upward face is recorded. Denote by  $X \in \{1,2\}$  the selected die, and  $Y \in \{0,1\}$  the outcome of rolling the die, say Y = 1 for blue, Y = 0 for red. Let us study the problem of predicting the outcome Y given X.

- 1. Is this a regression or a classification problem? Why?
- 2. Show that  $\eta(X) = \mathbb{P}(Y = 1|X)$ .
- 3. For the 0-1 cost function, what is the general form (expressed in terms of  $\eta$ ) of Bayes predictors and Bayes risk in this framework?
- 4. Derive  $\eta$  and Bayes predictors explicitly, and then show that Bayes risk is equal to  $\mathcal{R}_P^* = \frac{1}{6} + \frac{p}{3}$ .
- 5. Intuitively, why is Bayes risk an increasing function of p?

**Problem 2** Consider the regression framework with  $\mathcal{Y} = \mathbb{R}$ . Let  $F_{Y|X}(\cdot|x)$  be the conditional distribution function of Y|X=x. In this exercise, we assume the existence of the conditional PDF  $f_{Y|X=x}(\cdot|x)$ , which may be relaxed.

- 1. For the absolute value cost c(y, y') = |y y'| for  $y, y' \in \mathcal{Y}$ , let us show that  $f^* : x \mapsto \text{med}(Y|X = x)$  is a Bayes predictor, where med(Y|X = x) stands for the median of the distribution of Y given X = x:
  - (a) Fix  $x \in \mathcal{X}$ , and consider the function  $r_x : a \mapsto r_x(a) = \mathbb{E}[|a Y||X = x]$ . Show that for any  $a \in \mathbb{R}$ ,  $r'_x(a) = 2\mathbb{P}(Y \le a|X = x) 1$  and  $r''_x(a) = 2f_{Y|X=x}(a)$ .

Hint: Recall that for 
$$\varphi(x) = \int_{A(x)}^{B(x)} g(x,t)dt$$
 (assuming all functions are differentiable), 
$$\varphi'(x) = \int_{A(x)}^{B(x)} \frac{\partial g(x,t)}{\partial x} dt + B'(x)g(x,B(x)) - A'(x)g(x,A(x))$$

Note: This rule cannot be applied immediately to improper integrals. To be able to apply the rule, you could split the integrals  $\int_a^\infty y f_{Y|X}(y|x) = \int_a^M y f_{Y|X}(y|x) + \int_M^\infty y f_{Y|X}(y|x)$ .

- (b) Show that  $r_x$  admits a global minimum at  $a_x^* = \text{med}(Y|X=x)$ .
- (c) Deduce that  $\mathbb{E}[|f^*(X) Y|] \leq \mathbb{E}[|f(X) Y|]$  for any predictor  $f \in \mathcal{F}$  and conclude that  $f^*: x \mapsto \operatorname{med}(Y|X = x)$  is a Bayes predictor.
- 2. Derive a Bayes predictor when c is the asymmetric absolute value cost:

$$c(y,y') = c_-(y'-y)\mathbb{1}_{y < y'} + c_+(y-y')\mathbb{1}_{y \ge y'} \text{ for } y,y' \in \mathcal{Y}, \text{ with } c_-,c_+ \ge 0, \ c_- + c_+ > 0.$$

How does it relate to the Bayes predictor of the previous question?

**Problem 3** Let  $\mu_0, \mu_1 \in \mathbb{R}^d$  two vectors and  $\Sigma_0, \Sigma_1$  two symmetric positive definite matrices of size d. Let Y be a random variable such that  $\mathbb{P}(Y = 1) = 1 - \mathbb{P}(Y = 0) = p \in [0, 1]$ , and let X be a random variable such that  $X|Y = i \sim \mathcal{N}(\mu_i, \Sigma_i)$ , for  $i \in \{0, 1\}$ . We consider the classification problem of predicting Y given X with the 0-1 cost.

- 1. Recall the general form of Bayes classifiers in this framework (expressed in terms of  $\eta$ ).
- 2. Show that  $\eta(x) > 1/2 \iff \frac{\mathbb{P}(Y=1|X=x)}{\mathbb{P}(Y=0|X=x)} > 1$ .
- 3. For i = 0, 1, derive an expression of  $\mathbb{P}(Y = i | X = x)$  in terms of  $N_i(x)$  (the pdf of a multivariate normal with mean  $\mu_i$  and variance  $\Sigma_i$ ),  $f_X(x)$  and p.
- 4. Show that a Bayes classifier can be expressed as

$$f^*: x \in \mathbb{R}^d \mapsto \mathbb{1}_{x^\top A x + b^\top x + c > 0},$$

for some matrix A, vector b and constant c, depending on  $\mu_0, \mu_1, \Sigma_0, \Sigma_1$  and p.

Hint: Use the pdf of the multivariate normal distribution.

5. What is the geometric form of the decision boundary for this classifier? What if  $\Sigma_0 = \Sigma_1$ ?

**Problem 4** Consider the binary classification framework with  $\mathcal{Y} = \{0, 1\}$ . Let c the asymmetric 0-1 cost function:  $c(y, y') = w_{y'} \mathbb{1}_{y \neq y'}$ , for  $y, y' \in \{0, 1\}$ , with  $w_0, w_1 \geq 0$ ,  $w_0 + w_1 > 0$ . Show that  $f^* : x \in \mathcal{X} \mapsto \mathbb{1}_{\eta(x) > w_0/(w_0 + w_1)}$  is a Bayes predictor and derive Bayes risk, the expression of the excess risk and the set of all Bayes predictors.

1. Define the risk conditional on X,  $r_X(f) := \mathbb{E}[c(f(X), Y)|X]$ , for any classifier  $f \in \mathcal{F}$ . Show that  $r_X(f) = w_0 f(X)(1 - \eta(X)) + w_1(1 - f(X))\eta(X)$ .

- 2. Deduce that  $r_X(f) \ge \min \left( w_0(1 \eta(X)), w_1 \eta(X) \right)$ , and show that  $r_X(f^*) = \min \left( w_0(1 \eta(X)), w_1 \eta(X) \right).$
- 3. Show that  $f^*$  is a Bayes predictor and show that Bayes risk reads

$$\mathcal{R}_P^* = \mathbb{E}\Big[\min\Big(w_0(1 - \eta(X)), w_1\eta(X)\Big)\Big].$$

- 4. Recall the definition of the excess risk of a classifier  $f \in \mathcal{F}$  in terms of  $\mathcal{R}_{P}^{c}(f)$  and  $\mathcal{R}_{P}^{*}$ .
- 5. Show that

$$\ell(f^*, f) = (w_0 + w_1) \mathbb{E} \Big[ \mathbb{1}_{f(X) \neq f^*(X)} \Big| \frac{w_0}{w_0 + w_1} - \eta(X) \Big| \Big],$$

and deduce that all Bayes classifiers are almost surely equal to  $f^*$ .