

# Bayesian Classification

A simple application of  
**Bayes' formula**

CMU, 2006 fall, Tom Mitchell, Eric Xing, midterm, pr. 1.3

Suppose that in answering a question in a multiple choice test, an *examinee* either knows the answer, with probability  $p$ , or he guesses with probability  $1 - p$ .

Assume that the probability of answering a *question* correctly is 1 for an examinee who *knows* the answer and  $1/m$  for the examinee who *guesses*, where  $m$  is the number of *multiple choice alternatives*.

What is the probability that an examinee knew the answer to [such] a question, given that he has correctly answered it?

**Answer:**

$$\begin{aligned} P(knew|correct) &= \frac{P(correct|knew) \cdot P(knew)}{P(correct)} \\ &= \frac{P(correct|knew) \cdot P(knew)}{P(correct|knew) \cdot P(knew) + P(correct|guessed) \cdot P(guessed)}. \end{aligned}$$

Notice that in the denominator we had to consider the two ways (s)he can get a question correct: by knowing, or by guessing. Plugging in, we get:

$$\frac{p}{p + \frac{1}{m} \cdot (1 - p)} = \frac{mp}{mp + 1 - p}.$$

# Maximum A posteriori Probability (MAP) Hypotheses

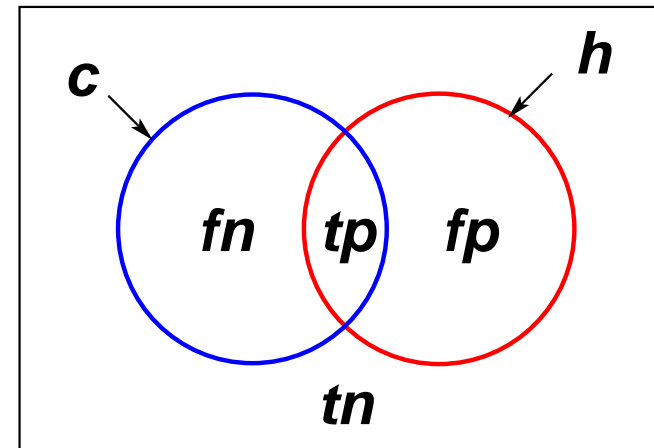
## Exemplifying

- the application of Bayes' theorem
- the notion of MAP (Maximum A posteriori Probability) hypotheses
- the computation of *expected values* for discrete random variables and
- the [use of] *sensitivity* and *specificity* of a test in a real-world application

CMU, 2009 fall, Geoff Gordon, HW1, pr. 2

There is a disease which affects 1 in 500 people. A 100.00 dollar blood **test** can help reveal whether a person has the disease. A positive outcome indicates that the person may have the disease.

The test has perfect **sensitivity** (*true positive rate*), i.e., a person who has the disease tests positive 100% of the time. However, the test has 99% **specificity** (*true negative rate*), i.e., a healthy person tests positive 1% of the time.



$$\text{sensitivity (or: recall): } \frac{tp}{tp + fn}$$

$$\text{specificity: } \frac{tn}{tn + fp}$$

a. A randomly selected individual is tested and the result is positive.

What is the *probability* of the individual having the disease?

b. There is a second more expensive test which costs 10, 000.00 dollars but is exact with 100% *sensitivity* and *specificity*.

If we require all people who test positive with the less expensive test to be tested with the more expensive test, what is the *expected cost* to check whether an individual has the disease?

c. A pharmaceutical company is attempting to decrease the cost of the second (perfect) test.

How much would it have to make the second test cost, so that the first test is no longer needed? That is, at what cost is it cheaper simply to use the perfect test alone, instead of screening with the cheaper test as described in part *b*?

**Answer:**

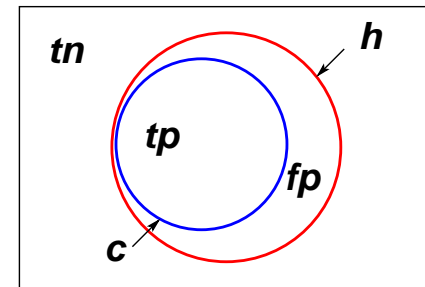
Let's define the following *random variables*:

$B$ :  $\begin{cases} 1/\text{true} & \text{for persons affected by that disease,} \\ 0/\text{false} & \text{otherwise;} \end{cases}$

$T_1$ : the result of the first test: + (in case of disease) or – (otherwise);

$T_2$ : the result of the second test: again + or –.

$$\textbf{Known facts: } \begin{cases} P(B) = \frac{1}{500} \\ P(T_1 = + \mid B) = 1, P(T_1 = + \mid \bar{B}) = \frac{1}{100}, \\ P(T_2 = + \mid B) = 1, P(T_2 = + \mid \bar{B}) = 0 \end{cases}$$



a.

$$\begin{aligned} P(B \mid T_1 = +) &\stackrel{TBayes}{=} \frac{P(T_1 = + \mid B) \cdot P(B)}{P(T_1 = + \mid B) \cdot P(B) + P(T_1 = + \mid \bar{B}) \cdot P(\bar{B})} \\ &= \frac{1 \cdot \frac{1}{500}}{1 \cdot \frac{1}{500} + \frac{1}{100} \cdot \frac{499}{500}} = \frac{100}{599} \approx 0.1669 \Rightarrow \end{aligned}$$

$P(\bar{B} \mid T_1 = +) = 0.8331 > P(B \mid T_1 = +)$ . Therefore,  $\bar{B}$  is the **MAP hypothesis**.



b.

Let's consider a new random variable:

$$C = \begin{cases} c_1 & \text{if the person only takes the first test} \\ c_1 + c_2 & \text{if the person takes the two tests} \end{cases}$$

$$\Rightarrow P(C = c_1) = P(T_1 = -) \text{ and } P(C = c_1 + c_2) = P(T_1 = +)$$

$$\begin{aligned} \Rightarrow E[C] &= c_1 \cdot (1 - P(T_1 = +)) + (c_1 + c_2) \cdot P(T_1 = +) \\ &= c_1 - c_1 \cdot P(T_1 = +) + c_1 \cdot P(T_1 = +) + c_2 \cdot P(T_1 = +) \\ &= c_1 + c_2 \cdot P(T_1 = +) \\ &= 100 + 10000 \cdot \frac{599}{50000} = 219.8 \approx 220\$ \end{aligned}$$

**Note:** Here above we used

$$\begin{aligned} P(T_1 = +) &\stackrel{\text{total probability form.}}{=} P(T_1 = + | B) \cdot P(B) + P(T_1 = + | \bar{B}) \cdot P(\bar{B}) \\ &= 1 \cdot \frac{1}{500} + \frac{1}{100} \cdot \frac{499}{500} = \frac{599}{50000} = 0.01198 \end{aligned}$$

**c.**

$c_n$  <sup>not.</sup> = the new price for the second test ( $T'_2$ )

$$\begin{aligned} c_n \leq E[C'] &= c_1 \cdot P(C = c_1) + (c_1 + c_n) \cdot P(C = c_1 + c_n) \\ &= c_1 + c_n \cdot P(T_1 = +) = 100 + c_n \cdot \frac{599}{50000} \end{aligned}$$

$$c_n = 100 + c_n \cdot 0.01198 \Rightarrow c_n \approx 101.2125.$$

## The “Monty’s haunted house” problem

- Exemplifying the application of Bayes’ theorem
- the notion of MAP (Maximum A posteriori Probability) hypotheses

CMU, 2009 fall, Geoff Gordon, HW1, pr. 1

You are in a haunted house and you are stuck in front of three doors. A ghost appears and tells you: “Your hope is behind one of these doors. There is only one door that opens to the outside and the two other doors have deadly monsters behind them. You must choose one door!” You choose the first door. The ghost tells you: “Wait! I will give you some more information.” The ghost opens the second door and shows you that there was a horrible monster behind it, then asks you: “Would you like to change your mind and take the third door instead?”

What’s better: to stick with the first door, or to change to the third door? For each of the following *strategies* used by the ghost, determine probabilities that the exit is behind the first and the third door, given that the ghost opened the second door.

- a. The ghost always opens a door you have not picked with a monster behind it. If both of the unopened doors hide monsters, he picks each of them with equal probability.
- b. The ghost has a slightly different strategy. If both of the unopened doors hide monsters, he always picks the second door.
- c. Finally, suppose that if both of the unopened doors hide monsters, the ghost always picks the third door.

## Answer

What we know:

$$P(O = 1) = P(O = 2) = P(O = 3) = \frac{1}{3} \quad (1)$$

$O$	$G$	$P(G \mid O)$		
		variant $a$	variant $b$	variant $c$
1	2	1/2	1	0
1	3	1/2	0	1
2	2	0	0	0
2	3	1	1	1
3	2	1	1	1
3	3	0	0	0

What we must compute:

$$P(O = 1 \mid G = 2) \stackrel{\text{Bayes F.}}{=} \frac{P(G = 2 \mid O = 1) \cdot P(O = 1)}{P(G = 2 \mid O = 1) \cdot P(O = 1) + P(G = 2 \mid O = 3) \cdot P(O = 3)}$$

$$P(O = 3 \mid G = 2) \stackrel{\text{Bayes F.}}{=} \frac{P(G = 2 \mid O = 3) \cdot P(O = 3)}{P(G = 2 \mid O = 3) \cdot P(O = 3) + P(G = 2 \mid O = 1) \cdot P(O = 1)}$$

Notice that we should have added  $P(G = 2 \mid O = 2) \cdot P(O = 2)$  at the denominator, but we know that it is 0 since  $P(G = 2 \mid O = 2) = 0$ .

Variant *a*:

$$P(O = 1 \mid G = 2) = \frac{\frac{1}{2} \cdot \frac{1}{3}}{\frac{1}{2} \cdot \frac{1}{3} + 1 \cdot \frac{1}{3}} = \frac{1}{3} \quad P(O = 3 \mid G = 2) = \frac{1 \cdot \frac{1}{3}}{1 \cdot \frac{1}{3} + \frac{1}{2} \cdot \frac{1}{3}} = \frac{2}{3}$$

Therefore, we should choose door 3.

Variant *b*:

$$P(O = 1 \mid G = 2) = \frac{1 \cdot \frac{1}{3}}{1 \cdot \frac{1}{3} + 1 \cdot \frac{1}{3}} = \frac{1}{2} \quad P(O = 3 \mid G = 2) = \frac{1 \cdot \frac{1}{3}}{1 \cdot \frac{1}{3} + 1 \cdot \frac{1}{3}} = \frac{1}{2}$$

Therefore, we can choose either door 1 or door 3.

Variant *c*:

$$P(O = 1 \mid G = 2) = 0 \quad P(O = 3 \mid G = 2) = \frac{1 \cdot \frac{1}{3}}{1 \cdot \frac{1}{3} + 0} = 1$$

Therefore, we should choose door 1.

## Alternative Solution (1) (in Romanian)

Echivalent, în cazul variantei  $a$ , pentru a determina maximumul dintre  $P(O = 1 \mid G = 2)$  și  $P(O = 3 \mid G = 2)$  ar fi fost suficient, conform formulei lui Bayes, să comparăm

$$P(G = 2 \mid O = 1) \cdot P(O = 1) \text{ și } P(G = 2 \mid O = 3) \cdot P(O = 3).$$

Mai mult, ținând cont de relația (1), aceasta revine la a compara

$$P(G = 2 \mid O = 1) \text{ și } P(G = 2 \mid O = 3).$$

Răspunsul poate fi citit imediat din tabelul de mai sus (vezi prima linie și penultima linie):  $O = 3$  este varianta pentru care se obține probabilitatea [a posteriori] maximă.

Altfel spus,  $O = 3$  este **ipoteza de probabilitate maximă a posteriori** (engl., maximum a posteriori probability (MAP) hypothesis).

Absolut similar se poate proceda și pentru variantele  $b$  și  $c$ .

**Observație:** În cazuri precum cel de mai sus ( $P(O = 1) = P(O = 2) = P(O = 3) = \frac{1}{3}$ ), ipoteza MAP coincide cu **ipoteza de verosimilitate maximă** (engl., maximum likelihood (ML) hypothesis).

## Alternative Solution (2) (in Romanian)

Echivalent, pentru **variantele  $b$  și  $c$**  putem răspunde la întrebare făcând următorul raționament, **fără a folosi formula lui Bayes:**

Ieșirea cea bună se poate găsi în spatele uneia dintre cele trei uși (vezi figura alăturată). Cum fantoma a deschis deja ușa cu numărul 2, una dintre aceste situații (și anume, a doua din figură) este eliminată, fiindcă în spatele ei este un monstru. În continuare, putem raționa în felul următor:

1	2	3
	M	M
M		M
M	M	

**Varianta  $b$ :** Întrucât fantoma alege ușa 2 cu probabilitate 1, putem afirma, (în lipsa unor alte informații) că ambele variante – 1 și 3 – au probabilități egale, și anume  $\frac{1}{2}$ .

Într-adevăr,

- fie ușa 1, cea aleasă de mine, dă înspre afară, iar atunci fantoma trebuie, conform principiului P2, să aleagă ușa 2;
- fie ușa 3 dă înspre afară, iar atunci, din nou conform principiului P2, fantoma trebuie să aleagă ușa 2;
- conform principiului P1, nu există o a treia posibilitate;
- nu dispun de alte informații pentru a decide între cele două situații de mai sus.

**Varianta  $c$ :** Știind că fantoma nu a deschis ușa 3 (care ar fi opțiunea corespunzătoare principiului P2), ci a ales ușa 2, înseamnă că nu a putut face altfel, deci ușa 3 reprezintă ieșirea.



