# 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

```
1 %matplotlib inline
import sys # system information
3 import matplotlib # plotting
4 import scipy as st # scientific computing
   import pandas as pd # data managing
6 import numpy as np # numerical comuptation
7 import scipy.optimize as opt
8 import sympy as sp
   import matplotlib.pyplot as plt
10 from scipy.special import erf
11 from numpy.linalg import inv, det
12 from scipy.linalg import block_diag
13 from scipy.stats import norm # for problem 2.17 (b)
14 from scipy.stats import multivariate_normal
15 # Matplotlib setting
  plt.rcParams['text.usetex'] = True
```

```
matplotlib.rcParams['figure.dpi']= 300
RES_GRID = 60
```

#### 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)

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

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

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

(8)

#### (2.4)

From Braga-Neto (2020, 17)

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

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

(11)

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

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

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

(2.9)

From Braga-Neto (2020, 18)

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

(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).

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

(2.34)

From Braga-Neto (2020, 25).

$$\epsilon^* = P(Y=0)\epsilon^0[\psi^*] + P(Y=1)\epsilon^1[\psi^*]$$
 (15)

$$= \sum_{\{x, |P(Y-1)n(x, |Y-1) > P(Y-0)n(x, |Y-0)\}} P(Y=0)p(x_k|Y=0)$$
 (16)

$$\epsilon^* = P(Y=0)\epsilon^0[\psi^*] + P(Y=1)\epsilon^1[\psi^*]$$

$$= \sum_{\{x_k|P(Y=1)p(x_k|Y=1) > P(Y=0)p(x_k|Y=0)\}} P(Y=0)p(x_k|Y=0)$$

$$+ \sum_{\{x_k|P(Y=1)p(x_k|Y=1) \le P(Y=0)p(x_k|Y=0)\}} P(Y=1)p(x_k|Y=1)$$
(15)
$$(16)$$

(2.36)

From Braga-Neto (2020, 25)

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

#### Problem 2.3

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

(a)

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

$$\epsilon^* = 0 \Leftrightarrow \eta(X) = 0 \text{ or } 1 \text{ with probability } 1.$$
 (18)

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

$$\psi^*(x) = \arg\max_{i} P(Y = i | X = x) = \begin{cases} 1, & \eta(x) > \frac{1}{2} \\ 0, & \text{otherwise} \end{cases}$$
 (19)

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

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

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

$$\epsilon^* = \epsilon[\psi^*(X)|X = x] \tag{20}$$

$$=I_{\psi^*(x)=0}P(Y=1|X=x)+I_{\psi^*(x)=1}P(Y=0|X=x) \eqno(21)$$

$$= \underbrace{I_{\psi^*(x)=0} e}_{=0} \underbrace{\eta(X)}_{=1} + \underbrace{I_{\psi^*(x)=1}}_{=1} \underbrace{(1 - \eta(X))}_{=0}$$
 (22)

$$=0 (23)$$

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

Similarly,

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

$$\epsilon^* = \epsilon[\psi^*(X)|X = x] \tag{24}$$

$$=I_{\psi^*(x)=0}P(Y=1|X=x)+I_{\psi^*(x)=1}P(Y=0|X=x) \eqno(25)$$

$$= \underbrace{I_{\psi^*(x)=0}}_{=1} \underbrace{\eta(X)}_{=0} + \underbrace{I_{\psi^*(x)=1}}_{=0} \underbrace{(1-\eta(X))}_{=1}$$
 (26)

$$=0 (27)$$

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

$$\eta(X) = Pr(Y = 1|X = x) = \begin{cases} 1, & f(X) = 1\\ 0, & f(X) = 0 \end{cases}$$
(28)

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  $x \in R^d$ . 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  $x \in R^d$ , 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

$$P(\psi(X) \neq Y | X = x) = 1 - \sum_{i=1}^{c-1} I_{\psi(x)=i} \eta_i(x) = 1 - \eta_{\psi(x)}(x)$$
 (29)

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

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

∴ We can derive the probability of error via

$$P(\psi(X) \neq Y | X = x) = 1 - P(\psi(X) = Y | X = x)$$
(31)

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

$$=1-\sum_{i=0}^{c-1}I_{\psi(x)=i}P(Y=i|X=x) \tag{33}$$

$$=1-\sum_{i=0}^{c-1}I_{\psi(x)=i}\eta_{i}(x) \tag{34}$$

Combining together, Equation 30 implies Equation 29.

