# Lecture 4: Probability and Bayesian Classifier

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- A key concept in the field in machine learning is that of uncertainty
  - Through noise on measurements
  - Through the finite size of data sets
- Probability theory provides a consistent framework for the quantification and manipulation of uncertainty
- Forms one of the central foundations for pattern recognition.

## Kolmogorov's Axioms of Probability (1933)

 To each sentence a, a numerical degree of belief between 0 and 1 is assigned

$$0 \le p(a) \le 1$$
  
  $p(true)=1, p(false)=0$ 

• The probability of disjunction is given by

$$p(a \lor b) = p(a) + p(b) - p(a \land b)$$

## Where do these numerical degrees of belief come from?

- Humans can *believe* in a subjective viewpoint from *experience*. This approach is called **Bayesian**
- For a finite sample we can estimate the true fraction. We count the *frequency* of an event in a *sample*. We do not know the true value because we cannot access the whole population of events. This approach is called **frequentist**
- From the true nature of the universe, for example, for a fair coin, the probability of heads is 0.5. This approach is related to the **Platonic** world of ideas. However, we can never verify whether a fair coin exists

- From the frequentist approach, one can determine the probability of an event a by counting
- If  $\Omega$  is the set of all possible events,  $p(\Omega) = 1$ , then  $\alpha \in \Omega$ .
- $card(\Omega)$  is the number of elements of the set  $\Omega$ , card(a) is the number of elements of the set a and

$$p(a) = \frac{card(a)}{card(\Omega)}$$

$$p(a \wedge b) = \frac{card(a \wedge b)}{card(\Omega)}$$

 Now we can define the posterior probability, the probability of a after the evidence b is obtained

$$p(a|b) = \frac{card(a \land b)}{card(b)}$$

using

$$p(a \wedge b) = \frac{card(a \wedge b)}{card(\Omega)}$$

• we get

$$p(a|b) = \frac{p(a \land b)}{p(b)}$$
  $p(b|a) = \frac{p(a \land b)}{p(a)}$ 

## Bayes' Rule

$$p(a|b) = \frac{p(a \land b)}{p(b)} \qquad p(b|a) = \frac{p(a \land b)}{p(a)}$$

The Bayes' rule follows from both equations

$$p(b|a) = \frac{p(a|b) \cdot p(b)}{p(a)}$$

## Law of Total Probability

• For mutually exclusive events  $b_1, ..., b_n$  with

$$\sum_{i=1}^{n} p(b_i) = 1$$

• the law of total probability is represented by

$$p(a) = \sum_{i=1}^{n} p(a) \wedge p(b_i) = \sum_{i=1}^{n} p(a, b_i)$$

$$p(a) = \sum_{i=1}^{n} p(a|b_i) \cdot p(b_i)$$

## The Rules of Probability

Sum Rule

$$p(X) = \sum_{Y} p(X, Y)$$

**Product Rule** 

$$p(X,Y) = p(Y|X)p(X)$$



## Bayes' Rule

$$p(a|b) = \frac{p(a \land b)}{p(b)} \qquad p(b|a) = \frac{p(a \land b)}{p(a)}$$

The Bayes' rule follows from both equations

$$p(b|a) = \frac{p(a|b) \cdot p(b)}{p(a)}$$

## Reverent Thomas Bayes (1702-1761)



- He set down his findings on probability in "Essay Towards Solving a Problem in the Doctrine of Chances" (1763), published posthumously in the Philosophical Transactions of the Royal Society of London.
  - The drawing after a portrait of Bayes used in a 1936 book, it is not known if the portrait is actually representing him.

## Bayes' Rule

$$p(h_k|D) = \frac{p(D|h_k) \cdot p(h_k)}{p(D)} = \frac{p(D, h_k)}{p(D)}$$

- $p(h_k)$  is called the **prior** (before)
  - For example, what is the probability of some illness in Portugal
- $p(D|h_k)$  is called **likelihood** and can can be easily estimated
  - For example, what is the probability that some illness generates some symptoms?
  - $p(D,h_k)$  is called **joint distribution**
- $p(h_k|D)$  is called **posterior probability**

## Bayes' Rule

$$p(h_k|D) = \frac{p(D|h_k) \cdot p(h_k)}{p(D)} = \frac{p(D, h_k)}{p(D)}$$

- Bayes rule can be used to determine the total posterior probability  $p(h_k|D)$  of hypothesis  $h_k$  given data D
  - For example, what is the probability that some illness is present?
- The most probable hypothesis  $h_k$  out of a set of possible hypothesis  $h_1$ ,  $h_2$ ,  $\cdots$  given some present data is according to the Bayes rule