## Exemplifying

- the application of Bayes' theorem
- the notion of MAP (Maximum A posteriori Probability) hypotheses

CMU, 2012 spring, Ziv Bar-Joseph, HW1, pr. 1.5

Mickey tosses a die multiple times, hoping for a 6.  
The sequence of his 10 tosses is 1, 3, 4, 2, 3, 3, 2, 5, 1, 6.  
Mickey is suspicious whether the die is biased towards 3 (or fair).

Conduct a simple analysis based on the Bayes theorem to inform on Mickey — to what degree is the die biased?  
Explain your reasoning.

Assume in general every 100 dice contain 5 unfair dice that are biased towards 3 with the probability distribution of the six faces (1, 2, 3, 4, 5, 6) as  $P = [0.1, 0.1, 0.5, 0.1, 0.1, 0.1]$ .

## Solution

**Definition for the notion of Maximum A posteriori Probability:**

$$h_{MAP} \stackrel{\text{def.}}{=} \operatorname{argmax}_{h \in H} P(h|D) \stackrel{\text{F.B.}}{=} \operatorname{argmax}_{h \in H} \frac{P(D|h) \cdot P(h)}{P(D)} = \operatorname{argmax}_{h \in H} P(D|h) \cdot P(h),$$

**Let us denote:**

- $D = \{1, 3, 4, 2, 3, 3, 2, 5, 1, 6\} = \{x_1, x_2, \dots, x_{10}\}$
- $H = \{FD, LD\}$ , where  $FD$  is the fair dice and  $LD$  is the loaded dice.

$$\begin{aligned}
P(D|FD) \cdot P(FD) &= P(x_1, x_2, \dots, x_{10}|FD) \cdot P(FD) \stackrel{i.i.d.}{=} \left( \prod_{i=1}^{10} P(x_i|FD) \right) \cdot P(FD) = \left( \frac{1}{6} \right)^{10} \cdot \frac{95}{100} \\
&= \frac{1}{2^{10} \cdot 3^{10}} \cdot \frac{19}{20}
\end{aligned}$$

$$\begin{aligned}
P(D|LD) \cdot P(LD) &= P(x_1, x_2, \dots, x_{10}|LD) \cdot P(LD) \stackrel{i.i.d.}{=} \left( \prod_{i=1}^{10} P(x_i|LD) \right) \cdot P(LD) \\
&= \left( \frac{1}{10} \cdot \frac{1}{2} \cdot \frac{1}{10} \cdot \frac{1}{10} \cdot \frac{1}{2} \cdot \frac{1}{2} \cdot \frac{1}{10} \cdot \frac{1}{10} \cdot \frac{1}{10} \cdot \frac{1}{10} \right) \cdot \frac{5}{100} = \frac{1}{10^7 \cdot 2^3} \cdot \frac{1}{20} = \frac{1}{2^{10} \cdot 5^7} \cdot \frac{1}{20}.
\end{aligned}$$

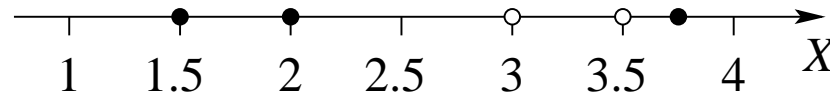
**In order to compare  $P(D|FD) \cdot P(FD)$  and  $P(D|LD) \cdot P(LD)$ , it is easier to firstly apply the  $\ln$ :**

$$\begin{aligned}
&\ln P(D|FD) \cdot P(FD) > \ln P(D|LD) \cdot P(LD) \Leftrightarrow \\
&\ln \frac{19}{3^{10}} > \ln \frac{1}{5^7} \Leftrightarrow \ln 19 - 10 \ln 3 > 7 \ln 5 \Leftrightarrow -8.0417 > -11.2661
\end{aligned}$$

**Note:** We could have directly computed the so-called **log-odds ratio**:

$$\ln \frac{P(LD|D)}{P(FD|D)} = \ln \frac{P(D|FD) \cdot P(FD)}{P(D|LD) \cdot P(LD)} = \dots = -3.2244 < 0 \text{ so we have to choose } FD.$$

Exemplifying  
*ML hypotheses and MAP hypotheses*  
using decision trees  
CMU, 2009 spring, Tom Mitchell, midterm, pr. 2.3-4



Let's consider the 1-dimensional data set shown above, based on the single real-valued attribute  $X$ . Notice there are two classes (values of  $Y$ ), and five data points.

Consider a special type of *decision trees* where leaves have *probabilistic labels*. Each leaf node gives the probability of each possible label, where the probability is the fraction of points at that leaf node with that label.

For *example*, a decision tree learned from the data set above with zero splits would say  $P(Y = 1) = 3/5$  and  $P(Y = 0) = 2/5$ . A decision tree with one split (at  $X = 2.5$ ) would say  $P(Y = 1) = 1$  if  $X < 2.5$ , and  $P(Y = 1) = 1/3$  if  $X \geq 2.5$ .

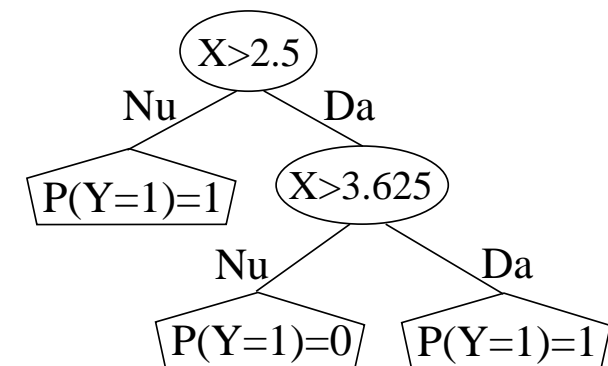
Solution:

- a. For the above data set, draw a tree that maximizes the *likelihood* of the data.

$T_{ML} = \operatorname{argmax}_T P_T(D)$ , where

$$P_T(D) \stackrel{\text{def.}}{=} P(D|T) \stackrel{i.i.d.}{=} \prod_{i=1}^5 P(Y = y_i | X = x_i, T),$$

where  $y_i$  is the label/class of the instance  $x_i$  ( $x_1 = 1.5$ ,  $x_2 = 2$ ,  $x_3 = 3$ ,  $x_4 = 3.5$ ,  $x_5 = 3.75$ .)



- b. Consider a prior probability distribution  $P(T)$  over trees that penalizes the number of splits in the tree.

$$P(T) \propto \left(\frac{1}{4}\right)^{\text{splits}(T)^2}$$

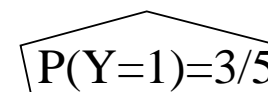
where  $T$  is a tree,  $\text{splits}(T)$  is the number of splits in  $T$ , and  $\propto$  means “is proportional to”.

For the same data set, give the MAP tree when using this prior,  $P(T)$ , over trees.

**Solution:**

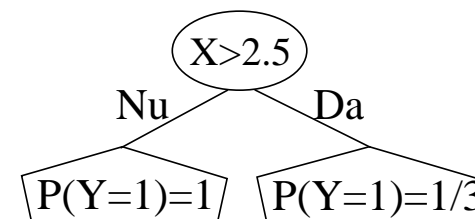
**0 nodes:**

$$P(T_0 \mid D) \propto \left(\frac{3}{5}\right)^3 \cdot \left(\frac{2}{5}\right)^2 \cdot \left(\frac{1}{4}\right)^0 = \frac{3^3 \cdot 2^2}{5^5} = \frac{108}{3125} = 0.0336$$



**1 node:**

$$P(T_1 \mid D) \propto 1^2 \cdot \left(\frac{2}{3}\right)^2 \cdot \frac{1}{3} \cdot \left(\frac{1}{4}\right)^1 = \frac{1}{27} = 0.037$$



**2 nodes:**

$$P(T_2) \propto \left(\frac{1}{4}\right)^4 \Rightarrow P(T_2 \mid D) \propto 1 \cdot \left(\frac{1}{4}\right)^4 = \frac{1}{256} = 0.0039 \Rightarrow \text{the MAP tree is } T_1.$$

# The Naive Bayes and Joint Bayes Algorithms



Exemplifying the application of  
Naive Bayes and Joint Bayes algorithms;  
the minimum number of parameters  
to be estimated for NB and respectively JB

CMU, 2008 fall, Eric Xing, HW1 pr. 2

Consider a classification problem, the table of observations for which is given nearby.  $X_1$  and  $X_2$  are two binary random variables which are the observed variables.  $Y$  is the class label which is observed for the training data given below. We will use the Naive Bayes classifier and the Joint Bayes classifier to classify a new instance after training on the data below, and compare the results.

$X_1$	$X_2$	$Y$	Counts
0	0	0	2
0	0	1	18
1	0	0	4
1	0	1	1
0	1	0	4
0	1	1	1
1	1	0	2
1	1	1	18

- Construct the Naive Bayes classifier given the data above. Use it to classify the instance  $X_1 = 0$ ,  $X_2 = 0$ .
- Construct the Joint Bayes classifier given the data above. Use it to classify the instance  $X_1 = 0$ ,  $X_2 = 0$ .

c. Compute the probabilities  $P(Y = 1|X_1 = 0, X_2 = 0)$  for the Naive Bayes classifier (let's denote it  $P_{NB}(Y = 1|X_1 = 0, X_2 = 0)$ ) and for the Joint Bayes classifier ( $P_{JB}(Y = 1|X_1 = 0, X_2 = 0)$ ).

Why is  $P_{NB}(Y = 1|X_1 = 0, X_2 = 0)$  different from  $P_{JB}(Y = 1|X_1 = 0, X_2 = 0)$ ? (*Hint: Compute  $P(X_1, X_2|Y)$ .*)

d. What happens to the difference between  $P_{NB}(Y = 1|X_1 = 0, X_2 = 0)$  and  $P_{JB}(Y = 1|X_1 = 0, X_2 = 0)$  if the table entries are changed to the nearby table?

(*Hint: Will the Naive Bayes assumption be more violated or less violated compared to the previous situation?*)

$X_1$	$X_2$	$Y$	Counts
0	0	0	3
0	0	1	9
1	0	0	3
1	0	1	9
0	1	0	3
0	1	1	9
1	1	0	3
1	1	1	9

e. Compare the number of independent parameters in the two classifiers. Instead of just two observed data variables, if there were  $n$  random binary observed variables  $\{X_1, \dots, X_n\}$ , what would be the number of parameters required for both classifiers?

From this, what can you comment about the rate of growth of the number of parameters for both models as  $n \rightarrow \infty$ ?

## Answer

a.

$$\hat{y}_{NB}(X_1 = 0, X_2 = 0) \stackrel{\text{def.}}{=} \operatorname{argmax}_{y \in \{0,1\}} P(X_1 = 0|Y = y) \cdot P(X_2 = 0|Y = y) \cdot P(Y = y)$$

$$p_0 \stackrel{\text{not.}}{=} P(X_1 = 0|Y = 0) \cdot P(X_2 = 0|Y = 0) \cdot P(Y = 0)$$

$$\stackrel{MLE}{=} \frac{6}{12} \cdot \frac{6}{12} \cdot \frac{12}{50} = \frac{3}{50} = \frac{6}{100}$$

$$p_1 \stackrel{\text{not.}}{=} P(X_1 = 0|Y = 1) \cdot P(X_2 = 0|Y = 1) \cdot P(Y = 1)$$

$$\stackrel{MLE}{=} \frac{19}{38} \cdot \frac{19}{38} \cdot \frac{38}{50} = \frac{19}{50}$$

$$p_0 < p_1 \Rightarrow \hat{y}_{NB}(X_1 = 0, X_2 = 0) = 1.$$

b.

$$\hat{y}_{JB}(X_1 = 0, X_2 = 0) \stackrel{\text{def.}}{=} \operatorname{argmax}_{y \in \{0,1\}} P(X_1 = 0, X_2 = 0 | Y = y) \cdot P(Y = y)$$

$$p'_0 \stackrel{\text{not.}}{=} P(X_1 = 0, X_2 = 0 \mid Y = 0) \cdot P(Y = 0) \stackrel{MLE}{=} \frac{2}{12} \cdot \frac{12}{50} = \frac{2}{50}$$

$$p'_1 \stackrel{\text{not.}}{=} P(X_1 = 0, X_2 = 0 \mid Y = 1) \cdot P(Y = 1) \stackrel{MLE}{=} \frac{18}{38} \cdot \frac{38}{50} = \frac{18}{50}$$

$$p'_0 < p'_1 \Rightarrow \hat{y}_{JB}(X_1 = 0, X_2 = 0) = 1.$$

c.

$$\begin{aligned}
P_{NB} &\stackrel{\text{not.}}{=} P(Y = 1 \mid X_1 = 0, X_2 = 0) \\
&\stackrel{\text{F. Bayes}}{=} \frac{P(X_1 = 0, X_2 = 0 \mid Y = 1) \cdot P(Y = 1)}{P(X_1 = 0, X_2 = 0 \mid Y = 1)P(Y = 1) + P(X_1 = 0, X_2 = 0 \mid Y = 0)P(Y = 0)} \\
&\stackrel{\text{indep. cdt.}}{=} \frac{P(X_1 = 0 \mid Y = 1) \cdot P(X_2 = 0 \mid Y = 1) \cdot P(Y = 1)}{P(X_1 = 0 \mid Y = 0) \cdot P(X_2 = 0 \mid Y = 0) \cdot P(Y = 0) + \\
&\quad P(X_1 = 0 \mid Y = 1) \cdot P(X_2 = 0 \mid Y = 1) \cdot P(Y = 1)} \\
&= \frac{p_1}{p_0 + p_1} = \frac{\frac{19}{100}}{\frac{6}{100} + \frac{19}{100}} = \frac{19}{25}
\end{aligned}$$

$$\begin{aligned}
P_{JB} &\stackrel{\text{not.}}{=} P(Y = 1 \mid X_1 = 0, X_2 = 0) \\
&\stackrel{\text{F. Bayes}}{=} \frac{P(X_1 = 0, X_2 = 0 \mid Y = 1) \cdot P(Y = 1)}{P(X_1 = 0, X_2 = 0 \mid Y = 1)P(Y = 1) + P(X_1 = 0, X_2 = 0 \mid Y = 0)P(Y = 0)} \\
&= \frac{p'_1}{p'_0 + p'_1} = \frac{\frac{18}{50}}{\frac{2}{50} + \frac{18}{50}} = \frac{18}{20}
\end{aligned}$$

$P_{NB} \neq P_{JB}$  because [in this case] the *conditional independence assumption* doesn't hold.