(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)

$$\epsilon = E[\epsilon[\psi(x)|X=x]] \tag{35}$$

$$=1 - \int_{R^d} P(\psi(X) = Y | X = x) p(x) dx \tag{36}$$

$$=1-\sum_{i=0}^{c-1}\int_{R^d}p(\psi(X)=i,Y=i|X=x)p(x)dx \tag{37}$$

$$=1-\sum_{i=0}^{c-1}\int_{R^d} \underbrace{p(\psi(X)=i|X=x)}_{\text{if } \{x|\psi(x)=i\};0, \text{ otherwise.}} p(Y=i|X=x)p(x)dx \tag{38}$$

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

$$=1-\sum_{i=0}^{c-1}\int_{\{x|\psi(x)=i\}}p(Y=i|X=x)p(x)dx \tag{40}$$

(c)

Prove that the Bayes classifier is given by

$$\psi^*(x) = \arg\max_{i=0,1,\dots,c-1} \eta_i(x), \quad x \in R^d$$
 (41)

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:

$$\epsilon[\psi|X=x] \ge \epsilon[\psi^*|X=x], \quad \text{for all } x \in \mathbb{R}^d$$
 (42)

From Equation 29, classifiers have the error rates:

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

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

Therefore,

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

$$(45)$$

$$= \sum_{i=1}^{c-1} (I_{\psi^*(x)=i} - I_{\psi(x)=i}) \eta_i(x)$$
 (46)

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

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

if  $i^* \neq i'$ 

$$P(\psi(X) \neq Y | X = x) - P(\psi^*(X) \neq Y | X = x) = (1 - 0)\eta_{i^*}(x) + (0 - 1)\eta_{i'}(x) \tag{47}$$

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

$$= \eta_{\max}(x) - \eta_{i'}(x) \tag{49}$$

$$\geq 0 \tag{50}$$

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 41.

(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  $i\neq i^*$ 

$$\epsilon[\psi^*] = E[\epsilon[\psi^*(x)|X=x]] \tag{51}$$

$$=1-\sum_{i=0}^{c-1}\int_{\{x\mid\psi^*(x)=i\}}\eta_i(x)p(x)dx \tag{52}$$

$$=1-\int_{\{x|\psi^{*}(x)=i^{*}\}}\eta_{\max}(x)p(x)dx \tag{53}$$

$$=1-E[\eta_{\max}(x)]\tag{54}$$

(e)

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

$$\max \epsilon[\psi^*] = 1 - \min E[\max_{i=0,1,\dots,c-1} \eta_i(X)]$$
 (55)

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

$$\min \max \eta(X) = \frac{1}{c} \tag{56}$$

Combining Equation 55 and Equation 56 together, the maximum Bayes error is  $1-\frac{1}{c}$ 

#### Problem 2.7

Consider the following univariate Gaussian class-conditional densities:

$$p(x|Y=0) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{(x-3)^2}{2})$$
 (57)

$$p(x|Y=1) = \frac{1}{3\sqrt{2\pi}} \exp(-\frac{(x-4)^2}{18})$$
 (58)

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("\psi^{*}(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");

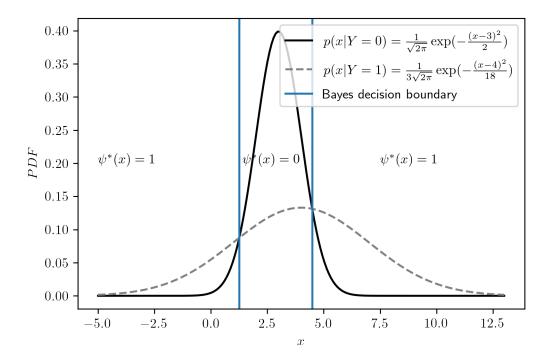


Figure 1: Univariate gaussian densities.

(b)

Determine the Bayes classifier.

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

$$\psi^*(x) = \begin{cases} 1, & D^*(x) > k^* \\ 0, & \text{otherwise} \end{cases}$$
 (59)

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 57 and Equation 58 into the forumula.

