# Homework 1

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### **Homework Description**

Course: ECEN649, Fall2022

Problems (from Chapter 2 in the book): 2.1, 2.3 (a,b), 2.4, 2.7, 2.9, 2.17 (a,b)

Note: the book is available electronically on the Evans library website.

• Deadline: Sept. 26th, 11:59 pm

# **Computational Environment Setup**

#### Third-party libraries

```
matplotlib inline
import sys # system information
import matplotlib # plotting
import scipy as st # scientific computing
import pandas as pd # data managing
import numpy as np # numerical comuptation
import matplotlib.pyplot as plt
from scipy.stats import multivariate_normal
from scipy.special import erf
import scipy.optimize as opt
from numpy.linalg import inv, det
# Matplotlib setting
plt.rcParams['text.usetex'] = True
matplotlib.rcParams['figure.dpi']= 300
```

#### Version

```
print(sys.version)
print(matplotlib.__version__)
print(st.__version__)
print(np.__version__)
print(pd.__version__)

3.8.12 (default, Oct 22 2021, 18:39:35)
[Clang 13.0.0 (clang-1300.0.29.3)]
3.3.1
1.5.2
1.19.1
1.1.1
```

#### Problem 2.1

Suppose that X is a discrete feature vector, with distribution concentrated over a countable set  $D = \{x^1, x^2, ...\}$  in  $R^d$ . Derive the discrete versions of (2.3), (2.4), (2.8), (2.9), (2.11), (2.30), (2.34), and (2.36)

Hint: Note that if X has a discrete distribution, then integration becomes summation,  $P(X=x_k)$ , for  $x_k \in D$ , play the role of p(x), and  $P(X=x_k|Y=y)$ , for  $x_k \in D$ , play the role of p(x|Y=y), for y=0,1.

# (2.3)

From Braga-Neto (2020, 16)

$$P(X \in E, Y = 0) = \int_{E} P(Y = 0)p(x|Y = 0)dx \tag{1}$$

$$P(X \in E, Y = 1) = \int_{E} P(Y = 1)p(x|Y = 1)dx \tag{2}$$

(3)

Let  $x_k = [x_1, \dots, x_d]$  be the feature vector of X in set  $D \in R^d,$ 

$$P(X \in D, Y = 0) = P(X = [x_1, \dots, x_d], Y = 0)$$
(4)

$$= \sum_{X \in D} P(Y=0) P(X=[x_1, \dots, x_d] | Y=0) \tag{5}$$

$$P(X \in D, Y = 1) = P(X = [x_1, \dots, x_d], Y = 1)$$
(6)

$$= \sum_{X \in D} P(Y=1)P(X=[x_1, \dots, x_d]|Y=1) \tag{7}$$

(8)

#### (2.4)

From Braga-Neto (2020, 17)

$$P(Y = 0|X = x_k) = \frac{P(Y = 0)p(X = x_k|Y = 0)}{p(X = x_k)}$$
(9)

$$=\frac{P(Y=0)p(X=x_k|Y=0)}{P(Y=0)p(X=x_k|Y=0)+P(Y=1)p(X=x_k|Y=1)} \tag{10}$$

(11)

$$P(Y=1|X=x_k) = \frac{P(Y=1)p(X=x_k|Y=1)}{p(X=x_k)} \tag{12}$$

$$=\frac{P(Y=1)p(X=x_k|Y=1)}{P(Y=0)p(X=x_k|Y=0)+P(Y=1)p(X=x_k|Y=1)} \tag{13}$$

(14)

#### (2.8)

From Braga-Neto (2020, 18)

$$\epsilon^0[\psi] = P(\psi(X) = 1|Y = 0) = \sum_{\{x_k|\psi(x) = 1\}} p(x_k|Y = 0)$$

$$\epsilon^1[\psi] = P(\psi(X) = 0 | Y = 1) = \sum_{\{x_k | \psi(x) = 1\}} p(x_k | Y = 1)$$

(2.9)

From Braga-Neto (2020, 18)

$$\epsilon[\psi] = \sum_{\{x|\psi(x)=1\}} P(Y=0) p(x_k|Y=0) + \sum_{\{x|\psi=0\}} P(Y=1) p(x_k|Y=1)$$

(2.11)

From Braga-Neto (2020, 19)

$$\epsilon[\psi] = E[\epsilon[\psi|X=x_k]] = \sum_{x_k \in D} \epsilon[\psi|X=x_k] p(x_k)$$

(2.30)

From Braga-Neto (2020, 24).

$$\epsilon^* = \sum_{x \in X} \left[ I_{\eta(X=x) \leq 1 - \eta(X=x)} \eta(X=x) + I_{\eta(X=x) > 1 - \eta(X=x)(1 - \eta(X=x))} \right] p(X=x)$$

(2.34)

From Braga-Neto (2020, 25).

$$\epsilon^* = P(Y=0)\epsilon^0[\psi^*] + P(Y=1)\epsilon^1[\psi^*] 
= \sum_{\{x|P(Y=1)p(x|Y=1)>P(Y=0)p(x|Y=0)\}} P(Y=0)p(x|Y=0) + \sum_{\{x|P(Y=1)p(x|Y=1)\leq P(Y=0)p(x|Y=0)\}} P(Y=1)p(x|Y=0) 
(15)$$
(15)

(2.36)

From Braga-Neto (2020, 25)

$$E[\eta(X)] = \sum_{x \in R^d} P(Y = 1 | X = x) p(x) = P(Y = 1)$$

# Problem 2.3

This problem seeks to characterize the case  $\epsilon^* = 0$ .