Indeed,

$$\left. \begin{aligned} P(X_1 = 0, X_2 = 0 \mid Y = 0) &\stackrel{MLE}{=} \frac{2}{12} \\ P(X_1 = 0 \mid Y = 0) \cdot P(X_2 = 0 \mid Y = 0) &\stackrel{MLE}{=} \frac{6}{12} \cdot \frac{6}{12} = \frac{1}{4} \end{aligned} \right\} \Rightarrow$$

$$\begin{aligned} \Rightarrow P(X_1 = 0, X_2 = 0 \mid Y = 0) &\neq P(X_1 = 0 \mid Y = 0) \cdot P(X_2 = 0 \mid Y = 0) \Rightarrow \\ \Rightarrow P(X_1, X_2 \mid Y) &\neq P(X_1 \mid Y) \cdot P(X_2 \mid Y) \end{aligned}$$

Therefore  $X_1$  and  $X_2$  are not conditionally independent w.r.t.  $Y$ .



d.

$$\begin{aligned}
P_{NB} &= P(Y = 1 \mid X_1 = 0, X_2 = 0) \\
&= \frac{P(X_1 = 0, X_2 = 0 \mid Y = 1) \cdot P(Y = 1)}{P(X_1 = 0, X_2 = 0 \mid Y = 1)P(Y = 1) + P(X_1 = 0, X_2 = 0 \mid Y = 0)P(Y = 0)} \\
&= \frac{P(X_1 = 0 \mid Y = 1) \cdot P(X_2 = 0 \mid Y = 1) \cdot P(Y = 1)}{P(X_1 = 0 \mid Y = 0) \cdot P(X_2 = 0 \mid Y = 0) \cdot P(Y = 0) + P(X_1 = 0 \mid Y = 1) \cdot P(X_2 = 0 \mid Y = 1) \cdot P(Y = 1)} \\
&= \frac{\frac{18}{36} \cdot \frac{18}{36} \cdot \frac{36}{48}}{\frac{6}{12} \cdot \frac{6}{12} \cdot \frac{12}{48} + \frac{18}{36} \cdot \frac{18}{36} \cdot \frac{36}{48}} = \frac{\frac{9}{48}}{\frac{3}{48} + \frac{9}{48}} = \frac{9}{12} = \frac{3}{4} \\
P_{JB} &= P(Y = 1 \mid X_1 = 0, X_2 = 0) \\
&= \frac{P(X_1 = 0, X_2 = 0 \mid Y = 1) \cdot P(Y = 1)}{P(X_1 = 0, X_2 = 0 \mid Y = 1)P(Y = 1) + P(X_1 = 0, X_2 = 0 \mid Y = 0)P(Y = 0)} \\
&= \frac{\frac{9}{36} \cdot \frac{36}{48}}{\frac{3}{12} \cdot \frac{12}{48} + \frac{9}{36} \cdot \frac{36}{48}} = \frac{\frac{9}{48}}{\frac{3}{48} + \frac{9}{48}} = \frac{9}{12} = \frac{3}{4}. \quad \text{Therefore, in this case } P_{NB} = P_{JB}.
\end{aligned}$$

In fact, it can be easily shown that for the newly given distribution the conditional independence assumption (for  $X_1$  and  $X_2$  w.r.t.  $Y$ ) holds. Therefore, the predictions made by Naive Bayes and Joint Bayes will coincide.

e. For our dataset, Naive Bayes needs to compute the following probabilities:

$$\begin{aligned}
 P(Y = 0) &\Rightarrow P(Y = 1) = 1 - P(Y = 0) \\
 P(X_1 = 0 \mid Y = 0) &\Rightarrow P(X_1 = 1 \mid Y = 0) = 1 - P(X_1 = 0 \mid Y = 0) \\
 P(X_1 = 0 \mid Y = 1) &\Rightarrow P(X_1 = 1 \mid Y = 1) = 1 - P(X_1 = 0 \mid Y = 1) \\
 P(X_2 = 0 \mid Y = 0) &\Rightarrow P(X_2 = 1 \mid Y = 0) = 1 - P(X_2 = 0 \mid Y = 0) \\
 P(X_2 = 0 \mid Y = 1) &\Rightarrow P(X_2 = 1 \mid Y = 1) = 1 - P(X_2 = 0 \mid Y = 1)
 \end{aligned}$$

Therefore, we will need only 5 values in order to fully construct the Naive Bayes classifier.

In the general case, when  $n$  input attributes / variables are given, we need to estimate  $P(Y)$ ,  $P(X_i \mid Y)$  and  $P(X_i \mid \neg Y)$  for  $i = \overline{1, n}$ , therefore  $2n + 1$  values / parameters.

For the Joint Bayes, we need to estimate

$$P(Y = 0) \Rightarrow P(Y = 1) = 1 - P(Y = 0)$$

$$\begin{aligned} P(X_1 = 0, X_2 = 0 \mid Y = 0) &\Rightarrow P(X_1 = 1, X_2 = 1 \mid Y = 0) = \\ P(X_1 = 0, X_2 = 1 \mid Y = 0) &1 - (P(X_1 = 0, X_2 = 0 \mid Y = 0) + P(X_1 = 0, X_2 = 1 \mid Y = 0) + \\ P(X_1 = 1, X_2 = 0 \mid Y = 0) &P(X_1 = 1, X_2 = 0 \mid Y = 0)). \end{aligned}$$

$$\begin{aligned} P(X_1 = 0, X_2 = 0 \mid Y = 1) &\Rightarrow P(X_1 = 1, X_2 = 1 \mid Y = 1) = \\ P(X_1 = 0, X_2 = 1 \mid Y = 1) &1 - (P(X_1 = 0, X_2 = 0 \mid Y = 1) + P(X_1 = 0, X_2 = 1 \mid Y = 1) + \\ P(X_1 = 1, X_2 = 0 \mid Y = 1) &P(X_1 = 1, X_2 = 0 \mid Y = 1)). \end{aligned}$$

For the general case, when  $n$  input variables are given, we will need to estimate  $P(Y)$ ,  $P(\tilde{X}_1, \dots, \tilde{X}_n \mid Y)$  and  $P(\tilde{X}_1, \dots, \tilde{X}_n \mid \neg Y)$ , where

$$\tilde{X}_i \in \{X_i, \neg X_i\} \forall i \in \overline{1, n}$$

and

$$(\tilde{X}_1, \dots, \tilde{X}_n) \neq (\neg X_1, \dots, \neg X_n).$$

Therefore,  $2(2^n - 1) + 1 = 2^{n+1} - 1$  values / parameters.

It can be seen that **Naive Bayes** uses a **linear number of parameters** (w.r.t.  $n$ , the number of input attributes), while **Joint Bayes** uses an **exponential number of parameters** (w.r.t. the same  $n$ ).

Exemplifying  
spam filtering using the Naive Bayes algorithm  
CMU, 2009 spring, Ziv Bar-Joseph, midterm, pr. 2

About  $\frac{2}{3}$  of your email is spam, so you downloaded an open source spam filter based on word occurrences that uses the Naive Bayes classifier.

Assume you collected the following regular and spam mails to train the classifier, and only three words are informative for this classification, i.e., each email is represented as a 3-dimensional binary vector whose components indicate whether the respective word is contained in the email.

'study'	'free'	'money'	Category	<i>count</i>
1	0	0	Regular	1
0	0	1	Regular	1
1	0	0	Regular	1
1	1	0	Regular	1
0	1	0	Spam	4
0	1	1	Spam	4

- a. You find that the spam filter uses a prior  $P(\text{spam}) = 0.1$ . Explain (in one sentence) why this might be sensible.
- b. Compute the Naive Bayes parameters, using Maximum Likelihood Estimation (MLE) and applying Laplace's rule ("add-one").
- c. Based on the prior and conditional probabilities above, give the model probability  $P(\text{spam} | s)$  that the sentence

$s = \text{"money for psychology study"}$

is spam.

## Answer:

a. It is worse for regular emails to be classified as spam than it is for spam email to be classified as regular email.

b. When **estimating the Naive Bayes parameters** from training data only using the **MLE** (maximum likelihood estimation) method we would have:

$$P(\text{study}|\text{spam}) = \frac{0}{8} = 0$$

$$P(\text{free}|\text{regular}) = \frac{1}{4}$$

$$P(\text{study}|\text{regular}) = \frac{3}{4}$$

$$P(\text{money}|\text{spam}) = \frac{4}{8} = \frac{1}{2}$$

$$P(\text{free}|\text{spam}) = \frac{8}{8} = 1$$

$$P(\text{money}|\text{regular}) = \frac{1}{4}$$

By applying **Laplace's rule ("add-one")** we get:

$$P(\text{study}|\text{spam}) = \frac{0 + 1}{8 + 2} = \frac{1}{10}$$

$$P(\text{study}|\text{regular}) = \frac{3 + 1}{4 + 2} = \frac{2}{3}$$

$$P(\text{free}|\text{spam}) = \frac{8 + 1}{8 + 2} = \frac{9}{10}$$

$$P(\text{free}|\text{regular}) = \frac{1 + 1}{4 + 2} = \frac{1}{3}$$

$$P(\text{money}|\text{spam}) = \frac{4 + 1}{8 + 2} = \frac{1}{2}$$

$$P(\text{money}|\text{regular}) = \frac{1 + 1}{4 + 2} = \frac{1}{3}$$

Notice that the occurrence of 2's at denominators corresponds to the number of values for each of the attributes used to describe the training instances.



### c. Classification of the message

$s = \text{“money for psychology study”},$

using the a priori probability  $P(\text{spam}) = 0.1$ :

$$P(\text{spam} \mid s) = P(\text{spam} \mid \text{study}, \neg \text{free}, \text{money})$$

$$\stackrel{\text{F. Bayes}}{=} \frac{P(\text{study}, \neg \text{free}, \text{money} \mid \text{spam}) \cdot P(\text{spam})}{P(\text{study}, \neg \text{free}, \text{money} \mid \text{spam})P(\text{spam}) + P(\text{study}, \neg \text{free}, \text{money} \mid \text{reg})P(\text{reg})}$$

$$P(\text{study}, \neg \text{free}, \text{money} \mid \text{spam}) \stackrel{\text{indep. cdt.}}{=} P(\text{study} \mid \text{spam}) \cdot P(\neg \text{free} \mid \text{spam}) \cdot P(\text{money} \mid \text{spam})$$

$$= \frac{1}{10} \cdot \frac{1}{10} \cdot \frac{1}{2} = \frac{1}{200}$$

$$P(\text{study}, \neg \text{free}, \text{money} \mid \text{reg}) \stackrel{\text{indep. cdt.}}{=} P(\text{study} \mid \text{reg}) \cdot P(\neg \text{free} \mid \text{reg}) \cdot P(\text{money} \mid \text{reg})$$

$$= \frac{2}{3} \cdot \frac{2}{3} \cdot \frac{1}{3} = \frac{4}{27}$$

Therefore,

$$P(\text{spam} \mid s) = \frac{\frac{1}{200} \cdot \frac{1}{10}}{\frac{1}{200} \cdot \frac{1}{10} + \frac{4}{27} \cdot \frac{9}{10}} \approx 0.0037$$

Notice that this is a small probability. However, without using Laplace's rule, it would be 0, due to the fact that the word *spam* did not appear in any of the spam emails in the training data.

**Naive Bayes and Joint Bayes:**  
**application when a joint probabilistic distribution**  
**(on input + output variables) is provided**

CMU, 2010 spring, T. Mitchell, E. Xing, A. Singh, midterm pr. 2.1

Consider the joint probability distribution over 3 boolean random variables  $x_1$ ,  $x_2$ , and  $y$  given in the nearby figure.

$x_1$	$x_2$	$y$	$P(x_1, x_2, y)$
0	0	0	0.15
0	0	1	0.25
0	1	0	0.05
0	1	1	0.08
1	0	0	0.10
1	0	1	0.02
1	1	0	0.20
1	1	1	0.15

a. Express  $P(y = 0 \mid x_1, x_2)$  in terms of  $P(x_1, x_2, y = 0)$  and  $P(x_1, x_2, y = 1)$ .

b. Compute the marginal probabilities which will be used by a Naive Bayes classifier. Fill in the following tables.

$y$	$P(y)$	$P(x_1   y)$	$x_1 = 0$	$x_1 = 1$	$P(x_2   y)$	$x_2 = 0$	$x_2 = 1$
$y = 0$		$y = 0$			$y = 0$		
$y = 1$		$y = 1$			$y = 1$		

c. Write out an expression for the value of  $P(y = 1 | x_1 = 1, x_2 = 0)$  predicted by the Naive Bayes classifier.

d. Write out an expression for the value of  $P(y = 1 | x_1 = 1, x_2 = 0)$  predicted by the Joint Bayes classifier.

e. The expressions you wrote down for parts (c) and (d) should be unequal. Explain why.