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

$$D^*(x) = \ln \frac{p(x|Y=1)}{p(x|Y=0)}$$
(60)

$$= -\ln \frac{\frac{1}{\sqrt{2\pi}} \exp(-\frac{(x-3)^2}{2})}{\frac{1}{3\sqrt{2\pi}} \exp(-\frac{(x-4)^2}{18})}$$
(61)

$$= -\ln\left[3 \cdot \exp(-\frac{(x-3)^2}{2} + \frac{(x-4)^2}{18})\right] \tag{62}$$

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

$$=\frac{4}{9}x^2 - \frac{23}{9}x - (\ln(3) + \frac{65}{18})\tag{64}$$

Thus, the Bayes classifier for distinguishing Equation 57 and Equation 58 is

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

with the boundaries

$$x = \begin{cases} \frac{1}{8}(23 - 3\sqrt{1 + 16\ln(3)}) &\approx 1.26\\ \frac{1}{8}(23 + 3\sqrt{1 + 16\ln(3)}) &\approx 4.49 \end{cases}$$
 (66)

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

$$\psi^*(x) = \begin{cases} 1, & \left[ x - \left( \frac{1}{8} (23 - 3\sqrt{1 + 16\ln(3)}) \right) \right] \left[ x - \left( \frac{1}{8} (23 + 3\sqrt{1 + 16\ln(3)}) \right) \right] > 0 \\ 0, & \text{otherwise} \end{cases}$$
 (67)

$$= \begin{cases} 1, x < (\frac{1}{8}(23 - 3\sqrt{1 + 16\ln(3)})) \lor x > (\frac{1}{8}(23 + 3\sqrt{1 + 16\ln(3)})) \\ 0, \text{ otherwise} \end{cases}$$
 (68)

$$\approx \begin{cases} 1, x < 1.26 \lor x > 4.49 \\ 0, \text{ otherwise} \end{cases}$$
 (69)

(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)

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

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

$$\epsilon^0[\psi^*(x)] = P(\psi(X) = 1|Y = 0)$$
(70)

$$= \int_{\{x|\psi(x)=1\}} p(x|Y=0)dx \tag{71}$$

$$= \int_{-\infty}^{b_1} p(x|Y=0)dx + \int_{b_2}^{\infty} p(x|Y=0)dx$$
 (72)

$$=F_{X_0}(b_1)+1-F_{X_0}(b_2) \tag{73}$$

$$= \frac{1}{2} \left[ 1 + erf\left(\frac{b_1 - \mu_0}{\sigma_0 \sqrt{2}}\right) \right] + 1 - \frac{1}{2} \left[ 1 + erf\left(\frac{b_2 - \mu_0}{\sigma_0 \sqrt{2}}\right) \right]$$
 (74)

$$=1+\frac{1}{2}(erf(\frac{b_{1}-\mu_{0}}{\sigma_{0}\sqrt{2}})-erf(\frac{b_{2}-\mu_{0}}{\sigma_{0}\sqrt{2}})) \tag{75}$$

<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

$$\epsilon^{1}[\psi^{*}(x)] = P(\psi(X) = 0|Y = 1)$$
(76)

$$= \int_{\{x|\psi(x)=0\}} p(x|Y=1)dx \tag{77}$$

$$= \int_{b_1}^{b_2} p(x|Y=1)dx \tag{78}$$

$$=F_{X_1}(b_2)-F_{X_1}(b1) \tag{79}$$

$$=\frac{1}{2}\left[erf(\frac{b_2-\mu_1}{\sigma_1\sqrt{2}})-erf(\frac{b_1-\mu_1}{\sigma_1\sqrt{2}})\right] \tag{80}$$

(81)