(a)

Prove the "Zero-One Law" for perfect discrimination:

$$\epsilon^* = 0 \Leftrightarrow \eta(X) = 0 \text{ or } 1 \text{ with probability } 1.$$
 (17)

The optimal Bayes classifier is defined in Braga-Neto (2020, 20). That is

$$\psi^*(x) = \arg\max_{i} P(Y = i | X = x) = \begin{cases} 1, & \eta(x) > \frac{1}{2} \\ 0, & \text{otherwise} \end{cases}$$
 (18)

**Part 1:**  $\eta(X) = 1$ 

$$\eta(X) = E[Y|X = x] = P(Y = 1|X = x) = 1$$

$$\because \eta(X) = 1 > \frac{1}{2} \because \psi^*(x) = 1$$

$$\epsilon^* = \epsilon[\psi^*(X)|X = x] \tag{19}$$

$$=I_{\eta h^*(x)=0}P(Y=1|X=x)+I_{\eta h^*(x)=1}P(Y=0|X=x)$$
(20)

$$= \underbrace{I_{\psi^*(x)=0}}_{=0} \underbrace{\eta(X)}_{=1} + \underbrace{I_{\psi^*(x)=1}}_{=1} \underbrace{(1-\eta(X))}_{=0}$$
 (21)

$$=0 (22)$$

**Part 2:**  $\eta(X) = 0$ 

Similarly,

$$: \eta(X) = 0 \le \frac{1}{2} : \psi^*(x) = 0$$

$$\epsilon^* = \epsilon[\psi^*(X)|X = x] \tag{23}$$

$$=I_{\psi^*(x)=0}P(Y=1|X=x)+I_{\psi^*(x)=1}P(Y=0|X=x) \tag{24}$$

$$= \underbrace{I_{\psi^*(x)=0}}_{=1} \underbrace{\eta(X)}_{=0} + \underbrace{I_{\psi^*(x)=1}}_{=0} \underbrace{(1-\eta(X))}_{=1}$$
 (25)

$$=0 (26)$$

In conclusion, both cases shows that  $\epsilon^* = 0$ .

(b)

Show that

 $\epsilon^* = 0 \Leftrightarrow$  there is a function f s.t. Y = f(X) with probability 1

$$\eta(X) = Pr(Y = 1|X = x) = \begin{cases} 1, & f(X) = 1\\ 0, & f(X) = 0 \end{cases}$$
 (27)

The sceneraio is same as Problem 3.7 (a).

- 1. Given  $\eta(X) = 1$ 
  - $\epsilon^* = 0$
- 2. Given  $\eta(X) = 0$ 
  - $\epsilon^* = 0$

 $\epsilon^* = 0$  for both cases.

#### Problem 2.4

This problem concerns the extension to the multiple-class case of some of the concepts derived in this chapter. Let  $Y \in \{0, 1, ..., c-1\}$ , where c is the number of classes, and let

$$\eta_i(x) = P(Y = i | X = x), \quad i = 0, 1, \dots, c - 1,$$

for each  $x \in \mathbb{R}^d$ . We need to remember that these probabilities are not indpendent, but satisfy  $\eta_0(x) + \eta_1(x) + \dots + \eta_{c-1}(x) = 1$ , for each  $x \in \mathbb{R}^d$ , so that one of the

functions is redundant. In the two-class case, this is made explicit by using a single  $\eta(x)$ , but using the redundant set above proves advantageous in the multiple-class case, as seen below.

Hint: you should answer the following items in sequence, using the previous answers in the solution of the following ones

(a)

Given a classifier  $\psi: R^d \to \{0, 1, \dots, c-1\}$ , show that its conditional error  $P(\psi(X) \neq Y | X = x)$  is given by

$$P(\psi(X) \neq Y | X = x) = 1 - \sum_{i=1}^{c-1} I_{\psi(x)=i} \eta_i(x) = 1 - \eta_{\psi(x)}(x)$$
 (28)

Use the "Law of Total Probability" (Braga-Neto 2020, sec. A.53),

$$P(\psi(X) = Y|X = x) + P(\psi(X) \neq Y|X = x) = 1$$
(29)

 $\div$  We can derive the probability of error via

$$P(\psi(X) \neq Y | X = x) = 1 - P(\psi(X) = Y | X = x)$$
(30)

$$=1-\sum_{i=0}^{c-1}P(\psi(x)=i,Y=i|X=x) \tag{31}$$

$$=1-\sum_{i=0}^{c-1}I_{\psi(x)=i}P(Y=i|X=x) \tag{32}$$

$$=1-\sum_{i=0}^{c-1}I_{\psi(x)=i}\eta_{i}(x) \tag{33}$$

Combining together, Equation 29 implies Equation 28.

(b)

Assuming that X has a density, show that the classification error of  $\psi$  is given by

$$\epsilon=1-\sum_{i=0}^{c-1}\int_{\{x\mid\psi(x)=i\}}\eta_i(x)p(x)dx.$$

Let  $\{x|\psi(x)=i\}$  be the set of  $\psi(x)=i$  in X.

