FTML project

TABLE DES MATIÈRES

1 BAYES ESTIMATOR AND BAYES RISK

Question 1 : Propose a supervised learning setting :

— input space $\mathcal{X}$

— output space $\mathcal{Y}$

— a random variable (X, Y) with a joint distribution.

— a loss function $l(x, y)$

$$l = \begin{cases} \mathcal{X} \times \mathcal{Y} \to \mathbb{R}_+ \\ (x, y) \mapsto l(x, y) \end{cases}$$

Compute the Bayes predictor and the Bayes risk associated with this setting.

We recall the definition of the Bayes predictor

$$f^*(x) = \arg\min_{y \in \mathcal{Y}} E[l(Y, y)|X = x] \tag{1}$$

Remark : you have to use a setting different than the settings seen during the course, in terms of input space $\mathcal{X}$ and output space $\mathcal{Y}$. However, you can use any classical loss function l (square loss, "0-1" loss, etc).

Question 2 : propose an estimator $\tilde{f}$, different than the Bayes estimator :

$$\tilde{f} = \begin{cases} \mathcal{X} \to \mathcal{Y} \\ x \mapsto \tilde{f}(x) \end{cases}$$

and run a simulation that gives a statistical approximation of its generalization error (risque réel), and compares it to the Bayes risk.

2 BAYES RISK WITH ABSOLUTE LOSS

We consider a supervised regression problem, $\mathcal{Y} = \mathbb{R}$. We have seen that when the loss used is the square loss $l_2(y, z) = (y - z)^2$, then the Bayes predictor is the conditional expectation :

$$f^*(x) = E\left[y|x = x\right] \tag{2}$$

The goal of this exercise is to determine $f^*(x)$ in a different situation where instead of using the square loss l_2, we use the absolute loss $l_1(y, z) = |y - z|$.

Question 1 : propose a setting where the Bayes predictor is different for the square loss and for the absolute loss.

Question 2 : General case : we consider a setting where for each value $x \in \mathcal{X}$, the conditional probability $P(Y|X = x)$ has a continuous density, noted $p_{Y|X=x}$, and that the conditional variable $Y|X = x$ has a moment of order 1. We note that for all $z \in \mathbb{R}$, this implies that $Y - z|X = x$ also has a moment of order 1 .

Determine the Bayes predictor, which means for a fixed x, determine

$$\begin{aligned} f^*(x) &= \arg\min_{z\in\mathbb{R}} E\left[|y - z||X = x\right] \\ &= \arg\min_{z\in\mathbb{R}}(g(z)) \end{aligned} \tag{3}$$

with

$$g(z) = \int_{y\in\mathbb{R}} |y - z| p_{Y|X=x}(y)dy \tag{4}$$

where $g(z)$ is correctly defined, according to the previous assumptions.

3 EXPECTED VALUE OF EMPIRICAL RISK

3.1 Reminder of the OLS setting

We consider the Ordinary least squares problem, and its

— $\mathcal{X} = \mathbb{R}^d$

— $\mathcal{Y} = \mathbb{R}$

— square loss :

$$l(y, y') = (y - y')^2$$

— hypothesis space :

$$F = \{x \mapsto x^T\theta, \theta \in \mathbb{R}^d\}$$

θ^T is the transposition of θ.

The dataset is stored in the **design matrix** $X \in \mathbb{R}^{n\times d}$.

$$X = \begin{pmatrix} x_1^T \\ \dots \\ x_i^T \\ \dots \\ x_n^T \end{pmatrix} = \begin{pmatrix} x_{11}, \dots, x_{1j}, \dots x_{1d} \\ \dots \\ x_{i1}, \dots, x_{ij}, \dots x_{id} \\ \dots \\ x_{n1}, \dots, x_{nj}, \dots x_{nd} \end{pmatrix}$$

The vector of predictions of the estimator writes $X\theta$. Hence,

$$\begin{aligned} R_n(\theta) &= \frac{1}{n}\sum_{i=1}^{n}(y_i - \theta^T x_i)^2 \\ &= \frac{1}{n}\|y - X\theta\|_2^2 \end{aligned}$$

With $y = (y_1, \ldots, y_n)^T$ being the vector containing the labels. $R_n(\theta)$ is a random variable that depends on y, X, θ.