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),

$$\epsilon[\psi^*(X)] = P(\psi(X) \neq Y) \tag{82}$$

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

$$= P(Y=0)P(\psi(X)=1|Y=0) + P(Y=1)P(\psi(X)=0|Y=1)$$
(84)

$$= P(Y=0)\epsilon^{0} + P(Y=1)\epsilon^{1}$$
(85)

$$=\frac{1}{2}(\epsilon^0 + \epsilon^1) \tag{86}$$

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

$$\psi_Q^*(x) = \begin{cases} 1, x^T A x + b^T x + c > 0 \\ 0, \text{ otherwise} \end{cases}$$
 (87)

where

$$A = \frac{1}{2}(\Sigma_0^{-1} - \Sigma_1^{-1}) \tag{88}$$

$$b = \Sigma_1^{-1} \mu_1 - \Sigma_0^{-1} \mu_0 \tag{89}$$

$$c = \frac{1}{2} (\mu_0^T \Sigma_0^{-1} \mu_0 - \mu_1^T \Sigma_1^{-1} \mu_1) + \frac{1}{2} \ln \frac{\det(\Sigma_0)}{\det(\Sigma_1)} + \ln \frac{P(Y=1)}{P(Y=0)}$$
(90)

Let x be the vector of sample values,

$$x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \tag{91}$$

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

 $<sup>^5</sup>$ 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 solveD(self):
            x0, x1 = sp.symbols('x0 x1')
51
            x = sp.Matrix([[x0],[x1]])
52
            return sp.simplify(x.T * bc.mA * x + bc.mb.T * x + bc.mc)
53
        def plot2D(self, psi_annotates=[[0.3,0.3], [0.7,0.7]]):
54
            fig, ax = plt.subplots()
            # Create girds
            xlist = np.linspace(-3.5, 3.5, RES_GRID)
            ylist = np.linspace(-3.5,3.5,RES_GRID)
59
            X, Y = np.meshgrid(xlist, ylist)
60
            pos = np.dstack((X,Y))
61
62
            # Compute Bayes classification
63
            Z = np.zeros(X.shape)
64
```