Use the multiplication rule (Braga-Neto 2020, sec. A1.3)

$$\epsilon = E[\epsilon[\psi(x)|X=x]] \tag{34}$$

$$=1 - \int_{R^d} P(\psi(X) = Y | X = x) p(x) dx \tag{35}$$

$$=1-\sum_{i=0}^{c-1}\int_{R^d}p(\psi(X)=i,Y=i|X=x)p(x)dx$$
(36)

$$=1-\sum_{i=0}^{c-1}\int_{R^d} \underbrace{p(\psi(X)=i|X=x)}_{\text{if } \{x|\psi(x)=i\};0, \text{ otherwise.}} p(Y=i|X=x)p(x)dx \tag{37}$$

$$=1-\sum_{i=0}^{c-1}\int_{\{x|\psi(x)=i\}}1\cdot p(Y=i|X=x)p(x)dx\tag{38}$$

$$=1-\sum_{i=0}^{c-1}\int_{\{x|\psi(x)=i\}}p(Y=i|X=x)p(x)dx \tag{39}$$

(c)

Prove that the Bayes classifier is given by

$$\psi^*(x) = \arg \max_{i=0, 1, \dots, c-1} \eta_i(x), \quad x \in \mathbb{R}^d$$
 (40)

Hint: Start by considering the difference between conditional expected errors  $P(\psi(X) \neq Y | X = x) - P(\psi^*(X) \neq Y | X = x)$ .

According to Braga-Neto (2020, 20), a Bayes classifier ( $\psi^*$ ) is defined as

$$\psi^* = \arg\min_{\psi \in \mathcal{C}} P(\psi(X) \neq Y)$$

over the set  $\mathcal{C}$  of all classifiers. We need to show that the error of any  $\psi \in \mathcal{C}$  has the conditional error rate:

$$\epsilon[\psi|X=x] \ge \epsilon[\psi^*|X=x], \quad \text{for all } x \in \mathbb{R}^d$$
 (41)

From Equation 28, classifiers have the error rates:

$$P(\psi^*(X) \neq |X = x) = 1 - \sum_{i=1}^{c-1} I_{\psi^*(x)=i} \eta_i(x) \tag{42}$$

$$P(\psi(X) \neq | X = x) = 1 - \sum_{i=1}^{c-1} I_{\psi(x)=i} \eta_i(x)$$
 (43)

Therefore,

$$P(\psi(X) \neq Y | X = x) - P(\psi^*(X) \neq Y | X = x) = (1 - \sum_{i=1}^{c-1} I_{\psi(x)=i} \eta_i(x)) - (1 - \sum_{i=1}^{c-1} I_{\psi^*(x)=i} \eta_i(x))$$
 (44)

$$= \sum_{i=1}^{c-1} (I_{\psi^*(x)=i} - I_{\psi(x)=i}) \eta_i(x)$$
 (45)

$$\begin{array}{ll} \bullet & I_{\psi^*(x)=i^*}=1 \text{ when } i^* \text{ satisfies } \eta_{i^*}(x)=\max_{i=0,1,\dots,c-1}\eta(x)=\eta_{\max}(x) \\ \bullet & I_{\psi(x)=i'}=1 \text{ when } \psi(x)=i' \text{ for } i'\in 0,1,\dots,c-1 \end{array}$$

• 
$$I_{\psi(x)=i'}=1$$
 when  $\psi(x)=i'$  for  $i'\in 0,1,\ldots,c-1$ 

if  $i^* \neq i'$ 

$$P(\psi(X) \neq Y | X = x) - P(\psi^*(X) \neq Y | X = x) = (1 - 0)\eta_{i^*}(x) + (0 - 1)\eta_{i'}(x) \tag{46}$$

$$= \eta_{i^*}(x) - \eta_{i'}(x) \tag{47}$$

$$= \eta_{\max}(x) - \eta_{i'}(x) \tag{48}$$

$$\geq 0 \tag{49}$$

if  $i^* = i'$ 

$$P(\psi(X) \neq Y | X = x) - P(\psi^*(X) \neq Y | X = x) = \eta_{i^*}(x) - \eta_{i'}(x) = 0$$

Therefore, there is no classifier  $\psi \in \mathcal{C}$  can have conditional error rate lower than Bayes classifier Equation 40.

(d)

Show that the Bayes error is given by

$$\epsilon^* = 1 - E[\max_{i=0,1,\dots,c-1} \eta_i(X)]$$

From Problem 2.4.b,

• Noted that,  $\{x|\psi^*(x)=i\}=\emptyset$  if  $i\neq i^*$ 

$$\epsilon[\psi^*] = E[\epsilon[\psi^*(x)|X=x]] \tag{50}$$

$$=1-\sum_{i=0}^{c-1}\int_{\{x\mid\psi^*(x)=i\}}\eta_i(x)p(x)dx \tag{51}$$

$$=1-\int_{\{x|\psi^{*}(x)=i^{*}\}}\eta_{\max}(x)p(x)dx \tag{52}$$

$$=1-E[\eta_{\max}(x)]\tag{53}$$

(e)

Show that the maximum Bayes error possible is  $1 - \frac{1}{c}$ .

$$\max \epsilon[\psi^*] = 1 - \min E[\max_{i=0,1,\dots,c-1} \eta_i(X)]$$
 (54)

also,

given

$$\eta_1(x) = \eta_2(x) = \dots = \eta_{c-1}(x)$$

Table 1: Parameters of Gaussian PDFs.

	Parameters	Values
0	\$\$\mu_0\$\$	3
1	\$\$\mu_1\$\$	4
2	$s\simeq 0$	1
3	$s_{\sigma_1}$	3

$$\sum_{i=1}^{c-1} \eta_i(x) = 1$$

we can get that

$$\min \max \eta(X) = \frac{1}{c} \tag{55}$$

Combining Equation 54 and Equation 55 together, the maximum Bayes error is  $1-\frac{1}{c}$ 

#### Problem 2.7

Consider the following univariate Gaussian class-conditional densities:

$$p(x|Y=0) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{(x-3)^2}{2})$$
 (56)

$$p(x|Y=1) = \frac{1}{3\sqrt{2\pi}} \exp(-\frac{(x-4)^2}{18})$$
 (57)

Assume that the classes are equally likely, i.e.,  $P(Y=0)=P(Y=1)=\frac{1}{2}$ 

The PDF of Guassian distribution is<sup>1</sup>

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}}\exp(-\frac{(x-\mu)^2}{2\sigma^2})$$

<sup>&</sup>lt;sup>1</sup>Gaussian PDF. WolframAlpha. URL: https://mathworld.wolfram.com/GaussianFunction.html

(a)

Draw the densities and determine the Bayes classifier graphically.