## Answer

a. Using the definition of conditional probability and then the total probability formula, we get:

$$P(y = 0 \mid x_1, x_2) = \frac{P(x_1, x_2, y = 0)}{P(x_1, x_2)} = \frac{P(x_1, x_2, y = 0)}{P(x_1, x_2, y = 0) + P(x_1, x_2, y = 1)}$$

b.

$y$	$P(y)$	$P(x_1 \mid y)$	$x_1 = 0$	$x_1 = 1$	$P(x_2 \mid y)$	$x_2 = 0$	$x_2 = 1$
$y = 0$	0.5	$y = 0$	0.40	0.60	$y = 0$	0.50	0.50
$y = 1$	0.5	$y = 1$	0.66	0.34	$y = 1$	0.54	0.46

**Explanations:**

i.  $P(y)$  was computed as a marginal probability, stating from the joint probability,  $P(x_1, x_2, y)$ :

$$\begin{aligned}
 P(y = 0) &= P(x_1 = 0, x_2 = 0, y = 0) + P(x_1 = 0, x_2 = 1, y = 0) + \\
 &\quad + P(x_1 = 1, x_2 = 0, y = 0) + P(x_1 = 1, x_2 = 1, y = 0) \\
 &= 0.15 + 0.05 + 0.1 + 0.2 = 0.5 \\
 P(y = 1) &= 1 - P(y = 0) = 0.5
 \end{aligned}$$

ii.  $P(x_1 | y)$  was computed using again the definition of conditional probability and then the total probability formula:

$$\begin{aligned}
 P(x_1 = 0 | y = 0) &= \frac{P(x_1 = 0, y = 0)}{P(y = 0)} = \frac{P(x_1 = 0, y = 0)}{P(x_1 = 0, y = 0) + P(x_1 = 1, y = 0)} \\
 P(x_1 = 0, y = 0) &= P(x_1 = 0, x_2 = 0, y = 0) + P(x_1 = 0, x_2 = 1, y = 0) = 0.15 + 0.05 = 0.2 \\
 P(x_1 = 1, y = 0) &= P(x_1 = 1, x_2 = 0, y = 0) + P(x_1 = 1, x_2 = 1, y = 0) = 0.1 + 0.2 = 0.3
 \end{aligned}$$

Therefore

$$P(x_1 = 0 | y = 0) = \frac{0.2}{0.2 + 0.3} = 0.4,$$

and

$$P(x_1 = 1 | y = 0) = 1 - P(x_1 = 0 | y = 0) = 0.6$$

Similarly,

$$\begin{aligned}
 P(x_1 = 0 | y = 1) &= \frac{P(x_1 = 0, y = 1)}{P(y = 1)} = \frac{0.25 + 0.08}{0.5} = 0.66 \Rightarrow \\
 P(x_1 = 1 | y = 1) &= 1 - P(x_1 = 0 | y = 1) = 0.34
 \end{aligned}$$

$P(x_2 | y)$  was calculated in a similar way.

c. The Naive Bayes classifier uses the *conditional independence assumption*. Therefore:

$$\begin{aligned}
 P(y = 1 \mid x_1 = 1, x_2 = 0) &\stackrel{\text{Bayes F.}}{=} \frac{P(x_1 = 1, x_2 = 0 \mid y = 1) \cdot P(y = 1)}{P(x_1 = 1, x_2 = 0)} \\
 &= \frac{P(x_1 = 1, x_2 = 0 \mid y = 1) \cdot P(y = 1)}{P(x_1 = 1, x_2 = 0 \mid y = 1)P(y = 1) + P(x_1 = 1, x_2 = 0 \mid y = 0)P(y = 0)} \stackrel{\text{cnd. indep.}}{=} \\
 &= \frac{P(x_1 = 1 \mid y = 1) \cdot P(x_2 = 0 \mid y = 1) \cdot P(y = 1)}{P(x_1 = 1 \mid y = 1)P(x_2 = 0 \mid y = 1)P(y = 1) + P(x_1 = 1 \mid y = 0)P(x_2 = 0 \mid y = 0)P(y = 0)} \\
 &= \frac{0.34 \cdot 0.54 \cdot 0.5}{0.34 \cdot 0.54 \cdot 0.5 + 0.6 \cdot 0.5 \cdot 0.5} = 0.38
 \end{aligned}$$

d. The Joint Bayes classifier doesn't use the *conditional independence assumption*. Therefore:

$$\begin{aligned}
 P(y = 1 \mid x_1 = 1, x_2 = 0) &= \frac{P(x_1 = 1, x_2 = 0, y = 1)}{P(x_1 = 1, x_2 = 0, y = 1) + P(x_1 = 1, x_2 = 0, y = 0)} \\
 &= \frac{0.02}{0.02 + 0.1} = 0.16
 \end{aligned}$$

e. The values calculated by the Naiv Bayes and respectively the Joint Bayes classifiers for  $P(y = 1 \mid x_1 = 1, x_2 = 0)$  are different because the conditional independence assumption does not hold.

Indeed,

$$P(x_1 = 0, x_2 = 0 \mid y = 0) = \frac{P(x_1 = 0, x_2 = 0, y = 0)}{P(y = 0)} = \frac{0.15}{0.5} = 0.3$$

while

$$P(x_1 = 0 \mid y = 0) \cdot P(x_2 = 0 \mid y = 0) = 0.4 \cdot 0.5 = 0.2 \neq 0.3$$

Therefore,  $x_1$  and  $x_2$  are not conditionally independent w.r.t.  $y$ .



Exemplifying

The computation of the *error rate* for the Naive Bayes algorithm

CMU, 2010 fall, Aarti Singh, HW1, pr. 4.2

Consider a simple learning problem of determining whether Alice and Bob from CA will go to hiking or not  $Y : Hike \in \{T, F\}$  given the weather conditions  $X_1 : Sunny \in \{T, F\}$  and  $X_2 : Windy \in \{T, F\}$  by a Naive Bayes classifier.

Using training data, we estimated the parameters

$$\begin{aligned} P(Hike) &= 0.5 \\ P(Sunny \mid Hike) &= 0.8, \quad P(Sunny \mid \neg Hike) = 0.7 \\ P(Windy \mid Hike) &= 0.4, \quad P(Windy \mid \neg Hike) = 0.5 \end{aligned}$$

Assume that the true distribution of  $X_1, X_2$ , and  $Y$  satisfies the Naive Bayes assumption of conditional independence with the above parameters.

a. What is the joint probability that Alice and Bob go to hiking and the weather is sunny and windy, that is  $P(Sunny, Windy, Hike)$ ?

**Solution:**

$$P(Sunny, Windy, Hike) \stackrel{cdt. indep.}{=} P(Sunny|Hike) \cdot P(Windy|Hike) \cdot P(Hike) = 0.8 \cdot 0.4 \cdot 0.5 = 0.16.$$

b. What is the expected error rate of the Naive Bayes classifier?

(Informally, the expected error rate is the probability that an “observation”/instance randomly generated according to the *true* probabilistic distribution of data is incorrectly classified by the Naive Bayes algorithm.)

**Solution:**

$X_1$	$X_2$	$Y$	$P(X_1, X_2, Y) = P(X_1 Y) \cdot P(X_2 Y) \cdot P(Y)$	$Y_{NB}(X_1, X_2)$	$P_{NB}(Y X_1, X_2)$
$F$	$F$	$F$	$0.3 \cdot 0.5 \cdot 0.5 = 0.075$	$F$	0.555556
$F$	$F$	$T$	$0.2 \cdot 0.6 \cdot 0.5 = \mathbf{0.060}$	$F$	0.444444
$F$	$T$	$F$	$0.3 \cdot 0.5 \cdot 0.5 = 0.075$	$F$	0.652174
$F$	$T$	$T$	$0.2 \cdot 0.4 \cdot 0.5 = \mathbf{0.040}$	$F$	0.347826
$T$	$F$	$F$	$0.7 \cdot 0.5 \cdot 0.5 = \mathbf{0.175}$	$T$	0.421686
$T$	$F$	$T$	$0.8 \cdot 0.6 \cdot 0.5 = 0.240$	$T$	0.578314
$T$	$T$	$F$	$0.7 \cdot 0.5 \cdot 0.5 = 0.175$	$F$	0.522388
$T$	$T$	$T$	$0.8 \cdot 0.4 \cdot 0.5 = \mathbf{0.160}$	$F$	0.477612

**Note:**

Joint probabilities corresponding to incorrect predictions are shown in bold.

$$\begin{aligned}
 \text{error} &\stackrel{\text{def.}}{=} E_P[I_{Y_{NB}(X_1, X_2) \neq Y}] \\
 &= \sum_{X_1, X_2, Y} I[Y_{NB}(X_1, X_2) \neq Y] \cdot P(X_1, X_2, Y) \\
 &= \mathbf{0.060} + \mathbf{0.040} + \mathbf{0.175} + \mathbf{0.160} = \mathbf{0.435}
 \end{aligned}$$

**Note:**

$I$  is the *indicator* function; its value is 1 whenever the associated condition (in our case,  $Y_{NB}(X_1, X_2) \neq Y$ ) is true, and 0 otherwise.

Next, suppose that we gather more information about weather conditions and introduce a new feature denoting whether the weather is  $X_3 : \text{Rainy}$  or not. Assume that each day the weather in CA can be either *Rainy* or *Sunny*. That is, it can not be both *Sunny* and *Rainy*. (Similarly, it can not be  $\neg \text{Sunny}$  and  $\neg \text{Rainy}$ ).

c. In the above new case, are any of the Naive Bayes assumptions violated? Why (not)? What is the joint probability that Alice and Bob go to hiking and the weather is sunny, windy and not rainy, that is  $P(\text{Sunny}, \text{Windy}, \neg \text{Rainy}, \text{Hike})$ ?

**Solution:**

The conditional independence of variables given the class label assumption of Naive Bayes is violated. Indeed, knowing if the weather is *Sunny* completely determines whether it is *Rainy* or not. Therefore, *Sunny* and *Rainy* are clearly NOT conditionally independent given *Hike*.

$$\begin{aligned}
 &P(\text{Sunny}, \text{Windy}, \neg \text{Rainy}, \text{Hike}) \\
 &= \underbrace{P(\neg \text{Rainy} | \text{Hike}, \text{Sunny}, \text{Windy})}_1 \cdot P(\text{Sunny}, \text{Windy} | \text{Hike}) \cdot P(\text{Hike}) \\
 &\stackrel{\text{cond. indep.}}{=} P(\text{Sunny} | \text{Hike}) \cdot P(\text{Windy} | \text{Hike}) \cdot P(\text{Hike}) \\
 &= 0.8 \cdot 0.4 \cdot 0.5 = 0.16.
 \end{aligned}$$

d. What is the expected error rate when the Naive Bayes classifier uses all three attributes? Does the performance of Naive Bayes improve by observing the new attribute Rainy? Explain why.

Solution:

$X_1$	$X_2$	$X_3$	$Y$	$P(X_1, X_2, Y)$	$P_{NB}(X_1, X_2, X_3, Y) = P(X_3 Y) \cdot P(X_1 Y) \cdot P(X_2 Y) \cdot P(Y)$	$Y_{NB}(X_1, X_2, X_3)$	$P_{NB}(Y X_1, X_2, X_3)$
$F$	$F$	$F$	$F$	0	$0.075 \cdot 0.7 = 0.0525$	$F$	0.522388
$F$	$F$	$F$	$T$	0	$0.060 \cdot 0.8 = 0.0480$	$F$	0.477612
$F$	$F$	$T$	$F$	0.075	$0.075 \cdot 0.3 = 0.0225$	$F$	0.652174
$F$	$F$	$T$	$T$	<b>0.060</b>	$0.060 \cdot 0.2 = 0.0120$	$F$	0.347826
$F$	$T$	$F$	$F$	0	$0.075 \cdot 0.7 = 0.0525$	$F$	0.621302
$F$	$T$	$F$	$T$	0	$0.040 \cdot 0.8 = 0.0320$	$F$	0.378698
$F$	$T$	$T$	$F$	0.075	$0.075 \cdot 0.3 = 0.0225$	$F$	0.737705
$F$	$T$	$T$	$T$	<b>0.040</b>	$0.040 \cdot 0.2 = 0.0080$	$F$	0.262295
$T$	$F$	$F$	$F$	<b>0.175</b>	$0.175 \cdot 0.7 = 0.0525$	$T$	0.389507
$T$	$F$	$F$	$T$	0.240	$0.240 \cdot 0.8 = 0.1920$	$T$	0.610493
$T$	$F$	$T$	$F$	0	$0.175 \cdot 0.3 = 0.0525$	$F$	0.522388
$T$	$F$	$T$	$T$	0	$0.240 \cdot 0.2 = 0.0480$	$F$	0.477612
$T$	$T$	$F$	$F$	<b>0.175</b>	$0.175 \cdot 0.7 = 0.0525$	$T$	0.489022
$T$	$T$	$F$	$T$	0.160	$0.160 \cdot 0.8 = 0.1280$	$T$	0.510978
$T$	$T$	$T$	$F$	0	$0.175 \cdot 0.3 = 0.0225$	$F$	0.621302
$T$	$T$	$T$	$T$	0	$0.060 \cdot 0.2 = 0.0120$	$F$	0.378698

The new error rate is:

$$E_P[I_{Y_{NB}(X_1, X_2, X_3) \neq Y}] = 0.060 + 0.040 + 0.175 + 0.175 = 0.45 > 0.435 \text{ (see question } b \text{)}.$$

*Important Remark:*

Please notice that we **always compute the error rate with respect to  $P$ , the true distribution**, and not  $P_{NB}$ , which is the distribution computed by Naive Bayes by using the conditional independence assumption.