```
for i in range(0, Z.shape[0]):
65
                 for j in range(0, Z.shape[1]):
66
                     x = np.matrix([X[i,j], Y[i,j]]).T
67
                     Z[i,j] = self.psi(x)
69
            # Compute Gaussia pdf
70
            rv0 = multivariate_normal(np.array(self.mu0.T)[0], self.sigma0)
71
            rv1 = multivariate_normal(np.array(self.mu1.T)[0], self.sigma1)
72
            Z0 = rv0.pdf(pos)
73
            Z1 = rv1.pdf(pos)
74
            # Plot contours
76
            cmap = plt.get_cmap('Set1', 2)
            ax.contour(X,Y,Z, cmap=cmap, levels=[0.9])
78
            ax.contour(X,Y,Z0, alpha=0.4)
79
            ax.contour(X,Y,Z1, alpha=0.4)
80
            ax.plot(self.mu0[0,0], self.mu0[1,0], marker="0", color="k",label="$\mu_0$")
            ax.plot(self.mu1[0,0], self.mu1[1,0], marker="o", color="gray",label="<math>\mbox{mu}_1")
            if psi_annotates==None:
                psi_annotates = [[self.mu0[0,0], self.mu0[1,0]], [self.mu1[0,0], self.mu1[1,0]]
84
85
            # Annotate decisions
86
            for ann in psi_annotates:
87
                 i = X[int(X.shape[0]*ann[0]), int(X.shape[1]*ann[1])]
88
                 j = Y[int(Y.shape[0]*ann[0]), int(Y.shape[1]*ann[1])]
                x = np.matrix([i, j]).T
                 if self.psi(x) > 0:
                     ax.annotate("\$\psi^{*}(x) = 1\$", (i, j))
92
                else:
93
                     ax.annotate("\$\psi^{*}(x) = 0$", (i, j))
94
95
            # legend and label settings
            ax.set_xlabel("$x_1$")
97
            ax.set_ylabel("$x_2$")
            ax.legend()
            return fig, ax
100
```

(a)

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

Matrix([[1.0\*x0 + 0.375\*x1\*\*2 - 1.69314718055995]])

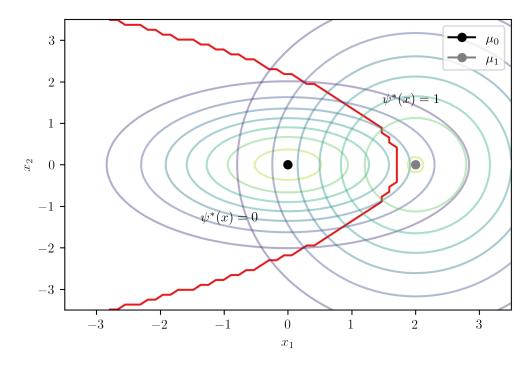


Figure 2: Bayes Classifier for 2D Gussian (a)

• The boundary is

$$D(x) = x_0 + 0.375 * x_1^2 - 1.69 = 0$$

(b)

Matrix([[0.125\*x0\*\*2 + 0.5\*x0 - 0.846573590279973]])

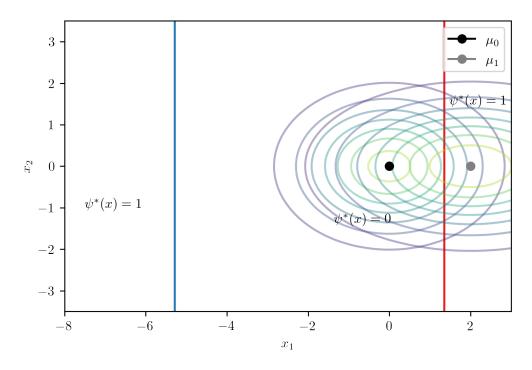


Figure 3: Bayes Classifier for 2D Gussian (b)

• Analytical solution to the boundary

$$D(x) = 0.125 * x_0^2 + 0.5 * x_0 - 0.85 = 0$$

• x = -5.28, 1.28 The solution are two vertical lines.

(c)

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

Matrix([[0.25\*x0\*\*2 + 0.25\*x1\*\*2 - 0.693147180559945]])

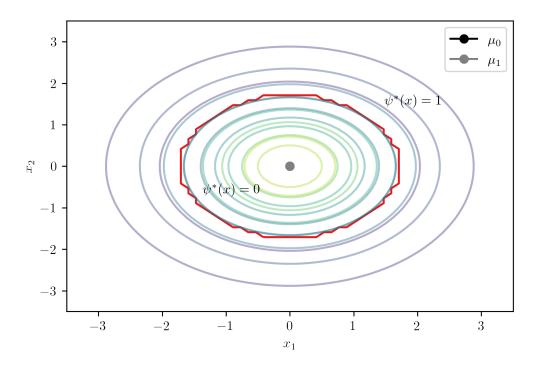


Figure 4: Bayes Classifier for 2D Gussian (c)

• Analytical solution to the boundary

$$D(x) = 0.25 * x_0^2 + 0.25 * x_1^2 - 0.69 = 0$$

The solution is a *circle*.

(d)

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

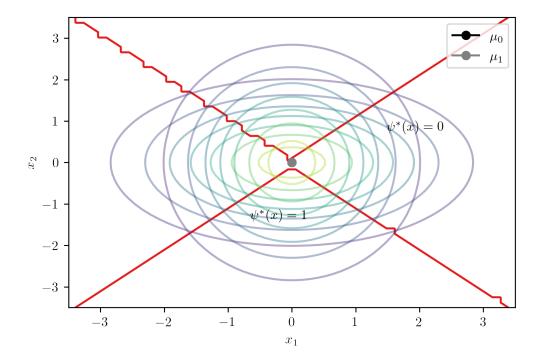


Figure 5: Bayes Classifier for 2D Gussian (d)

• Analytical solution to the boundary

$$D(x) = -0.25x_0^2 + 0.25 * x_1^2 = 0$$

• Noted that  $D([0,0]^T)=0$ , then  $\phi^*([0,0]^T)=0$  for the origin.

# 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

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

$$(92)$$

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

$$\epsilon_L^* = \Phi(-\frac{\delta}{2}) \tag{93}$$

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

$$\Sigma_{d \times d} = \begin{bmatrix} \Sigma_{l_1 \times l_1}(\sigma_1^2, \rho_1) & 0 & \cdots & 0 \\ 0 & \Sigma_{l_2 \times l_2}(\sigma_2^2, \rho_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Sigma_{l_k \times l_k}(\sigma_k^2, \rho_k) \end{bmatrix}$$
(94)

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

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

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

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

The element-wised summation of all terms in  $\Sigma_{l_k \times l_k}(\sigma_i^2, \rho_i)$  is

$$\begin{split} sum(\Sigma_{l_k \times l_k}(\sigma_k^2, \rho_k)) &= \frac{1}{\sigma_i^2 (1 - \rho_k) (1 + (l_k - 1) \rho_k)} (-l_k^2 \rho_k + l_k (1 + (l_k - 1) \rho_k)) \\ &= \frac{l_k (1 - \rho_k)}{\sigma_k^2 (1 - \rho_k) (1 + (l_k - 1) \rho_k)} \end{split} \tag{98}$$

Thus, the inverse of covariance matrix is

$$\Sigma_{d \times d}^{-1} = \begin{bmatrix} \Sigma_{l_1 \times l_1}^{-1}(\sigma_1^2, \rho_1) & 0 & \cdots & 0 \\ 0 & \Sigma_{l_2 \times l_2}^{-1}(\sigma_2^2, \rho_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Sigma_{l_k \times l_k}^{-1}(\sigma_k^2, \rho_k) \end{bmatrix}$$
(100)

Combining together,

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

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

$$= \Phi\left(\sum_{i=1}^{k}\frac{l_{i}(1 - \rho_{i})}{\sigma_{i}^{2}(1 - \rho_{i})(1 + (l_{i} - 1)\rho_{i})}\right)$$

$$(101)$$

(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  $\rho$ .

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  $\rho = 0, 0.25, 0.5, 0.75$  (plot one curve for each value). Confirm that the Bayes error increasese monotonically with  $\sigma$  from 0 to 0.5 for each value of  $\rho$ , and that Bayes error for larger  $\rho$  is uniformly larger than that for smaller  $\rho$ . The latter fact shows that correlation between the features is detrimental to classification.

As shown in Figure 6, the correlation does have the detrimental effect on classification, and monotoniously increases Bayes error.