- The plot is dispayed in Figure 1.
- The decision bounding was determined by the right intersection of both distributions. I applied Brent's method to find the intersection<sup>2</sup>.
  - Intuitively, the intersection on the right has the minimum  $\epsilon^0$  to the right and  $\epsilon^1$  to the left.

```
class Gauss:
       def __init__(self, scale, mean, var):
2
          self.scale = scale
3
          self.mean = mean
4
          self.var = var
       def pdf(self, x):
          return 1/(self.scale*np.sqrt(2*np.pi))*np.exp(-1*(x-self.mean)**2/self.var)
       def plot(self, ax, x_bound=[-5,13], nticks=200, **args):
          xs = np.linspace(x_bound[0], x_bound[1], nticks)
          ps = [self.pdf(x) for x in xs]
10
          ax.plot(xs, ps, **args)
11
12
13
   g0 = Gauss(1,3,2)
14
   g1 = Gauss(3,4,18)
16
   ## Boundaries
17
   dec_x = [1.26, 4.49] # see problem 2.7 (b) for derivation
18
19
   ## Plotting
20
   fig, ax = plt.subplots()
^{21}
   g0.plot(ax, color="black", label="$p(x|Y=0) = \frac{1}{\sqrt{2}}}\\ (x-3)^2 = \frac{1}{\sqrt{2}}
   ax.axvline(x=dec_x[0], label="Bayes decision boundary")
24
   ax.axvline(x=dec_x[1])
25
   ax.set_xlabel("$x$")
26
   ax.set_ylabel("$PDF$")
27
   ax.annotate("\frac{*}{x}=1$", (7.5,0.2))
   ax.annotate("\pi^{*}(x)=1", (-5,0.2))
   ax.annotate("\pi^{*}(x)=0", (1.4,0.2))
```

 $<sup>{}^2 \</sup>texttt{scipy.optimize.brentq}. \ \, \text{https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.brentq.html} \\$ 

# ax.legend(loc="upper right");

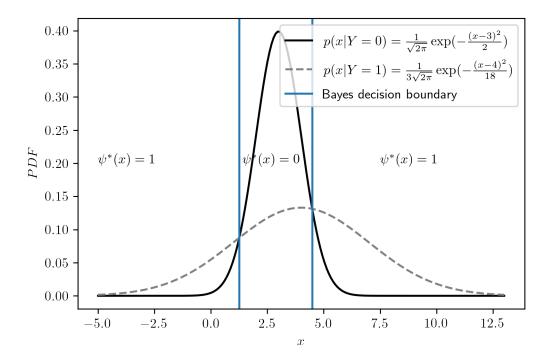


Figure 1: Univariate gaussian densities.

(b)

Determine the Bayes classifier.

According to Braga-Neto (2020, 22), the Bayes classifier can be defined by

$$\psi^*(x) = \begin{cases} 1, & D^*(x) > k^* \\ 0, & \text{otherwise} \end{cases}$$
 (58)

where  $D^*(x) = \ln \frac{p(x|Y=1)}{p(x|Y=0)}$ ,  $k^* = \ln \frac{P(Y=0)}{P(Y=1)}$ . Now, take Equation 56 and Equation 57 into the forumula.

$$k^* = \ln \frac{1}{1} = 0$$

$$D^*(x) = \ln \frac{p(x|Y=1)}{p(x|Y=0)}$$
(59)

$$= \ln \frac{\frac{1}{\sqrt{2\pi}} \exp(-\frac{(x-3)^2}{2})}{\frac{1}{3\sqrt{2\pi}} \exp(-\frac{(x-4)^2}{18})}$$
(60)

$$= \ln \left[ 3 \cdot \exp(-\frac{(x-3)^2}{2} + \frac{(x-4)^2}{18}) \right] \tag{61}$$

$$= \ln 3 - \frac{(x-3)^2}{2} + \frac{(x-4)^2}{18} \tag{62}$$

$$= \frac{-4}{9}x^2 + \frac{23}{9}x + (\ln(3) - \frac{65}{18}) \tag{63}$$

Thus, the Bayes classifier for distinguishing Equation 56 and Equation 57 is

$$\psi^*(x) = \begin{cases} 1, & \frac{-4}{9}x^2 + \frac{23}{9}x + (\ln(3) - \frac{65}{18}) > 0\\ 0, & \text{otherwise} \end{cases}$$
 (64)

with the boundaries

$$x = \begin{cases} \frac{1}{8}(23 - 3\sqrt{1 + 16\ln(3)}) & \approx 1.26\\ \frac{1}{8}(23 + 3\sqrt{1 + 16\ln(3)}) & \approx 4.49 \end{cases}$$
 (65)

Noted that there are two boundaries for  $D^*(x) = 0$  becasue  $D^*(x)$  is a second order equation of x.

$$\psi^*(x) = \begin{cases} 1, & \left[ x - \left( \frac{1}{8} (23 - 3\sqrt{1 + 16 \ln(3)}) \right) \right] \left[ x - \left( \frac{1}{8} (23 + 3\sqrt{1 + 16 \ln(3)}) \right) \right] > 0 \\ 0, & \text{otherwise} \end{cases}$$
 (66)

$$= \begin{cases} 1, x < (\frac{1}{8}(23 - 3\sqrt{1 + 16\ln(3)})) \lor x > (\frac{1}{8}(23 + 3\sqrt{1 + 16\ln(3)})) \\ 0, \text{ otherwise} \end{cases}$$
 (67)

$$\approx \begin{cases} 1, x < 1.26 \lor x > 4.49 \\ 0, \text{ otherwise} \end{cases}$$
 (68)

(c)

Determine the specificity and sensitivity of the Bayes classifier.