Here above, the Naive Bayes classifier performance drops because the conditional independence assumptions do not hold for the correlated features.

## How bad/naive is Naive Bayes?

CMU, 2010 spring, E. Xing, T. Mitchell, A. Singh, midterm, pr. 2.1

Clearly Naive Bayes makes what, in many cases, are overly strong assumptions. But even if those assumptions aren't true, is it possible that Naive Bayes is still pretty good? *Here we will use a simple example to explore the limitations of Naive Bayes.*

Let  $X_1$  and  $X_2$  be i.i.d. Bernoulli(0.5) random variables, and let  $Y \in \{1, 2\}$  be some deterministic function of the values of  $X_1$  and  $X_2$ .

- a. Find a function  $Y$  for which the Naive Bayes classifier has a 50% error rate. Given the value of  $Y$ , how are  $X_1$  and  $X_2$  correlated?
- b. Show that for every function  $Y$ , the Naive Bayes classifier will perform no worse than the one above. *Hint:* there are many  $Y$  functions, but because of symmetries in the problem you only need to analyze a few of them.



## Răspuns

a. Considerăm  $Y$  definit conform tabelului alăturat.

$X_1$	$X_2$	$Y$
0	0	1
0	1	2
1	0	2
1	1	1

*Observație:* Dacă se consideră valoarea lui  $Y$  fixată (fie 1, fie 2), atunci putem să stabilim o regulă astfel încât dacă îl cunoaștem pe  $X_1$  să-l determinăm pe  $X_2$  (și invers).<sup>a</sup> Altfel spus,  $X_1$  este unic determinat de  $X_2$  (și invers) dată fiind o valoare fixată a lui  $Y$ . Deci condiția de independență condițională este încălcată. Mai mult, în acest caz avem maximul posibil de „dependență” între cele două variabile (în raport cu  $Y$ ).

Pe slide-ul următor vom calcula rata erorii înregistrate de algoritmul Bayes Naiv pe datele din tabelul de mai sus.

---

<sup>a</sup>Pentru  $Y = 1$ , regula este:  $X_2$  are aceeași valoare ca și  $X_1$ . Pentru  $Y = 2$ , regula este:  $X_1$  și  $X_2$  au valori complementare.

Bayes Naiv estimează valoarea lui  $Y$  astfel:

$$\hat{y} = \operatorname{argmax}_{y \in \{1,2\}} P(X_1 | Y = y)P(X_2 | Y = y)P(Y = y)$$

Pentru  $X_1 = 0, X_2 = 0$ , algoritmul compară următoarele două valori:

$$\begin{aligned} p_1 &= P(X_1 = 0 | Y = 1)P(X_2 = 0 | Y = 1)P(Y = 1) = \frac{1}{2} \cdot \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{8} \\ p_2 &= P(X_1 = 0 | Y = 2)P(X_2 = 0 | Y = 2)P(Y = 2) = \frac{1}{2} \cdot \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{8} \end{aligned}$$

Cum  $p_1 = p_2$ , algoritmul va alege una dintre ele cu o probabilitate de 0.5. Deoarece valoarea lui  $Y$  este 1 din tabel, înseamnă că algoritmul va alege greșit în 50% din cazuri.

Pentru celelalte 3 cazuri,  $(X_1 = 0, X_2 = 1)$ ,  $(X_1 = 1, X_2 = 0)$  și  $(X_1 = 1, X_2 = 1)$ , se observă ușor că se obțin de asemenea valori egale, iar algoritmul va alege pentru  $Y$  una dintre valorile 1 sau 2 cu o probabilitate de 0.5.

Deci pentru această definiție a lui  $Y$  rata erorii este de 50%.

b. Vom calcula rata erorii pentru fiecare dintre cele 3 moduri de definire a lui  $Y$  care nu a fost studiat.

<b>Cazul 1:</b>	$X_1$	$X_2$	$Y$	Este similar cu cazul:	$Y$
	0	0	1		2
	0	1	1		2
	1	0	1		2
	1	1	1		2

- Pentru  $X_1 = 0, X_2 = 0$ , algoritmul compară:

$$p_1 = P(X_1 = 0 | Y = 1)P(X_2 = 0 | Y = 1)P(Y = 1) = \frac{2}{4} \cdot \frac{2}{4} \cdot 1 = \frac{1}{4}$$

$$p_2 = P(X_1 = 0 | Y = 2)P(X_2 = 0 | Y = 2)P(Y = 2) = 0 \cdot 0 \cdot 0 = 0$$

Cum  $p_1 > p_2$  algoritmul alege pentru  $Y$  valoarea 1, ceea ce este corect.

- Pentru celelalte 3 cazuri,  $(X_1 = 0, X_2 = 1)$ ,  $(X_1 = 1, X_2 = 0)$  și  $(X_1 = 1, X_2 = 1)$ , se observă că se obțin aceleași valori pentru  $p_1$  și  $p_2$  ca mai sus, deci algoritmul alege (în mod corect) pentru  $Y$  valoarea 1.

Așadar, am obținut că rata erorii este în acest caz 0.

<b>Cazul 2:</b>	$X_1$	$X_2$	$Y$	<b>Cazuri similare:</b>	$Y$	$Y$	$Y$	$Y$	$Y$	$Y$	$Y$
	0	0	1		1	1	2	2	2	2	1
	0	1	1		1	2	1	2	2	1	2
	1	0	1		2	1	1	2	1	2	2
	1	1	2		1	1	1	1	2	2	2

- Pentru  $X_1 = 0, X_2 = 0$ :

$$\left. \begin{aligned} p_1 &= P(X_1 = 0 | Y = 1)P(X_2 = 0 | Y = 1)P(Y = 1) = \frac{2}{3} \cdot \frac{2}{3} \cdot \frac{3}{4} = \frac{1}{3} \\ p_2 &= P(X_1 = 0 | Y = 2)P(X_2 = 0 | Y = 2)P(Y = 2) = 0 \cdot 0 \cdot \frac{1}{4} = 0 \end{aligned} \right\} \Rightarrow \hat{y} = 1$$

- Pentru  $X_1 = 0, X_2 = 1$ :

$$\left. \begin{aligned} p_1 &= P(X_1 = 0 | Y = 1)P(X_2 = 1 | Y = 1)P(Y = 1) = \frac{2}{3} \cdot \frac{1}{3} \cdot \frac{3}{4} = \frac{1}{6} \\ p_2 &= P(X_1 = 0 | Y = 2)P(X_2 = 1 | Y = 2)P(Y = 2) = 0 \cdot 1 \cdot \frac{1}{4} = 0 \end{aligned} \right\} \Rightarrow \hat{y} = 1$$

- Pentru  $X_1 = 1, X_2 = 0$ :

$$\left. \begin{aligned} p_1 &= P(X_1 = 1 \mid Y = 1)P(X_2 = 0 \mid Y = 1)P(Y = 1) = \frac{1}{3} \cdot \frac{2}{3} \cdot \frac{3}{4} = \frac{1}{6} \\ p_2 &= P(X_1 = 1 \mid Y = 2)P(X_2 = 0 \mid Y = 2)P(Y = 2) = 1 \cdot 0 \cdot \frac{1}{4} = 0 \end{aligned} \right\} \Rightarrow \hat{y} = 1$$

- Pentru  $X_1 = 1, X_2 = 1$ :

$$\left. \begin{aligned} p_1 &= P(X_1 = 1 \mid Y = 1)P(X_2 = 1 \mid Y = 1)P(Y = 1) = \frac{1}{3} \cdot \frac{1}{3} \cdot \frac{3}{4} = \frac{1}{12} \\ p_2 &= P(X_1 = 1 \mid Y = 2)P(X_2 = 1 \mid Y = 2)P(Y = 2) = 1 \cdot 1 \cdot \frac{1}{4} = \frac{1}{4} \end{aligned} \right\} \Rightarrow \hat{y} = 2$$

Deci rata erorii este 0 pentru această definiție a lui  $Y$ .

<b>Cazul 3:</b>	$X_1$	$X_2$	$Y$	<b>Cazuri similare:</b>	$Y$	$Y$	$Y$
	0	0	1		2	1	2
	0	1	2		1	1	2
	1	0	1		2	2	1
	1	1	2		1	2	1

- Pentru  $X_1 = 0, X_2 = 0$ :

$$p_1 = \frac{1}{2} \cdot 1 \cdot \frac{1}{2} = \frac{1}{4}, p_2 = \frac{1}{2} \cdot 0 \cdot \frac{1}{2} = 0 \Rightarrow p_1 > p_2 \Rightarrow \hat{y} = 1 \text{ (corect)}$$

- Pentru  $X_1 = 0, X_2 = 1$ :

$$p_1 = \frac{1}{2} \cdot 0 \cdot \frac{1}{2} = 0, p_2 = \frac{1}{2} \cdot 1 \cdot \frac{1}{2} = \frac{1}{4} \Rightarrow p_1 < p_2 \Rightarrow \hat{y} = 2 \text{ (corect)}$$

- Pentru  $X_1 = 1, X_2 = 0$ :

$$p_1 = \frac{1}{2} \cdot 1 \cdot \frac{1}{2} = \frac{1}{4}, p_2 = \frac{1}{2} \cdot 0 \cdot \frac{1}{2} = 0 \Rightarrow p_1 > p_2 \Rightarrow \hat{y} = 1 \text{ (corect)}$$

- Pentru  $X_1 = 1, X_2 = 1$ :

$$p_1 = \frac{1}{2} \cdot 0 \cdot \frac{1}{2} = 0, p_2 = \frac{1}{2} \cdot 1 \cdot \frac{1}{2} = \frac{1}{4} \Rightarrow p_1 < p_2 \Rightarrow \hat{y} = 2 \text{ (corect)}$$

Prin urmare, rata erorii este 0 și în acest caz.

<b>Cazul 4:</b> (cel de la punctul a)	$X_1$	$X_2$	$Y$	Este similar cu cazul:	$Y$
	0	0	1		2
	0	1	2		1
	1	0	2		1
	1	1	1		2

**Concluzie:** Doar pentru 2 moduri (cazul 4) de definire a lui  $Y$  rata erorii este de 50%; pentru celelalte 14 moduri (cazurile 1, 2, 3) rata erorii este 0.

Unlike Naive Bayes,  
the Joint Bayes classifier has 0 training error rate for  
all boolean functions

(and even all mathematically defined functions on categorical attributes);

“in-between Naive and Joint” Bayesian classifiers

CMU, 2004 fall, T. Mitchell, Z. Bar-Joseph, HW3, pr. 1.2



Suppose we have a function  $y = (A \wedge B) \vee \neg(B \vee C)$ , where  $A, B, C$  are independent binary random variables, each having a 50% chance of being 0.

a. How many parameters a Naive Bayes classifier needs to estimate (without counting  $P(\neg x)$  as a parameter if  $P(x)$  is already counted as an estimated parameter)?

What will be the error rate of the Naive Bayes classifier (assuming infinite training data)?

b. How many parameters a joint Bayes classifier needs to estimate? What will be the error rate of the joint Bayes classifier (assuming infinite training data)?

c. Consider a Bayes classifier that assumes that  $A$  is independent of  $C$  when conditioned on  $B$  and on  $y$  (unlike a Naive Bayes classifier that assumes that  $A, B, C$  are all independent of each other when conditioned on  $y$ ).

Show that this Bayes classifier will need to estimate fewer parameters than a joint Bayes classifier, but will still have the same error rate (assuming infinite training data). Compute the error rate of this classifier.

## Computing

The *sample complexity* of the Naive Bayes and Joint Bayes Classifiers

CMU, 2010 spring, Eric Xing, Tom Mitchell, Aarti Singh, HW2, pr. 1.1

A big reason we use the Naive Bayes classifier is that it requires less training data than the Joint Bayes Classifier. This exercise should give you a “feeling” for how great the disparity really is.

Imagine that each *instance* is an independent “*observation*” of the multi-variate random variable  $\bar{X} = (X_1, \dots, X_d)$ , where the  $X_i$  are i.i.d. and Bernoulli of parameter  $p = 0.5$ .

To train the Joint Bayes classifier, we need to see every value of  $\bar{X}$  “enough” times; training the Naive Bayes classifier only requires seeing both values of  $X_i$  “enough” times.

**Main Question:** How many “observations”/instances are needed until, with probability  $1 - \varepsilon$ , we have seen every variable we need to see at least once?

Note: To train the classifiers well would require more than this, but for this problem we only require one observation.

Hint: You may want to use the following *inequalities*:

- For any  $k \geq 1$ ,  $(1 - 1/k)^k \leq e^{-1}$
- For *any* events  $E_1, \dots, E_k$ ,  $Pr(E_1 \cup \dots \cup E_k) \leq \sum_{i=1}^k Pr(E_i)$ .  
(This is called the “union bounds” property.)

Consider the Naive Bayes classifier.

- a. Show that if  $N$  observations have been made, the probability that a given value of  $X_i$  (either 0 or 1) has *not* been seen is  $\leq \frac{1}{2^{N-1}}$ .
- b. Show that if more than  $N_{NB} = 1 + \log_2 \left( \frac{d}{\varepsilon} \right)$  observations have been made, then the probability that *any*  $X_i$  has not been observed in both states is  $\leq \varepsilon$ .

