# INFO-F-422: Statistical foundations of machine learning

Theory exam: 1st session

Gianluca Bontempi, Computer Science Department, ULB

This assessment counts for 40% of your grade. Student cannot use the handbook. Only material for writing (e.g. graph paper) and a pocket calculator are accepted.

#### 1 Question (2 points)

- 1. Mention in which case a combination of estimators can be beneficial
- 2. Prove it analytically (Use a red ink to identify the random variables in the demonstration).
- 3. Discuss at least 2 techniques that are based on this principle (at most 10 lines per technique : use of pseudo code is welcome)

**Solution :** The student could discuss for instance the bagging and the Random Forest learning technique.

## 2 Question (1 point)

Derive the bias/variance/noise decomposition of the test error in a regression problem. Use a red ink to identify the random variables in the demonstration.

## 3 Question (1,5 points)

Let us consider a fraud detection problem. Suppose we collect the following transactional dataset where  $\mathbf{v}=1$  means that the transaction came from a suspicious web site and  $\mathbf{f}=1$  means that the transaction is fraudulent.

$$\begin{array}{c|cccc} & \mathbf{f} = 1 & \mathbf{f} = 0 \\ \hline \mathbf{v} = 1 & 500 & 1000 \\ \mathbf{v} = 0 & 1 & 10000 \\ \end{array}$$

1. Estimate the following quantities by using the frequency as estimator of probability:

— Prob 
$$\{ \mathbf{f} = 1 \}$$

**Solution :** Prob 
$$\{\mathbf{f} = 1\} = 501/11501 = 0.043$$

$$--\operatorname{Prob}\left\{\mathbf{v}=0\right\}$$

**Solution :** Prob 
$$\{\mathbf{v} = 0\} = 10001/11501 = 0.869$$

$$--\operatorname{Prob}\left\{\mathbf{f}=1|\mathbf{v}=1\right\}$$

**Solution :** Prob 
$$\{\mathbf{f} = 1 | \mathbf{v} = 1\} = 500/1500 = 1/3$$

$$-\operatorname{Prob}\left\{\mathbf{v}=1|\mathbf{f}=1\right\}$$

**Solution**: Prob 
$$\{\mathbf{f} = 1 | \mathbf{v} = 1\} = 500/501$$

2. Use the Bayes theorem to compute Prob  $\{\mathbf{v}=1|\mathbf{f}=1\}$  and show that the result is identical to the one computed before.

**Solution**: Prob {
$$\mathbf{f} = 1 | \mathbf{v} = 1$$
} =  $\frac{1/3(1500/11501)}{501/11501} = 500/501$ 

3. Suppose you make a classifier that returns always  $\mathbf{f} = 1$ : what would have been its specificity, sensitivity and precision for the collected dataset?

$$SE=TP/(TP+FN)=1$$

$$SP=TN/(FP+TN)=0$$

$$PR = TP/(TP + FP) = 501/11501$$

#### Question (2 points) 4

Consider a regression task with two inputs  $\mathbf{x}_1$ ,  $\mathbf{x}_2$  and output  $\mathbf{y}$ . Suppose we observe the following training set

$X_1$	$X_2$	Y
-0.2	0 .1	1
0.1	0	0.5
1	-0.3	1.2
0.1	0.2	1
-0.4	0.4	0.5
0.1	0.1	0
1	-1	1.1

1. Fit a multivariate linear model with  $\beta_0 = 0$  to the dataset.

Fit a multivariate linear model with Solution : 
$$X^T X = \begin{bmatrix} 2.23 & -1.45 \\ -1.45 & 1.31 \end{bmatrix}$$

$$(X^T X)^{-1} = \begin{bmatrix} 1.599 & 1.77 \\ 1.77 & 2.72 \end{bmatrix}$$

$$(X^T X)^{-1} = \begin{bmatrix} 1.599 & 1.77 \\ 1.77 & 2.72 \end{bmatrix}$$

$$X^TY = \begin{bmatrix} 2.05 \\ -0.96 \end{bmatrix}$$

$$X^{T}Y = \begin{bmatrix} 2.05 \\ -0.96 \end{bmatrix}$$
$$\beta = (X^{T}X)^{-1}X^{T}Y = \begin{bmatrix} 1.58 \\ 1.016 \end{bmatrix}$$