Hint: use the standard Gaussian CDF  $\psi(x)$ 

Let left and right boundaries be  $\frac{1}{8}(23-3\sqrt{1+16\ln(3)})=b_1$  and  $\frac{1}{8}(23+3\sqrt{1+16\ln(3)})=b_2$ ,

Table 2: The definition of sensitivity and specificity from Braga-Neto (2020, 18)

$$\frac{\text{Sensitivity}}{1 - \epsilon^1 [\psi]} \quad \frac{\text{Specificity}}{1 - \epsilon^0 [\psi]}$$

The standard normal CDF is<sup>3</sup>. Use the definition of  $\epsilon^0[\psi]$  and  $\epsilon^1[\psi]$  in Braga-Neto (2020, 18)

$$F(x) = p(X < x) = \frac{1}{2} \left[ 1 + erf(\frac{x - \mu}{\sigma\sqrt{2}}) \right]$$

$$\epsilon^0[\psi^*(x)] = P(\psi(X) = 1|Y = 0) \tag{69}$$

$$= \int_{\{x|\psi(x)=1\}} p(x|Y=0)dx \tag{70}$$

$$= \int_{-\infty}^{b_1} p(x|Y=0)dx + \int_{b_2}^{\infty} p(x|Y=0)dx$$
 (71)

$$=F_{X_0}(b_1)+1-F_{X_0}(b_2) \tag{72}$$

$$= \frac{1}{2} \left[ 1 + erf\left(\frac{b_1 - \mu_0}{\sigma_0 \sqrt{2}}\right) \right] + 1 - \frac{1}{2} \left[ 1 + erf\left(\frac{b_2 - \mu_0}{\sigma_0 \sqrt{2}}\right) \right]$$
 (73)

$$= 1 + \frac{1}{2} (erf(\frac{b_1 - \mu_0}{\sigma_0 \sqrt{2}}) - erf(\frac{b_2 - \mu_0}{\sigma_0 \sqrt{2}})) \tag{74}$$

<sup>&</sup>lt;sup>3</sup>Normal distribution. Wiki URL: https://en.wikipedia.org/wiki/Normal\_distribution

Table 3: Exact values of type 0 and type 1 error rates.

	Error statistics	Value
0	epsilon_0	0.108752
1	epsilon_1	0.384628
2	Sensitivity	0.615372
3	Specificity	0.891248
4	Overall Bayes error	0.246690

$$\epsilon^{1}[\psi^{*}(x)] = P(\psi(X) = 0|Y = 1)$$
(75)

$$= \int_{\{x|\psi(x)=0\}} p(x|Y=1)dx \tag{76}$$

$$= \int_{b_1}^{b_2} p(x|Y=1)dx \tag{77}$$

$$=F_{X_1}(b_2)-F_{X_1}(b1) \tag{78}$$

$$=\frac{1}{2}\left[erf(\frac{b_2-\mu_1}{\sigma_1\sqrt{2}})-erf(\frac{b_1-\mu_1}{\sigma_1\sqrt{2}})\right] \tag{79}$$

(80)

The exact values of error estimation are shown in Table 3 (epsilon\_0 is  $\epsilon_0$ , and epsilon\_1  $\epsilon_1$ ). Specificity and sensitivity are calculated with their definitions shown in Table 2,

```
# Calculation of error statistics
def nerf(b, mu, std):
    return erf( (b - mu) / (std*np.sqrt(2)))

b1 = (1/8)*(23-3*np.sqrt(1+16*np.log(3)))
b2 = (1/8)*(23+3*np.sqrt(1+16*np.log(3)))
e0 = 1 + 0.5*(nerf(b1,mu0, std0) - nerf(b2,mu0, std0))
e1 = 0.5*(nerf(b2,mu1, std1) - nerf(b1, mu1, std1))

sensi = 1 - e1
spec = 1 - e0
bayesError = 0.5*(e0+e1)
```

Table 4: Exact values of Bayes error.

	Error statistics	Value
0	Overall Bayes error	0.24669

(d)

Determine the overall Bayes error.

Use the derivation in Braga-Neto (2020, 18),

$$\epsilon[\psi^*(X)] = P(\psi(X) \neq Y) \tag{81}$$

$$= P(\psi(X) = 1, Y = 0) + P(\psi(X) = 0, Y = 1)$$
(82)

$$= P(Y=0)P(\psi(X)=1|Y=0) + P(Y=1)P(\psi(X)=0|Y=1)$$
(83)

$$=P(Y=0)\epsilon^0 + P(Y=1)\epsilon^1 \tag{84}$$

$$=\frac{1}{2}(\epsilon^0 + \epsilon^1) \tag{85}$$

The excat Bayes error is displayed in Table 4.

#### Problem 2.9

Obtain the optimal decision boundary in the Gaussian model with P(Y=0)=P(Y=1) and

In each case draw the optimal decision boundary, along with the class means and class conditional density contours, indicating the 0- and 1-decision regions.