```
# Implementation
def get_VecM(length, val):
    return np.ones((1, length)).T * val

class GeneralMultiGaussian:
    def __init__(self, d, l, sig, rho, Imu0=0, Imu1=1):
        self.d = d
        self.l = l
        self.sig = sig
        self.rho = rho
```

```
self.Imu0 = Imu0
11
            self.Imu1 = Imu1
12
            self.mu0 = get_VecM(d, Imu0)
13
            self.mu1 = get_VecM(d, Imu1)
14
            # cluster of covariance matrix
            self.subCovInv = self.cluster_cov_inv()
16
            self.CovInv = self.cov_inv()
17
18
       def cluster_cov_inv(self):
19
            sig = self.sig
20
            1 = self.1
21
            rho = self.rho
22
            scale = 1/((sig**2)*(1-rho)*(1+(l-1)*rho))
23
            diag_val = 1 + (1-2)*rho
            covInv = np.ones((1,1)) * (-1*rho)
25
            covInv = np.matrix(covInv)
26
            np.fill_diagonal(covInv, diag_val)
27
            return scale*covInv
28
29
       def cov_inv(self):
30
            d = self.d; l = self.l
            subMs = [self.subCovInv for i in range(0,int(d/l)+1)]
            return block_diag(*subMs)[0:d, 0:d]
33
34
       def bayesError(self):
35
            mu0 = self.mu0
36
            mu1 = self.mu1
37
            mud = mu1 - mu0
            CovInv = self.CovInv
            delta = -0.5 * np.sqrt(mud.T @ CovInv @ mud)
40
            return norm.cdf(delta)
41
42
43
   # Parameter Setting
44
   sigs = np.linspace(0.01, 3, 50)
   d = 20
   1 = 4
   rhos = [0, 0.25, 0.5, 0.75]
49
   # Measurement of Bayes errors
50
   errorD = dict()
51
   for rho in rhos:
```