We assume that X is **injective.** Necessary, $d \leqslant n$. As we have seen in the class, the ordinary least squares estimator, that minimizes the empirical risk, given X and y, is defined as :

$$\hat{\theta} = (X^T X)^{-1} X^T y \tag{5}$$

3.2 Statistical setting

3.2.1 *Linear model*

In the **linear model**, we assume that

$$y = X\theta^* + \epsilon \tag{6}$$

where ϵ is a vector of centered Gaussian noise with variance matrix $\sigma^* I_n$. Equivalently this can be written in the following formulation :

$$y_i = \theta^{*T} x_i + \epsilon_i, \forall i \in [1, n]$$

and ϵ_i is a centered noise (or error) ($E[\epsilon_i] = 0$) with variance σ^2. The noise is independent for all i. Hence, both y and $\hat{\theta}$ are random variables and depend on ϵ.

3.2.2 *Fixed design*

In the **fixed design** setting, X is **deterministic and fixed.** Hence, now all expectations are with respect to ϵ (or equivalently, to y) and to θ. In this setting, given θ, we can define the **fixed design risk**, as done during the class.

$$\begin{aligned} R_X(\theta) &= E_y[\frac{1}{n}\sum_{i=1}^{n}(y_i - \theta^T x_i)^2] \\ &= E_y[\frac{1}{n}\|y - X\theta\|_2^2] \\ &= E_y[R_n(\theta)] \end{aligned} \tag{7}$$

In the previous expression, the expectation is with respect to $y = (y_1, \ldots, y_n)^T$. This quantity is itself a random variable that depends on θ.

3.3 Objective

We want to show that in the linear model, fixed design we have

Proposition 1.

$$E[R_X(\hat{\theta})] = \frac{n-d}{n}\sigma^2 \tag{8}$$

In this expression, both y and $\hat{\theta}$ are random variables, that are not independent, as $\hat{\theta}$ is the OLS estimator. The expectation is over the distribution of both variables.

3.4 Exercise

We note $\|.\| = \|.\|_2$.

Step 1 : Show that :

$$\mathbb{E}\left[R_n(\hat{\theta})\right] = \mathbb{E}_\epsilon\left[\frac{1}{n}\|(I_n - X(X^TX)^{-1}X^T)\epsilon\|^2\right] \tag{9}$$

where $\mathbb{E}_\epsilon$ means that the expected value is over ϵ.

Step 2 : Let $A \in \mathbb{R}^{n,n}$. Show that

$$\sum_{(i,j)\in[1,n]^2} A_{ij}^2 = tr(A^TA) \tag{10}$$

Step 3 : Show that

$$\mathbb{E}_\epsilon\left[\frac{1}{n}\|A\epsilon\|^2\right] = \frac{\sigma^2}{n}tr(A^TA) \tag{11}$$

Step 4 : We note

$$A = I_n - X(X^TX)^{-1}X^T \tag{12}$$

Show that

$$A^TA = A \tag{13}$$

Step 5 : Conclude.

3.5 Simulation

Step 6 : Still in the same setting, what is the expected value of $\frac{||y-X\hat{\theta}||_2^2}{n-d}$?

Step 7 : Produce a numerical simulation that estimates σ^2 thanks to the result of step 6. Check that the result is consistent with the theoretical value you have chosen.

4 REGRESSION

Perform a regression on the dataset stored in **FTML/Project/data/regression/**.

— The inputs x are stored in **inputs.npy**.

— The labels y are stored in **labels.npy**

You are free to choose the regression method. **However**, it is required that you explain and discuss your approach in your report. For instance, you could discuss :

— the performance of several methods that you tried.

— the choice of the hyperparameters and the method to choose them.

— the optimization method.

We have seen several types of regressors during the class.

You may use libraries, but if you do so, it is required that you explain their usage in your report.

The Bayes estimator for this dataset and the square loss reaches a R2 score of approximately 0.88. Your objective should be to obtain a R2 score superior than 0.84 on a test subset or as a cross validation score.

https://fr.wikipedia.org/wiki/Coefficient_de_d%C3%A9termination

https://scikit-learn.org/stable/modules/generated/sklearn.metrics.r2_score.html

https://scikit-learn.org/stable/modules/cross_validation.html

5 CLASSIFICATION

Same instructions as in 4, except that this time a classification has to be performed and the data and the dataset is stored in **FTML/Project/data/classification/**.

We have seen several types of classifiers during the class.

Your objective should be to obtain a mean accuracy superior than 0.85 on a test set or as a cross validation score.

https://scikit-learn.org/stable/modules/model_evaluation.html#accuracy-score

6 ORGANIZATION

Number of students per group : 4.

Submission deadline : **June 17th 2022**.

The project must be shared through a github repo, sent by email with contributions from all students. The repo should contain :

— the pdf report.

— the python files for exercice 1

— the python files for exercice 3

— the python files for the regression problem 4.

— the python files for the classification problem 5.

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