Since  $\Sigma_0 \neq \Sigma_1$  happens in the following subproblems, these are heteroskedastic cases. As mentioned in Braga-Neto (2020, sec. 2.5.2). The Bayes classifier is

$$\psi_Q^*(x) = \begin{cases} 1, x^T A x + b^T x + c > 0 \\ 0, \text{ otherwise} \end{cases}$$
 (86)

where

$$A = \frac{1}{2}(\Sigma_0^{-1} - \Sigma_1^{-1}) \tag{87}$$

$$b = \Sigma_1^{-1} \mu_1 - \Sigma_0^{-1} \mu_0 \tag{88}$$

$$c = \frac{1}{2} (\mu_0^T \Sigma_0^{-1} \mu_0 - \mu_1^T \Sigma_1^{-1} \mu_1) + \frac{1}{2} \ln \frac{\det(\Sigma_0)}{\det(\Sigma_1)} + \ln \frac{P(Y=1)}{P(Y=0)}$$
(89)

Let x be the vector of sample values,

$$x = \begin{bmatrix} x_1 \\ x_0 \end{bmatrix} \tag{90}$$

The following is the Python implementation with NumPy<sup>4</sup> <sup>5</sup>.

```
def compose(U,D):
2
       return U.transpose()@inv(D)@U
   def mA(sigma0, sigma1):
       sigma0_inv = inv(sigma0)
       sigma1_inv = inv(sigma1)
       return 0.5*(sigma0_inv - sigma1_inv)
   def mb(sigma0, sigma1, mu0, mu1):
       sigma0_inv = inv(sigma0)
10
       sigma1_inv = inv(sigma1)
11
       return sigma1_inv@mu1 - sigma0_inv@mu0
12
13
   def mc(sigma0, sigma1, mu0, mu1, Py):
14
       return 0.5*(compose(mu0, sigma0) - compose(mu1, sigma1)) +\
15
           0.5*np.log(det(sigma0)/det(sigma1)) +\
16
                np.log(Py/(1-Py))
17
18
   def BayesBound(x, sigma0, sigma1, mu0, mu1, Py):
19
       xax = x.transpose() @ mA(sigma0, sigma1)@x
20
       bx = mb(sigma0, sigma1, mu0, mu1).transpose() @ x
       c = mc(sigma0, sigma1, mu0, mu1, Py)
22
23
```

<sup>&</sup>lt;sup>4</sup>There is a well-written documentation for matrix operation: https://numpy.org/doc/stable/user/absolute\_beginners.html#creatir matrices

<sup>&</sup>lt;sup>5</sup>the contour plot for Gaussian process is referred to https://gist.github.com/gwgundersen/90dfa64ca29aa8c3833dbc6b03de44be.

```
return float(xax + bx + c)
24
25
   class GaussianBayesClassifier:
26
        def __init__(self, sigma0, sigma1, mu0, mu1, Py):
27
            self.sigma0 = sigma0
28
            self.sigma1 = sigma1
29
            self.mu0 = mu0
30
            self.mu1 = mu1
31
            self.Py = Py
32
            # Inferred Matrix
            self.mA = mA(sigma0, sigma1)
            self.mb = mb(sigma0, sigma1, mu0, mu1)
36
            self.mc = mc(sigma0, sigma1, mu0, mu1, Py)
37
38
        def BayesBound(self, x):
39
            return BayesBound(x, self.sigma0, self.sigma1, self.mu0, self.mu1, self.Py)
40
        def psi(self, x):
            11 11 11
            Bayes classification
44
            11 11 11
45
            pred = 0
46
            if self.BayesBound(x) > 0:
47
                pred = 1
            return pred
49
        def plot2D(self, psi_annotates=[[0.3,0.3], [0.7,0.7]]):
51
            fig, ax = plt.subplots()
52
53
            # Create girds
54
            xlist = np.linspace(-3.5,3.5,40)
            ylist = np.linspace(-3.5,3.5,40)
            X, Y = np.meshgrid(xlist, ylist)
            pos = np.dstack((X,Y))
59
            # Compute Bayes classification
60
            Z = np.zeros(X.shape)
61
            for i in range(0, Z.shape[0]):
62
                for j in range(0, Z.shape[1]):
63
                    x = np.matrix([X[i,j], Y[i,j]]).T
64
```

```
Z[i,j] = self.psi(x)
65
66
            # Compute Gaussia pdf
67
            rv0 = multivariate_normal(np.array(self.mu0.T)[0], self.sigma0)
            rv1 = multivariate normal(np.array(self.mu1.T)[0], self.sigma1)
69
            Z0 = rv0.pdf(pos)
70
            Z1 = rv1.pdf(pos)
71
72
            # Plot contours
73
            cmap = plt.get_cmap('Set1', 2)
            ax.contour(X,Y,Z, cmap=cmap, levels=[0.9])
            ax.contour(X,Y,Z0, alpha=0.4)
            ax.contour(X,Y,Z1, alpha=0.4)
            ax.plot(self.mu0[0,0], self.mu0[1,0], marker="0", color="k",label="$\mu_0$")
78
            ax.plot(self.mu1[0,0], self.mu1[1,0], marker="o", color="gray",label="<math>\mbox{mu}_1")
79
            if psi_annotates==None:
80
                psi_annotates = [[self.mu0[0,0], self.mu0[1,0]], [self.mu1[0,0], self.mu1[1,0]]]
            # Annotate decisions
            for ann in psi_annotates:
                i = X[int(X.shape[0]*ann[0]), int(X.shape[1]*ann[1])]
85
                j = Y[int(Y.shape[0]*ann[0]), int(Y.shape[1]*ann[1])]
86
                x = np.matrix([i, j]).T
87
                if self.psi(x) > 0:
88
                    ax.annotate("$\pi^{*}(x) = 1$", (i, j))
                else:
                    ax.annotate("$\pi^{*}(x) = 0$", (i, j))
            # legend and label settings
93
            ax.set_xlabel("$x_1$")
94
            ax.set_ylabel("$x_2$")
95
            ax.legend()
96
```