**Solution:**

$$\text{a. } P(\text{component } X_i \text{ not seen in both states}) = \left(\frac{1}{2}\right)^N + \left(\frac{1}{2}\right)^N = \frac{2}{2^N} = \frac{1}{2^{N-1}}$$

$$\text{b. } P(\text{any component not seen in both states})$$

$$\leq \sum_{i=1}^d P(\text{component } X_i \text{ not seen in both states})$$

$$= \sum_{i=1}^d \frac{1}{2^{N_{NB}-1}} = d \cdot \frac{1}{2^{N_{NB}-1}} = d \cdot \frac{1}{2^{1+\log_2 \frac{d}{\varepsilon}-1}} = d \cdot \frac{1}{2^{\log_2 \frac{d}{\varepsilon}}} = d \cdot \frac{1}{\frac{d}{\varepsilon}} = d \cdot \frac{\varepsilon}{d} = \varepsilon$$

Consider the Joint Bayes classifier.

- c. Let  $\bar{x}$  be a particular value of  $\bar{X}$ . Show that after  $N$  observations, the probability that we have never seen  $\bar{x}$  is  $\leq e^{-N/2^d}$ .
- d. Using the “union bounds” property, show that if more than  $N_{JB} = 2^d \ln \left( \frac{2^d}{\varepsilon} \right)$  observations have been made, then the probability that *any* value of  $\bar{X}$  has not been seen is  $\leq \varepsilon$ .

**Solution:**

- c.  $P(\bar{x} \text{ not seen in } N \text{ observations})$

$$= \left(1 - \frac{1}{2^d}\right)^N = \left[\left(1 - \frac{1}{2^d}\right)^{2^d}\right]^{N/2^d} \leq \left(\frac{1}{e}\right)^{N/2^d} = e^{-N/2^d}$$

- d.  $P(\text{any } \bar{x} \text{ not seen in } N_{JB} \text{ observations})$

$$\begin{aligned} &\leq \sum_{\bar{x}} P(\bar{x} \text{ not seen in } N_{JB} \text{ observations}) \\ &\leq \sum_{\bar{x}} e^{-N_{JB}/2^d} = 2^d \cdot e^{-N_{JB}/2^d} = 2^d \cdot e^{-\ln \frac{2^d}{\varepsilon}} = 2^d \cdot \frac{1}{e^{\ln \frac{2^d}{\varepsilon}}} = \frac{2^d}{\frac{2^d}{\varepsilon}} = \varepsilon \end{aligned}$$

- e. Let  $d = 2$  and  $\varepsilon = 0.1$ . What are the values of  $N_{NB}$  and  $N_{JB}$ ?  
 What about  $d = 5$ ?  
 And  $d = 10$ ?

**Solution:**

$$\varepsilon = 0.1, d = 2 \Rightarrow \begin{cases} N_{NB} = 1 + \log_2 \frac{2}{0.1} = 1 + \log_2 20 \approx 5.32 \\ N_{JB} = 2^2 \cdot \ln \frac{2^2}{0.1} = 4 \cdot \ln 40 \approx 14.75 \end{cases}$$

$$\varepsilon = 0.1, d = 5 \Rightarrow \begin{cases} N_{NB} = 1 + \log_2 \frac{5}{0.1} = 1 + \log_2 50 \approx 6.64 \\ N_{JB} = 2^5 \cdot \ln \frac{2^5}{0.1} = 32 \cdot \ln 320 \approx 184.58 \end{cases}$$

$$\varepsilon = 0.1, d = 10 \Rightarrow \begin{cases} N_{NB} = 1 + \log_2 \frac{10}{0.1} = 1 + \log_2 100 \approx 7.64 \\ N_{JB} = 2^{10} \cdot \ln \frac{2^{10}}{0.1} = 1024 \cdot \ln 10240 \approx 9455.67 \end{cases}$$

The relationship between [the decision rules of]  
*Naive Bayes and Logistic Regression*;  
the case of Boolean input variables

CMU, 2005 fall, Tom Mitchell, Andrew Moore, HW2, pr. 2

CMU, 2009 fall, Carlos Guestrin, HW1, pr. 4.1.2

CMU, 2009 fall, Geoff Gordon, HW4, pr. 1.2

CMU, 2012 fall, Tom Mitchell, Ziv Bar-Joseph, HW2, pr. 3.a



a. [NB and LR: the relationship between the decision rules]

In Tom's draft chapter (*Generative and discriminative classifiers: Naive Bayes and logistic regression*) it has been proved that when  $Y$  follows a Bernoulli distribution and  $X = (X_1, \dots, X_d)$  is a vector of Gaussian variables, then under certain assumptions the Gaussian Naive Bayes classifier implies that  $P(Y|X)$  is given by the logistic function with appropriate parameters  $w$ . So,

$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_{i=1}^d w_i X_i)}.$$

and therefore,

$$P(Y = 0|X) = \frac{\exp(w_0 + \sum_{i=1}^d w_i X_i)}{1 + \exp(w_0 + \sum_{i=1}^d w_i X_i)}$$

Consider instead the case where  $Y$  is Boolean (more generally, Bernoulli) and  $X = (X_1, \dots, X_d)$  is a vector of Boolean variables. Prove for this case also that  $P(Y|X)$  follows this same form and hence that Logistic Regression is also the discriminative counterpart to a Naive Bayes generative classifier over Boolean features.

**Note:** **Discriminative classifiers** learn the parameters of  $P(Y|X)$  directly, whereas **generative classifiers** instead learn the parameters of  $P(X|Y)$  and  $P(Y)$ .

*Hints:*

1. Simple notation will help. Since the  $X_i$ 's are Boolean variables, you need only one parameter to define,  $P(X_i|Y = y_k)$ , for each  $i = 1, \dots, d$ .

Define  $\theta_{i1} = P(X_i = 1|Y = 1)$ , in which case  $P(X_i = 0|Y = 1) = 1 - \theta_{i1}$ . Similarly, use  $\theta_{i0}$  to denote  $P(X_i = 1|Y = 0)$ .

2. Notice that with the above notation you can represent  $P(X_i|Y = 1)$  as follows:

$$P(X_i|Y = 1) = \theta_{i1}^{X_i} (1 - \theta_{i1})^{(1-X_i)},$$

except the cases when  $\theta_{i1} = 0$  and  $X_i = 0$ , respectively  $\theta_{i1} = 1$  and  $X_i = 1$ . Note that when  $X_i = 1$  the second term is equal to 1 because its exponent is zero. Similarly, when  $X_i = 0$  the first term is equal to 1 because its exponent is zero.

## Solution

$$P(Y = 1|X = x) \stackrel{B.F.}{=} \frac{P(X = x|Y = 1) P(Y = 1)}{\sum_{y' \in \{0,1\}} P(X = x|Y = y') P(Y = y')}$$

$$= \frac{1}{1 + \frac{P(X = x|Y = 0)P(Y = 0)}{P(X = x|Y = 1)P(Y = 1)}}$$

$$= \frac{1}{1 + \exp \left( \ln \frac{P(X = x|Y = 0)P(Y = 0)}{P(X = x|Y = 1)P(Y = 1)} \right)}$$

$$= \frac{1}{1 + \exp \left( \ln \frac{P(X_1 = x_1, \dots, X_d = x_d|Y = 0)P(Y = 0)}{P(X_1 = x_1, \dots, X_d = x_d|Y = 1)P(Y = 1)} \right)}$$

$$\stackrel{cond. indep.}{=} \frac{1}{1 + \exp \left( \ln \frac{P(Y=0)}{P(Y=1)} + \sum_{i=1}^d \ln \frac{P(X_i=x_i|Y=0)}{P(X_i=x_i|Y=1)} \right)}$$

### *Conditions:*

1.  $P(X = x|Y = 1) P(Y = 1) \neq 0$ ;
2.  $P(X = x|Y = 0) P(Y = 0) \neq 0$ ;
3.  $P(X = x_i|Y = 0) \neq 0$  and  $P(X = x_i|Y = 1) \neq 0$ .

**Prior probabilities are:**  $P(Y = 1) = \pi$  and  $P(Y = 0) = 1 - \pi$ .

**Also, each  $X_i$  follows a Bernoulli distribution:**

$P(X_i|Y = 1) = \theta_{i1}^{X_i}(1 - \theta_{i1})^{(1-X_i)}$ , and  $P(X_i|Y = 0) = \theta_{i0}^{X_i}(1 - \theta_{i0})^{(1-X_i)}$ .

**So,**

$$\begin{aligned}
 P(Y = 1|X = x) &= \frac{1}{1 + \exp \left( \ln \frac{1 - \pi}{\pi} + \sum_{i=1}^d \ln \frac{\theta_{i0}^{X_i}(1 - \theta_{i0})^{(1-X_i)}}{\theta_{i1}^{X_i}(1 - \theta_{i1})^{(1-X_i)}} \right)} \\
 &= \frac{1}{1 + \exp \left( \ln \frac{1 - \pi}{\pi} + \sum_{i=1}^d \left( X_i \ln \frac{\theta_{i0}}{\theta_{i1}} + (1 - X_i) \ln \frac{1 - \theta_{i0}}{1 - \theta_{i1}} \right) \right)} \\
 &= \frac{1}{1 + \exp \left( \ln \frac{1 - \pi}{\pi} + \sum_{i=1}^d \ln \frac{1 - \theta_{i0}}{1 - \theta_{i1}} + \sum_{i=1}^d X_i \left( \ln \frac{\theta_{i0}}{\theta_{i1}} - \ln \frac{1 - \theta_{i0}}{1 - \theta_{i1}} \right) \right)}
 \end{aligned}$$

**Therefore, in order to reach  $P(Y = 1|X = x) = 1/(1 + \exp(w_0 + \sum_{i=1}^d w_i X_i))$ , we can set**

$$w_0 = \ln \frac{1 - \pi}{\pi} + \sum_{i=1}^d \ln \frac{1 - \theta_{i0}}{1 - \theta_{i1}} \quad \text{and} \quad w_i = \ln \frac{\theta_{i0}}{\theta_{i1}} - \ln \frac{1 - \theta_{i0}}{1 - \theta_{i1}} \quad \text{for } i = 1, \dots, d.$$

## Note

Although here we derived for  $P(Y|X)$  a form which is specific to Logistic Regression starting from the decision rule (better said, from the expression of  $P(Y = 1|X)$ ) used by Naive Bayes, this does not mean that Logistic Regression itself uses the conditional independence assumption.

b. [Relaxing the conditional independence assumption]

To capture interactions between features, the Logistic Regression model can be supplemented with extra terms. For example, a term can be added to capture a dependency between  $X_1$  and  $X_2$ :

$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + w_{1,2}X_1X_2 + \sum_{i=1}^n w_iX_i)}$$

Similarly, the conditional independence assumptions made by Naive Bayes can be relaxed so that  $X_1$  and  $X_2$  are not assumed to be conditionally independent. In this case, we can write:

$$P(Y|X) = \frac{P(Y) P(X_1, X_2|Y) \prod_{i=3}^n P(X_i|Y)}{P(X)}$$

Prove that for this case, that  $P(Y|X)$  follows the same form as the logistic regression model supplemented with the extra term that captures the dependency between  $X_1$  and  $X_2$  (and hence that the supplemented Logistic Regression model is the discriminative counterpart to this generative classifier).

***Hints:***

1. Using simple notation will help here as well. You need more parameters than before to define  $P(X_1, X_2, Y)$ . So let's define  $\beta_{ijk} = P(X_1 = i, X_2 = j, Y = k)$ , for each  $i, j$  and  $k$ .

2. The above notation can be used to represent  $P(X_1, X_2|Y = k)$  as follows:

$$P(X_1, X_2|Y = k) = (\beta_{11k})^{X_1 X_2} (\beta_{10k})^{X_1(1-X_2)} (\beta_{01k})^{(1-X_1)X_2} (\beta_{00k})^{(1-X_1)(1-X_2)}$$

for  $k \in \{0, 1\}$ , except for the cases when  $\beta_{11k} = 0$  and  $X_1 X_2 = 0$ , or  $\beta_{10k} = 0$  and  $X_1(1 - X_2) = 0$ , or  $\beta_{01k} = 0$  and  $(1 - X_1)X_2 = 0$ , or  $\beta_{00k} = 0$  and  $(1 - X_1)(1 - X_2) = 0$ .