```
errorD[rho] = np.zeros(len(sigs))
53
54
   for rho in errorD.keys():
55
       for (i, sig) in enumerate(sigs):
56
            gm = GeneralMultiGaussian(d, 1, sig, rho)
57
            err = gm.bayesError()
58
            errorD[rho][i] = err
59
60
   # Plotting
61
   fig, ax = plt.subplots()
   for rho in rhos:
       ax.plot(sigs, errorD[rho], label="$\\rho={}$".format(rho))
   ax.set_xlabel("$\\sigma$")
   ax.set_ylabel("Bayes Error")
66
   ax.legend();
67
```

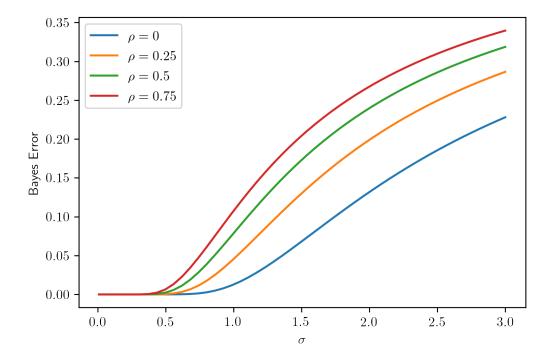


Figure 6: The relation of Bayes error with standard deviation and covariance.

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  $\rho=0,0.25,0.5,0.75$  (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.

The plot is shown in Figure 7.

```
# Parameter setting
   ds = np.arange(4, 40, 4, dtype=int)
   sig = 1
   # Measure errors
   errorD2 = dict()
   for rho in rhos:
       errorD2[rho] = np.zeros(len(ds))
10
   for rho in errorD2.keys():
11
       for (i, d) in enumerate(ds):
12
           gm = GeneralMultiGaussian(d, 1, sig, rho)
           err = gm.bayesError()
14
           errorD2[rho][i] = err
15
16
17
   # Plotting
   fig, ax = plt.subplots()
   for rho in rhos:
19
       ax.plot(ds, errorD2[rho], label="$\\rho={}$".format(rho))
   ax.set_xlabel("$d$")
21
   ax.set_ylabel("Bayes Error")
   ax.legend();
```

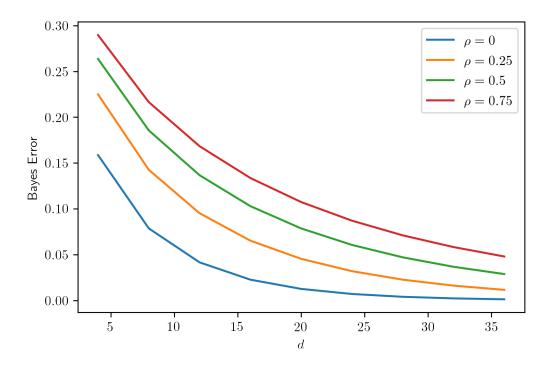


Figure 7: Bayes error as a function of dimension.

iii.

Plot the Bayes error as a function of the correlation  $\rho \in [0,1]$  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  $\rho = 0$ , which shows that the Bayes error is very sensitive to correlation in the near-independent region.

The plot is show in Figure 8.

```
# Parameter setting
d = 20
ls = [1,2,4,10]
sig = 2
rhos = np.linspace(0.,0.99,40)

# Measure errors
errorD3 = dict()
for l in ls:
```

```
errorD3[1] = np.zeros(len(rhos))
10
11
   for l in ls:
12
       for (i, rho) in enumerate(rhos):
13
            gm = GeneralMultiGaussian(d, 1, sig, rho)
14
            err = gm.bayesError()
15
            errorD3[1][i] = err
16
17
   # Plotting
18
   fig, ax = plt.subplots()
19
   for 1 in 1s:
       ax.plot(rhos, errorD3[1], label="$\\l={}$".format(1))
   ax.set_xlabel("$\\rho$")
   ax.set_ylabel("Bayes Error")
23
   ax.legend();
24
```

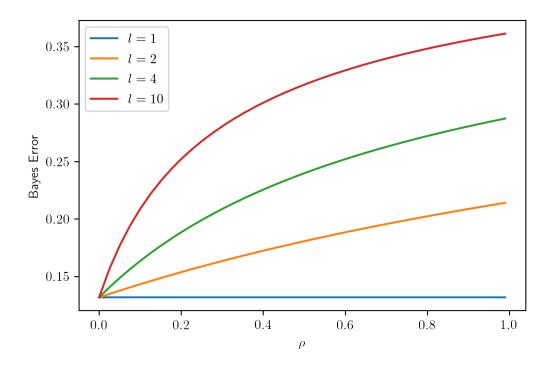


Figure 8: Bayes error as a function of correlation.

### References

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