(a)

$$\mu_0 = (0,0)^T, \mu_1 = (2,0)^T, \Sigma_0 = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}, \Sigma_1 = \begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix}$$

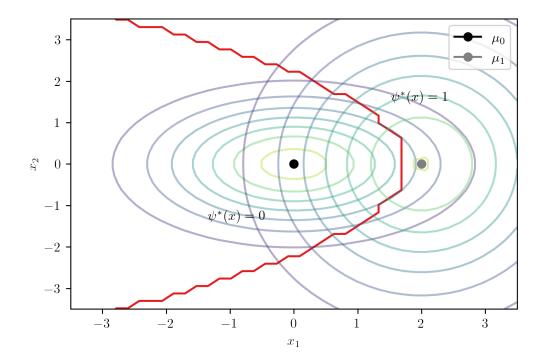


Figure 2: Bayes Classifier for 2D Gussian (a)

(b)

$$\mu_0 = (0,0)^T, \mu_1 = (2,0)^T, \Sigma_0 = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}, \Sigma_1 = \begin{pmatrix} 4 & 0 \\ 0 & 1 \end{pmatrix}$$

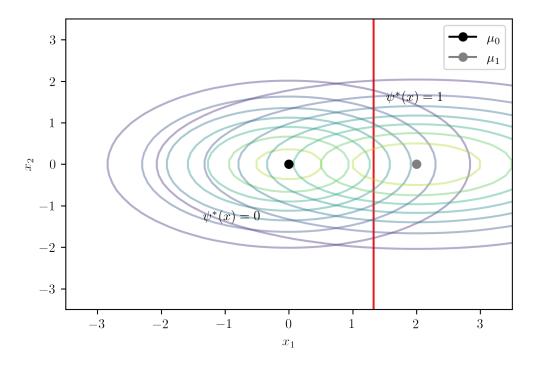


Figure 3: Bayes Classifier for 2D Gussian (b)

(c)

$$\mu_0 = (0,0)^T, \mu_1 = (0,0)^T, \Sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \Sigma_1 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

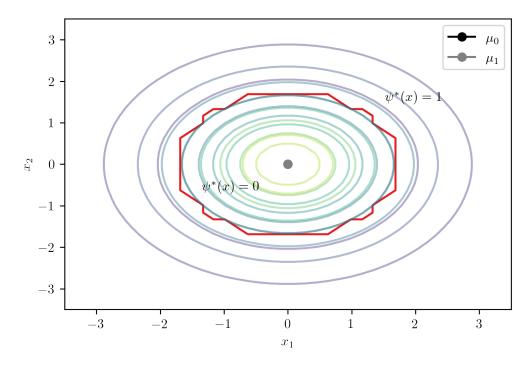


Figure 4: Bayes Classifier for 2D Gussian (c)

(d)

$$\mu_0 = (0,0)^T, \mu_1 = (0,0)^T, \Sigma_0 = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}, \Sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$

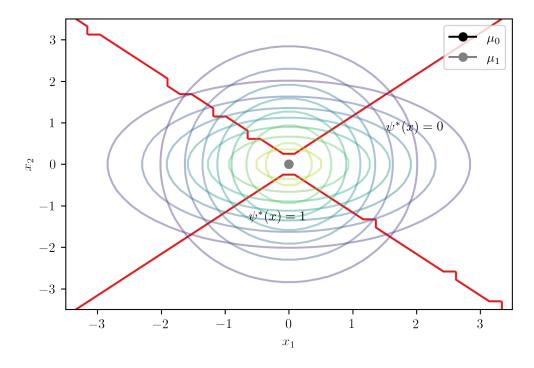


Figure 5: Bayes Classifier for 2D Gussian (d)

# Python Assignment: Problem 2.17

This problem concerns the Gaussian model for synthetic data generation in Braga-Neto (2020, sec. A8.1).

(a)

Derive a general expression for the Bayes error for the homosked astic case with  $\mu_0=(0,\dots,0), \mu_1=(1,\dots,1),$  and P(Y=0)=P(Y=1). Your answer should be in terms of  $k,\sigma_1^2,\dots,\sigma_k^2,l_1,\dots,l_k,$  and  $\rho_1,\dots,\rho_k.$ 

Hint: Use the fact that

$$\begin{bmatrix} 1 & \sigma & \cdots & \sigma \\ \sigma & 1 & \cdots & \sigma \\ \vdots & \vdots & \ddots & \vdots \\ \sigma & \sigma & \cdots & 1 \end{bmatrix}_{l \times l}^{-1} = \frac{1}{(1-\sigma)(1+(l-1)\sigma)} \begin{bmatrix} 1+(l-2)\sigma & -\sigma \cdots & -\sigma \\ -\sigma & 1+(l-2)\sigma & \cdots & -\sigma \\ \vdots & \vdots & \ddots & \vdots \\ -\sigma & -\sigma & \cdots & 1+(l-2) & \sigma \end{bmatrix}$$

$$(91)$$

Use Equation 2.53 in Braga-Neto (2020, 31). Given P(Y=0) = P(Y=1) = 0.5, then

$$\epsilon_L^* = \Phi(-\frac{\delta}{2}) \tag{92}$$

where  $\delta = \sqrt{(\mu_1 - \mu_0)^T \Sigma^{-1} (\mu_1 - \mu_0)}$ .