## Solution

$$\begin{aligned}
P(Y = 1|X) &\stackrel{B.F.}{=} \frac{P(X|Y = 1)P(Y = 1)}{P(X|Y = 1)P(Y = 1) + P(X|Y = 0)P(Y = 0)} \\
&= \frac{1}{1 + \frac{P(X|Y = 0)P(Y = 0)}{P(X|Y = 1)P(Y = 1)}} \\
&= \frac{1}{1 + \exp\left(\ln \frac{P(X|Y = 0)P(Y = 0)}{P(X|Y = 1)P(Y = 1)}\right)} \\
&\stackrel{cdtl. indep.}{=} \frac{1}{1 + \exp\left(\ln \frac{P(X_1, X_2|Y = 0) \prod_{i=3}^d P(X_i|Y = 0)P(Y = 0)}{P(X_1, X_2|Y = 1) \prod_{i=3}^d P(X_i|Y = 1)P(Y = 1)}\right)} \\
&= \frac{1}{1 + \exp\left(\ln \frac{1 - \pi}{\pi} + \sum_{i=3}^d \ln \frac{P(X_i|Y = 0)}{P(X_i|Y = 1)} + \ln \frac{P(X_1, X_2|Y = 0)}{P(X_1, X_2|Y = 1)}\right)} \\
&= \frac{1}{1 + \exp\left(\ln \frac{1 - \pi}{\pi} + \sum_{i=3}^d \ln \frac{\theta_{i0}^{X_i} (1 - \theta_{i0})^{(1-X_i)}}{\theta_{i1}^{X_i} (1 - \theta_{i1})^{(1-X_i)}} + \ln \frac{(\beta_{110})^{X_1 X_2} (\beta_{100})^{X_1 (1-X_2)} (\beta_{010})^{(1-X_1) X_2} (\beta_{000})^{(1-X_1)(1-X_2)}}{(\beta_{111})^{X_1 X_2} (\beta_{101})^{X_1 (1-X_2)} (\beta_{011})^{(1-X_1) X_2} (\beta_{001})^{(1-X_1)(1-X_2)}}\right)} \\
&= \frac{1}{1 + \exp\left(\ln \frac{1 - \pi}{\pi} + \sum_{i=3}^d \left(X_i \left(\ln \frac{\theta_{i0}}{\theta_{i1}} + \ln \frac{1 - \theta_{i1}}{1 - \theta_{i0}}\right) + \ln \frac{1 - \theta_{i1}}{1 - \theta_{i0}}\right) + \ln \frac{\beta_{000}}{\beta_{001}} + w_1 X_1 + w_2 X_2 + w_{1,2} X_1 X_2\right)}
\end{aligned}$$

### *Conditions:*

- 1.**  $P(X = x|Y = 1) P(Y = 1) \neq 0$ ;
- 2.**  $P(X = x|Y = 0) P(Y = 0) \neq 0$ ;
- 3.**  $P(X_1 X_2|Y = 0) \neq 0$  **and**  $P(X_1 X_2|Y = 1) \neq 0$ ;  $P(X_i|Y = 0) \neq 0$  **and**  $P(X_i|Y = 1) \neq 0$ .



with

$$\begin{aligned}
 w_0 &= \ln \frac{1 - \pi}{\pi} + \sum_{i=3}^d \ln \frac{1 - \theta_{i1}}{1 - \theta_{i0}} + \ln \frac{\beta_{000}}{\beta_{001}} \\
 w_1 &= \ln \frac{\beta_{100}}{\beta_{101}} + \ln \frac{\beta_{001}}{\beta_{000}} \\
 w_2 &= \ln \frac{\beta_{010}}{\beta_{011}} + \ln \frac{\beta_{001}}{\beta_{000}} \\
 w_{1,2} &= \ln \frac{\beta_{110}}{\beta_{111}} + \ln \frac{\beta_{101}}{\beta_{100}} + \ln \frac{\beta_{011}}{\beta_{010}} + \ln \frac{\beta_{000}}{\beta_{001}} \\
 w_i &= \ln \frac{\theta_{i0}}{\theta_{i1}} + \ln \frac{1 - \theta_{i1}}{1 - \theta_{i0}} \text{ for } i = 3, \dots, d.
 \end{aligned}$$

# Gaussian Bayesian Classification

Exemplifying the Gaussian [Naive] Bayes algorithm on data from  $\mathbb{R}$   
CMU, 2001 fall, Andrew Moore, midterm, pr. 3.a

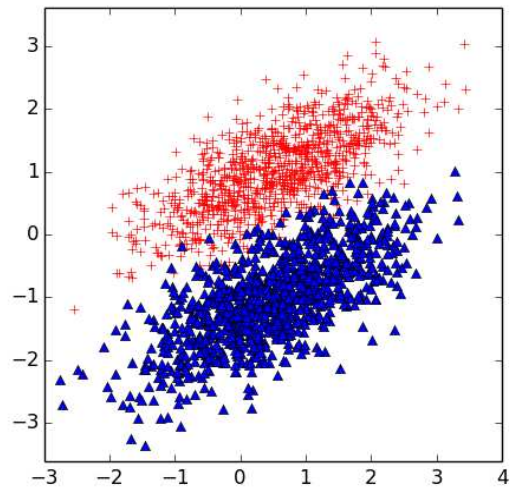
Suppose you have the nearby training set with one real-valued input  $X$  and a categorical output  $Y$  that has two values.

$X$	$Y$
0	$A$
2	$A$
3	$B$
4	$B$
5	$B$
6	$B$
7	$B$

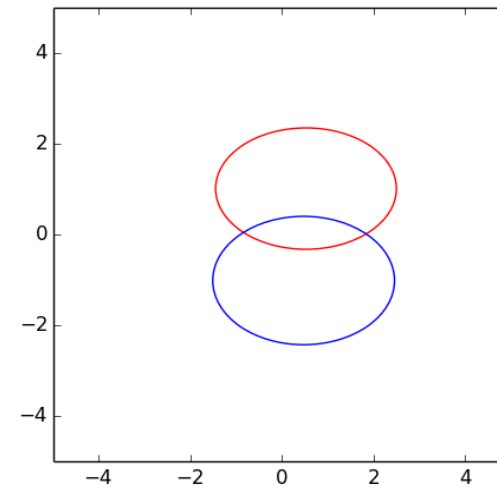
a. You must learn from this data the parameters of the Gaussian Bayes classifier. Write your answer in the following table.

$\mu_A =$	$\sigma_A^2 =$	$P(Y = A) =$
$\mu_B =$	$\sigma_B^2 =$	$P(Y = B) =$

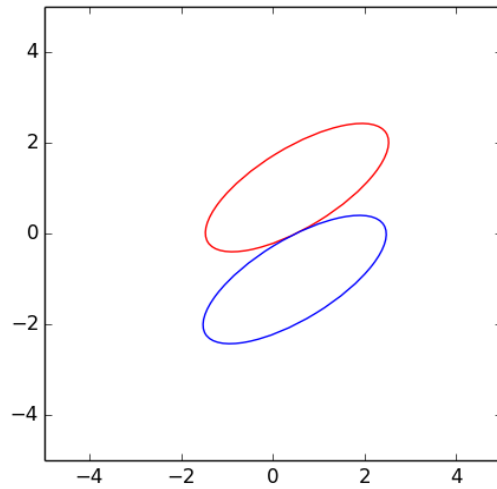
- b. Using the notation  $\alpha = p(X = 2|Y = A)$  and  $\beta = p(X = 2|Y = B)$ ,
- What is  $p(X = 2, Y = A)$ ? (Answer in terms of  $\alpha$ .)
  - What is  $p(X = 2, Y = B)$ ? (Answer in terms of  $\beta$ .)
  - What is  $p(X = 2)$ ? (Answer in terms of  $\alpha$  and  $\beta$ .)
  - What is  $p(Y = A|X = 2)$ ? (Answer in terms of  $\alpha$  and  $\beta$ .)
  - How would the point  $X = 2$  be classified by the Gaussian Bayes algorithm? (Answer in terms of  $\alpha$  and  $\beta$ .)



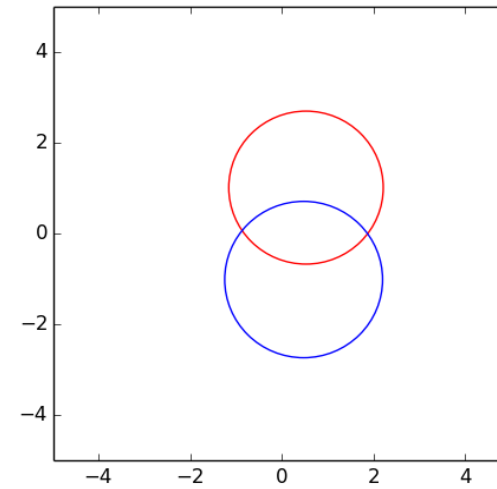
(A) Data



(B)



(C)



(D)

### Solution:

- a. (C) is the truth.
- b. (B) corresponds to the Gaussian Naive Bayes estimates. [LC: Here follows the explanation:]  
Because the Gaussian Naive Bayes model assume independence of the two features conditioned on the class label, the estimated model should be aligned with the axes. Both (B) and (D) satisfy this, but only in (B) the width and height of the oval, which are proportional to the standard deviation of each axis, matched the data.
- c. (C) gives the lowest training error.

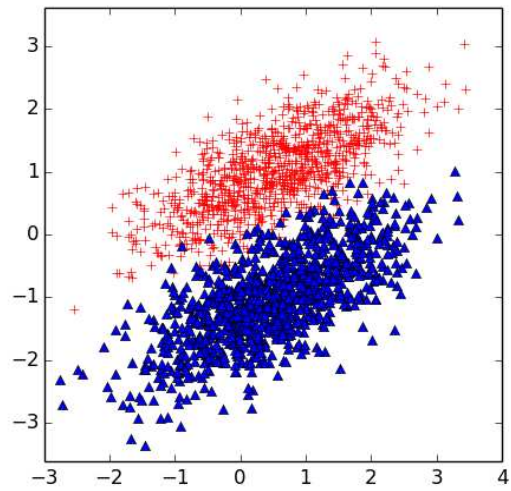
Exemplifying the Gaussian [Naive] Bayes algorithm on data from  $\mathbb{R}^2$

CMU, 2014 fall, W. Cohen, Z. Bar-Joseph, HW2, pr. 5.c

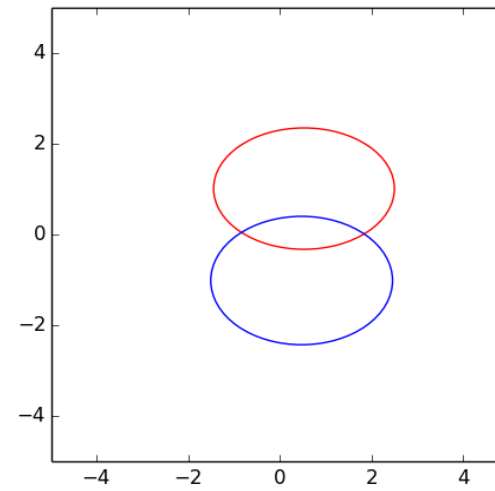


In a two dimensional case, we can visualize how Gaussian Naive Bayes behaves when input features are correlated. A data set is shown in Figure (A), where red points are in Class 0, blue points are in Class 1. The conditional distributions are two-dimensional Gaussians. In (B), (C) and (D), the ellipses represent conditional distributions for each class. The centers of ellipses show the means, and the contours show the boundary of two standard deviations.

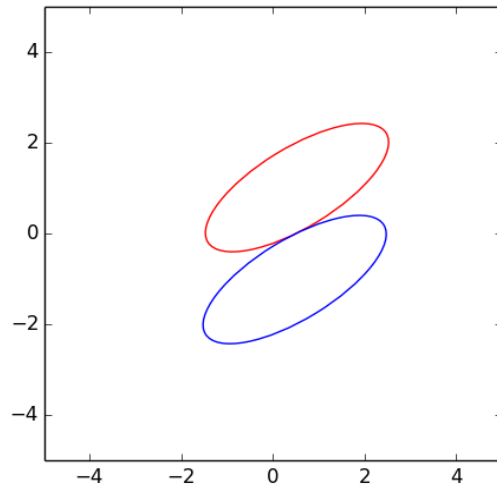
- a. Which of them is most likely to be the true conditional distribution?
- b. Which of them is most likely to be estimates by a Gaussian Naive Bayes model?
- c. If we assume the prior probabilities for both classes are equal, which model will achieve a higher accuracy on the training data?



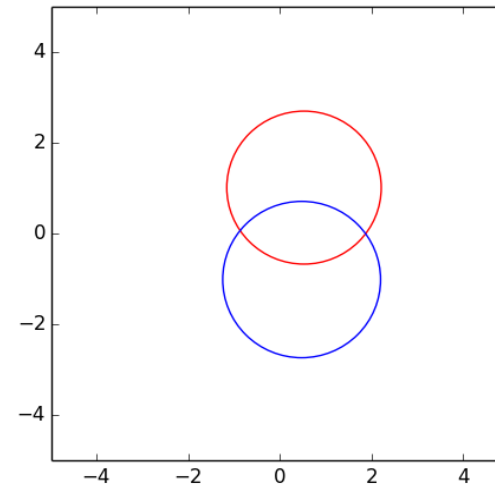
(A) Data



(B)



(C)



(D)

### Solution:

- a. (C) is the truth.
- b. (B) corresponds to the Gaussian Naive Bayes estimates. [LC: Here follows the explanation:]  
Because the Gaussian Naive Bayes model assume independence of the two features conditioned on the class label, the estimated model should be aligned with the axes. Both (B) and (D) satisfy this, but only in (B) the width and height of the oval, which are proportional to the standard deviation of each axis, matched the data.
- c. (C) gives the lowest training error.

**Estimating the parameters for  
Gaussian Naive Bayes and Full/Joint Gaussian Naive Bayes algorithms**

CMU, 2014 fall, W. Cohen, Z. Bar-Joseph, HW2, pr. 5.ab

Consider a Gaussian Naive Bayes model, where the conditional distribution of each feature is a one-dimensional Gaussian,  $X^{(j)}|Y \sim N(\mu_Y^{(j)}, (\sigma_Y^{(j)})^2)$ ,  $j = 1, \dots, d$ .

a. Given  $n$  independent training data points,  $\{(X_1, Y_1), \dots, (X_n, Y_n)\}$ , give a maximum-likelihood estimate (MLE) of the conditional distribution of feature  $X^{(j)}$ ,  $j = 1, \dots, d$ .