2. Compute the mean squared training error.

Solution: 
$$e = Y - X\beta = \begin{bmatrix} 1.21 \\ 0.34 \\ -0.08 \\ 0.64 \\ 0.73 \\ -0.26 \\ 0.54 \end{bmatrix}$$

$$MSE=0.41$$

3. Suppose you use a correlation-based ranking strategy for ranking the features. What would be the top ranked variable?

Solution: Since

$$\rho_{X_1Y} = \frac{\sum_{i=1}^{N} (X_{i1} - \mu_1)(Y_i - \mu_Y)}{\sqrt{\sum_{i=1}^{N} (X_{i1} - \mu_1)^2 (Y_i - \mu_Y)^2}} = 0.53$$

and

$$\rho_{X_2Y} = \frac{\sum_{i=1}^{N} (X_{i2} - \mu_2)(Y_i - \mu_Y)}{\sqrt{\sum_{i=1}^{N} (X_{i2} - \mu_2)^2 (Y_i - \mu_Y)^2}} = -0.48$$

where  $\mu_1 = 0.24, \mu_2 = -0.07, \mu_Y = 0.75, X_1$  is the top ranked variable.

Hint:

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix} \Rightarrow A^{-1} = \frac{1}{a_{11}a_{22} - a_{12}^2} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{12} & a_{11} \end{bmatrix}$$

#### 5 Question (3,5 points)

Let us consider a classification task with 3 binary inputs and one binary output. Suppose we collected the following training set

$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{y}$
1	1	0	1
0	0	1	0
0	1	0	0
1	1	1	1
0	0	0	0
0	1	0	0
0	1	1	0
0	0	1	0
0	0	0	0
0	1	0	0
1	1	1	1

1. Estimate the following quantities by using the frequency as estimator of probability

 $--\operatorname{Prob}\left\{ \mathbf{y}=1\right\}$ 

Solution:  $Prob\{y = 1\} = 3/11$ 

- Prob  $\{\mathbf{y} = 1 | \mathbf{x}_1 = 0\}$ 

**Solution**: Prob  $\{y = 1 | x_1 = 0\} = 0$ 

- Prob  $\{\mathbf{y} = 1 | \mathbf{x}_1 = 0, \mathbf{x}_2 = 0, \mathbf{x}_3 = 0\}$ 

**Solution**: Prob  $\{y = 1 | \mathbf{x}_1 = 0, \mathbf{x}_2 = 0, \mathbf{x}_3 = 0\} = 0$ 

2. Consider a Naive Bayes classifier and compute its classifications if the same dataset is used also for testing

**Solution:** Note that the values of  $\mathbf{x}_1$  are identical to the ones of  $\mathbf{y}$ . Then Prob  $\{\mathbf{x}_1 = A | \mathbf{y} = \neg A\} = 0$ . It follows that if use a Naive Bayes and the test dataset is equal to the training set all the predictions will coincide with the values of  $\mathbf{x}_1$ . The training error is then zero

3. Trace the ROC curve associated to the Naive Bayes classifier if the same dataset is used also for testing. (Hint: make the assumption that the denominator of the Bayes formula is 1 for all test points)

Solution : Since all the predictions are correct the ROC curve is equal to 1 for all FPR values

#### Bonus question (1,5 points)

The points of the bonus question will be taken into account only if the students got at least 8 points in the previous questions

Consider the data set in Question 4 and let us fit to it a radial basis function with 2 basis functions having as parameters  $\mu^{(1)} = [0,0]$  and  $\mu^{(2)} = [1,1]$ . The equation of the basis function is

$$\rho(x,\mu) = \prod_{i=1}^{2} exp^{-(x_i - \mu_i)^2}$$

where  $x_i$  ( $\mu_i$ ) stands for the *i*th coordinate of the vector x ( $\mu$ ).

The student should return the equation of the radial basis function.

**Solution :** The equation of the RBF is  $h(x) = \sum_{j=1}^{2} w_j \rho^{(j)}(x, \mu^{(j)})$ The only unknown terms are the weights  $w_1$  and  $w_2$  which should be estimated by least-squares solving the equation Y = RW where  $W = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$  and

$$R = \begin{bmatrix} \rho^{(1)}(x_1, \mu^{(1)}) & \rho^{(2)}(x_1, \mu^{(2)}) \\ & \ddots & \\ \rho^{(1)}(x_N, \mu^{(1)}) & \rho^{(2)}(x_N, \mu^{(2)}) \end{bmatrix}$$

For our dataset

$$R = \begin{bmatrix} 0.95 & 0.11 \\ 0.99 & 0.16 \\ 0.34 & 0.18 \\ 0.95 & 0.23 \\ 0.73 & 0.10 \\ 0.98 & 0.20 \\ 0.14 & 0.02 \end{bmatrix}$$

By solving the least-squares  $W = (R^T R)^{-1} R^T Y$  we obtain  $w_1 = 0.02, w_2 = 3.94$