$$\Sigma_{d \times d} = \begin{bmatrix} \Sigma_{l_1 \times l_1}(\sigma_1^2, \rho_1) & 0 & \cdots & 0 \\ 0 & \Sigma_{l_2 \times l_2}(\sigma_2^2, \rho_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Sigma_{l_k \times l_k}(\sigma_k^2, \rho_k) \end{bmatrix}$$
(93)

where  $l_1 + \dots + l_k = d$ .

$$\Sigma_{l_k \times l_k}(\sigma_i^2, \rho_i) = \sigma_i^2 \begin{bmatrix} 1 & \rho_i & \cdots & \rho_i \\ \rho_i & 1 & \cdots & \rho_i \\ \vdots & \vdots & \ddots & \vdots \\ \rho_i & \rho_i & \cdots & 1 \end{bmatrix}$$

$$\Sigma_{l_k \times l_k}^{-1}(\sigma_i^2, \rho_i) = \frac{1}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} \begin{bmatrix} 1 + (l_k - 2)\sigma_i & -\sigma_i & \cdots & -\sigma_i \\ -\sigma_i & 1 + (l_k - 2)\sigma_i & \cdots & -\sigma_i \\ \vdots & \vdots & \ddots & \vdots \\ -\sigma_i & -\sigma_i & \cdots & 1 + (l_k - 2)\sigma_i \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1 + (l_k - 2)\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} & \frac{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} & \cdots & \frac{\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} \\ \vdots & \vdots & \ddots & \vdots \\ -\sigma_i & -\sigma_i & \cdots & \frac{-\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} & \cdots & \frac{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1 + (l_k - 2)\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} & \frac{-\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} & \cdots & \frac{-\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} \\ \vdots & \vdots & \ddots & \vdots \\ -\sigma_i & \cdots & \frac{-\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} & \cdots & \frac{1 + (l_k - 2)\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1 + (l_k - 2)\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} & \cdots & \frac{-\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} \\ \vdots & \vdots & \ddots & \vdots \\ -\sigma_i & \cdots & \frac{-\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} & \cdots \\ \frac{-\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} & \cdots & \frac{-\sigma_i}{\sigma_i^2 (1 - \sigma_i)(1 + (l_k - 1)\sigma_i)} \\ \end{bmatrix}$$

Thus, the inverse of covariance matrix is

$$\Sigma_{d \times d}^{-1} = \begin{bmatrix} \Sigma_{l_1 \times l_1}^{-1}(\sigma_1^2, \rho_1) & 0 & \cdots & 0 \\ 0 & \Sigma_{l_2 \times l_2}^{-1}(\sigma_2^2, \rho_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Sigma_{l_1 \times l_2}^{-1}(\sigma_k^2, \rho_k) \end{bmatrix}$$
(97)

Combining together,

$$\epsilon_{L}^{*} = \Phi(\frac{-1}{2}\delta) = \frac{-1}{2}\sqrt{(\mu_{1} - \mu_{0})^{T}\Sigma^{-1}(\mu_{1} - \mu_{0})}$$

$$= \frac{-1}{2}\sqrt{\underbrace{\begin{bmatrix} 1 & \cdots & 1 \end{bmatrix}}_{1 \times d} \underbrace{\begin{bmatrix} \sum_{l_{1} \times l_{1}}^{-1}(\sigma_{1}^{2}, \rho_{1}) & 0 & \cdots & 0 \\ 0 & \sum_{l_{2} \times l_{2}}^{-1}(\sigma_{2}^{2}, \rho_{2}) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sum_{l_{k} \times l_{k}}^{-1}(\sigma_{k}^{2}, \rho_{k}) \end{bmatrix}}_{d \times 1}\underbrace{\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}}_{d \times 1}$$

$$(98)$$

(b)

Specialize the previous formula for equal-sized blocks  $l_1 = \cdots = l_k = l$  with equal correlations  $\rho_1 = \cdots = \rho_k = \rho$ , and constant variance  $\sigma_1^2 = \cdots, \sigma_k^2 = \sigma^2$ . Write the resulting formula in terms of  $d, l, \sigma$  and  $\sigma$ .

i.

Using the python function norm.cdf in the scipy.stats module, plot the Bayes error as a function of  $\sigma \in [0.01, 3]$  for d = 20, l = 4, and four different correlation values  $\sigma = 0, 0.25, 0.5, 0.75$  (plot one curve for each value). Confirm that the Bayes error increasese monotonically with  $\sigma$  from 0 to 0.5 for each value of  $\sigma$ , and that Bayes error for large  $\sigma$  is uniformly larger than that for smaller  $\sigma$ . The latter fact shows that correlation between the features is detrimental to classification.

ii.

Plot the Bayes error as a function of  $d=2,4,6,8,\ldots,40$ , with fixed block size l=4 and variance  $\sigma^2=1$  and  $\sigma=0,0.25,0.5,0.75$  (plot one curve for each value). Confirm that the Bayes error decreases monotonically to 0 with increasing dimensionality, with faster convergence for smaller correlation values.

iii.

Plot the Bayes error as a function of the correlation  $\sigma \in [0,1]$  for constant variance  $\sigma^2 = 2$  and fixed d = 20 with varying block size l = 1, 2, 4, 10 (plot one curve for each value). Confirm that the Bayes error increases monotonically with increasing correlation. Notice that the rate of increase is particularly large near  $\sigma = 0$ , which shows that the Bayes error is very sensitive to correlation in the near-independent region.

# References

Braga-Neto, Ulisses. 2020. Fundamentals of Pattern Recognition and Machine Learning. Springer.