**Solution:**

**The likelihood of the samples in Class 0 is**

$$\begin{aligned} L(X_{i,0}^{(j)} | \mu_0^{(j)}, (\sigma \mu_0^{(j)})^2) &= \prod_{i=1}^{n_0} \frac{1}{\sqrt{2\pi} \sigma_0^{(j)}} \exp \left( -\frac{(X_{i,0}^{(j)} - \mu_0^{(j)})^2}{2(\sigma_0^{(j)})^2} \right) \\ &= \left( \frac{1}{\sqrt{2\pi} \sigma_0^{(j)}} \right)^{n_0} \exp \left( -\sum_{i=1}^{n_0} \frac{(X_{i,0}^{(j)} - \mu_0^{(j)})^2}{2(\sigma_0^{(j)})^2} \right) \end{aligned}$$

**and the log-likelihood is**

$$\ln L = -n_0 \ln \sigma_0^{(j)} - \frac{1}{2(\sigma_0^{(j)})^2} \sum_{i=1}^{n_0} (X_{i,0}^{(j)} - \mu_0^{(j)})^2 + \text{constant}$$

**Taking the partial derivatives of the log-likelihood, we have**

$$\begin{aligned} \frac{\partial \ln L}{\partial \mu_0^{(j)}} = 0 &\Leftrightarrow \sum_{i=1}^{n_0} (X_{i,0}^{(j)} - \mu_0^{(j)}) = 0 \Leftrightarrow \mu_0^{(j)} = \frac{1}{n_0} \sum_{i=1}^{n_0} X_{i,0}^{(j)} \\ \frac{\partial \ln L}{\partial \sigma_0^{(j)}} = 0 &\Leftrightarrow -\frac{n_0}{\sigma_0^{(j)}} + \frac{1}{(\sigma_0^{(j)})^3} \sum_{i=1}^{n_0} (X_{i,0}^{(j)} - \mu_0^{(j)})^2 = 0 \Leftrightarrow (\sigma \mu_0^{(j)})^2 = \frac{1}{n_0} \sum_{i=1}^{n_0} (X_{i,0}^{(j)} - \hat{\mu}_0^{(j)})^2 \end{aligned}$$

**Similarly, one can derive the MLE for the parameters in Class 1.**

b. Suppose the prior of  $Y$  is already given. How many parameters do you need to estimate in Gaussian Naive Bayes model?

**Solution:**

For each class, there are 2 parameters (the mean and variance) for each feature, therefore there are  $2 \cdot 2d = 4d$  parameters for all features in the two classes.

c. In a full/Joint Gaussian Bayes model, we assume that the conditional distribution  $\Pr(X|Y)$  is a multidimensional Gaussian,  $X|Y \sim \mathcal{N}(\mu_Y, \Sigma_Y)$ , where  $\mu \in \mathbb{R}^d$  is the mean vector and  $\Sigma \in \mathbb{R}^{d \times d}$  is the covariance matrix.

Again, suppose the prior of  $Y$  is already given. How many parameters do you need to estimate in a full/Joint Gaussian Bayes model?

**Solution:**

For each class, there are  $d$  parameters for the mean,  $d(d+1)/2$  parameters for the covariance matrix, because the covariance matrix is symmetric. Therefore, the number of parameters is  $2 \cdot (d + d(d+1)/2) = d(d+3)$  in total for the two classes.

## Proving

the relationship between the decision rules for

*Gaussian Naive Bayes* and the *Logistic Regression* algorithm

when the covariance matrices are diagonal and identical

i.e.,  $\sigma_{0i}^2 = \sigma_{1i}^2$  for  $i = 1, \dots, d$

CMU, 2009 spring, Ziv Bar-Joseph, HW2, pr. 2

Assume a two-class ( $Y \in \{0, 1\}$ ) Naive Bayes model over the  $d$ -dimensional real-valued input space  $\mathbb{R}^d$ , where the input variables  $X|Y = 0 \in \mathbb{R}^d$  are distributed as

$$\text{Gaussian}(\mu_0 = \langle \mu_{01}, \dots, \mu_{0d} \rangle, \sigma = \langle \sigma_1, \dots, \sigma_d \rangle)$$

and  $X|Y = 1 \in \mathbb{R}^d$  as

$$\text{Gaussian}(\mu_1 = \langle \mu_{11}, \dots, \mu_{1d} \rangle, \sigma = \langle \sigma_1, \dots, \sigma_d \rangle)$$

i.e., the inputs given the class have different means but identical variance for both classes.



Prove that, given the conditions stated above, the conditional probability  $P(Y = 1|X = x)$ , where  $X = (X_1, \dots, X_d)$  and  $x = (x_1, \dots, x_d)$  can be written in a similar form to Logistic Regression:

$$\frac{1}{1 + \exp(w_0 + w \cdot x)}$$

with the parameters  $w_0 \in \mathbb{R}$  and  $w = (w_1, \dots, w_d) \in \mathbb{R}^d$  chosen in a suitable way.

As a consequence, the decision rule for the Gaussian Bayes classifier supported by this model the decision rule has a linear form.

## Solution

$$\begin{aligned}
 P(Y = 1|X = x) &\stackrel{B.F.}{=} \frac{P(X = x|Y = 1) P(Y = 1)}{\sum_{y' \in \{0,1\}} P(X = x|Y = y') P(Y = y')} \\
 &= \frac{1}{1 + \frac{P(X = x|Y = 0)P(Y = 0)}{P(X = x|Y = 1)P(Y = 1)}} \\
 &= \frac{1}{1 + \exp \left( \ln \frac{P(X = x|Y = 0)P(Y = 0)}{P(X = x|Y = 1)P(Y = 1)} \right)} \\
 &= \frac{1}{1 + \exp \left( \underbrace{\ln \frac{P(X_1 = x_1, \dots, X_d = x_d|Y = 0)P(Y = 0)}{P(X_1 = x_1, \dots, X_d = x_d|Y = 1)P(Y = 1)}}_{\text{exponent}} \right)}
 \end{aligned}$$

$$\begin{aligned}
\text{exponent} & \stackrel{\text{cond. indep.}}{=} \ln \frac{P(Y=0)}{P(Y=1)} + \sum_{i=1}^d \ln \frac{P(X_i=x_i|Y=0)}{P(X_i=x_i|Y=1)} \\
& = \ln \frac{P(Y=0)}{P(Y=1)} + \sum_{i=1}^d \ln \left( \frac{\frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{(x_i-\mu_{i0})^2}{2\sigma_i^2}\right)}{\frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{(x_i-\mu_{i1})^2}{2\sigma_i^2}\right)} \right) \\
& = \ln \frac{P(Y=0)}{P(Y=1)} + \sum_{i=1}^d \left( \frac{(x_i-\mu_{i1})^2}{2\sigma_i^2} - \frac{(x_i-\mu_{i0})^2}{2\sigma_i^2} \right) \\
& = \ln \frac{P(Y=0)}{P(Y=1)} + \sum_{i=1}^d \frac{2x_i(\mu_{0i}-\mu_{1i}) + (\mu_{1i}^2 - \mu_{0i}^2)}{2\sigma_i^2} \\
& = \ln \frac{P(Y=0)}{P(Y=1)} + \sum_{i=1}^d \left( \frac{x_i(\mu_{0i}-\mu_{1i})}{\sigma_i^2} + \frac{(\mu_{1i}^2 - \mu_{0i}^2)}{2\sigma_i^2} \right) \\
& = \underbrace{\ln \frac{P(Y=0)}{P(Y=1)} + \sum_{i=1}^d \frac{(\mu_{1i}^2 - \mu_{0i}^2)}{2\sigma_i^2}}_{w_0} + \sum_{i=1}^d \underbrace{\frac{\mu_{0i}-\mu_{1i}}{\sigma_i^2}}_{w_i} x_i
\end{aligned}$$

**In conclusion,**

$$P(Y = 1|X = x) = \frac{1}{1 + e^{(w \cdot x + w_0)}}$$

**with**

$$w_0 = \ln \frac{P(Y = 0)}{P(Y = 1)} + \sum_{i=1}^d \frac{(\mu_{1i}^2 - \mu_{0i}^2)}{2\sigma_i^2} \text{ and } w_i = \frac{\mu_{0i} - \mu_{1i}}{\sigma_i^2}, i = 1, \dots, d$$

**Note that**

$$P(Y = 0|X = x) = \frac{e^{(w \cdot x + w_0)}}{1 + e^{(w \cdot x + w_0)}}$$

**and**

$$P(Y = 1|X = x) > P(Y = 0|X = x) \Leftrightarrow w \cdot x + w_0 < 0$$

Since the coefficients  $w_i$  for  $i = 1, \dots, d$  do not depend on  $x_i$ , it follows that this *decision rule* of Gaussian Naive Bayes [in the conditions stated in the beginning of this problem] is a linear rule, like in Logistic Regression.

However, this relationship does not mean that there is a one-to-one correspondence between the parameters  $w_i$  of Gaussian Naive Bayes (GNB) and the parameters  $w_i$  of logistic regression (LR) because LR is discriminative and therefore doesn't model  $P(X)$ , while GNB does model  $P(X)$ .

To be more specific, note that the coefficients  $w_i$  in the GNB decision rules should be divided by  $P(x_1, \dots, x_d)$  in order to correspond to  $P(Y = 1|X = x)$ , which means that then they will not anymore be independent of  $x_i$ , like the LR coefficients.

Proving  
the relationship between  
*The full Gaussian Bayes* algorithm and *Logistic Regression*  
when  $\Sigma_0 = \Sigma_1$

CMU, 2011 spring, Tom Mitchell, HW2, pr. 2.2

Let's make the following *assumptions*:

1.  $Y$  is a boolean variable following a Bernoulli distribution, with parameter  $\pi = P(Y = 1)$  and thus  $P(Y = 0) = 1 - \pi$ .
2.  $X = \langle X_1, X_2, \dots, X_n \rangle$  is a vector of random variables *not* conditionally independent given  $Y$ , and  $P(X|Y = k)$  follows a *multivariate normal distribution*  $N(\mu_k, \Sigma)$ .

Note that  $\mu_k$  is the  $n \times 1$  mean vector depending on the value of  $Y$ , and  $\Sigma$  is the  $n \times n$  covariance matrix, which does not depend on  $Y$ . We will write/use the density of the multivariate normal distribution in vector/matrix notation.

$$\mathcal{N}(x; \mu, \Sigma) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} \exp \left( -\frac{1}{2} (x - \mu)^\top \Sigma^{-1} (x - \mu) \right)$$

Is the form of  $P(Y|X)$  implied by such this [not-so-naive] Gaussian Bayes classifier [LC: similar to] the form used by logistic regression?

Derive the form of  $P(Y|X)$  to prove your answer.

We start with:

$$\begin{aligned}
 P(Y = 1|X) &= \frac{P(X|Y = 1) P(Y = 1)}{P(X|Y = 1) P(Y = 1) + P(X|Y = 0) P(Y = 0)} \\
 &= \frac{1}{1 + \frac{P(Y = 0) P(X|Y = 0)}{P(Y = 1) P(X|Y = 1)}} = \frac{1}{1 + \exp\left(\ln \frac{P(Y = 0) P(X|Y = 0)}{P(Y = 1) P(X|Y = 1)}\right)} \\
 &= \frac{1}{1 + \exp\left(\ln \frac{P(Y = 0)}{P(Y = 1)} + \ln \frac{P(X|Y = 0)}{P(X|Y = 1)}\right)}
 \end{aligned}$$

Next we will focus on the term  $\ln \frac{P(X|Y = 0)}{P(X|Y = 1)}$ :

$$\ln \frac{P(X|Y = 0)}{P(X|Y = 1)} = \ln \frac{\frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}}}{\frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}}} + \ln \exp[(\star)] = \ln \exp[(\star)] = (\star)$$

where  $(\star)$  is the formulation obtained as the difference between the exponential parts of two multivariate Gaussian densities  $P(X|Y = 0)$  and  $P(X|Y = 1)$ .



$$\begin{aligned}
(\star) &= \frac{1}{2}[(X - \mu_1)^\top \Sigma^{-1}(X - \mu_1) - (X - \mu_0)^\top \Sigma^{-1}(X - \mu_0)] \\
&= (\mu_0^\top - \mu_1^\top) \Sigma^{-1} X + \frac{1}{2} \mu_1^\top \Sigma^{-1} \mu_1 - \frac{1}{2} \mu_0^\top \Sigma^{-1} \mu_0
\end{aligned}$$

As a result, we have:

$$\begin{aligned}
P(Y = 1|X) &= \frac{1}{1 + \exp \left( \ln \frac{1 - \pi}{\pi} + \frac{1}{2} \mu_1^\top \Sigma^{-1} \mu_1 - \frac{1}{2} \mu_0^\top \Sigma^{-1} \mu_0 + (\mu_0^\top - \mu_1^\top) \Sigma^{-1} X \right)} \\
&= \frac{1}{1 + \exp(w_0 + w^\top X)}
\end{aligned}$$

where  $w_0 = \ln \frac{1 - \pi}{\pi} + \frac{1}{2} \mu_1^\top \Sigma^{-1} \mu_1 - \frac{1}{2} \mu_0^\top \Sigma^{-1} \mu_0$  is a scalar,  
and  $w = \Sigma^{-1}(\mu_0 - \mu_1)$  is a  $d \times 1$  a parameter vector.

**Note that**  $((\mu_0^\top - \mu_1^\top) \Sigma^{-1})^\top = ((\mu_0 - \mu_1)^\top \Sigma^{-1})^\top = (\Sigma^{-1})^\top ((\mu_0 - \mu_1)^\top)^\top = \Sigma^{-1}(\mu_0 - \mu_1)$  **because**  $\Sigma^{-1}$  **is symmetric.**

( $\Sigma$  is symmetric because it is a covariance matrix, and therefore  $\Sigma^{-1}$  is also symmetric.)

In conclusion,  $P(Y|X)$  has the form of the logistic regression (in vector and matrix notation).