## Maximum a Posteriori (MAP) Hypothesis

•  $p(h_k|D)$  and  $p(D,h_k)$  are related in a linear manner  $p(h_k|D) \propto p(D|h_k) \cdot p(h_k)$ posterior  $\propto$  likelihood  $\times$  prior

 $\bullet$  to determine the  $maximum\ posteriori\ hypothesis\ h_{MAP}$  we maximize

$$h_{MAP} = \arg\max_{h_k} \frac{p(D|h_k) \cdot p(h_k)}{p(D)}$$

• we can see, the maximization is independent of p(D), it follows

$$h_{MAP} = \arg\max_{h_k} p(D|h_k) \cdot p(h_k)$$

## Maximum Likelihood (ML) hypothesis

- If we assume  $p(h_k) = p(h_v)$  for all  $h_k$  and  $h_v$ , then we can further
- simplify, and choose the maximum likelihood (ML) hypothesis

$$h_{ML} = \arg\max_{h_k} p(D|h_k)$$

## Bayesian Interpretation

- In the Bayesian (or epistemological) interpretation, probability measures a "degree of belief" and Bayes' rule links the degree of belief in a proposition before and after accounting for evidence
- with prior probability  $p(h_k)$
- $p(D|h_k)$  represents the likelihood of the data D if we assume  $h_k$  to be true
  - if we, in fact, observe D, we can update our belief about  $h_k$  through the rule

$$p(h_k|D) = \frac{p(D|h_k) \cdot p(h_k)}{p(D)}$$

## Bayesian Interpretation and bias

Objective likelihood is biased by the prior belief

posterior  $\propto$  likelihood  $\times$  prior= likelihood  $\times$  bias

- Bias is a disproportionate weight in favor of or against an idea or thing, usually in a way that is closed-minded, prejudicial, or unfair.
- Biases can be innate or learned. People may develop biases for or against an individual, a group, or a belief.

### Cancer screening

- Cancer screening aims to detect cancer before symptoms appear
- This may involve for example a blood test.
- Suppose that a patient tests positive...
- The test is secure because in **99** percent of the cases the test returns a correct positive result (= positive) in which a rare form of cancer is actually present.
- Should the doctor tell the patient, that he has cancer?

- The test has correct negative result (= negative) in 99 percent of the cases where the rare form of cancer is not present
- It is also known that 0.001 of the entire population have the rare form of cancer (h = cancer)
- p(cancer) = 0.001,  $p(\neg cancer) = 0.999$
- p(positive | cancer) = 0.99,  $p(positive | \neg cancer) = 0.01$ ,
- p(negative | cancer) = 0.01,  $p(negative | \neg cancer) = 0.99$

• We determine  $h_{map}$  according to the linear relation

posterior ∝ likelihood × prior

 $p(cancer|positive) \propto p(positive|cancer) \cdot p(cancer) = 0.99 \cdot 0.001$  $p(\neg cancer|positive) \propto \cdot p(positive|\neg cancer) \cdot p(\neg cancer) = 0.01 \cdot 0.999$ 

It follows

$$h_{map} = \neg cancer$$

 $p(cancer|positive) \propto p(positive|cancer) \cdot p(cancer) = 0.99 \cdot 0.001$  $p(\neg cancer|positive) \propto \cdot p(positive|\neg cancer) \cdot p(\neg cancer) = 0.01 \cdot 0.999$ 

It follows

$$h_{map} = \neg cancer$$

- So, despite the positive result, we are still more confident that the patient is healthy than otherwise.
- The right thing to do would be to another test to try to accumulate more evidence in favor of the hypothesis that patient has the disease.

 $p(positive, cancer) = p(positive | cancer) \cdot p(cancer) = 0.99 \cdot 0.001$  $p(positive, \neg cancer) = p(positive | \neg cancer) \cdot p(\neg cancer) = 0.01 \cdot 0.999$ 

$$p(positive | cancer) = \frac{p(positive, cancer)}{p(positive, cancer) + p(positive, \neg cancer)}$$

*law of total probability:*  $p(positive) = p(positive, cancer) + p(positive, \neg cancer)$ 

$$p(positive | cancer) = \frac{p(positive | cancer) \cdot p(cancer)}{p(positive)}$$

## Estimating p(h)

Let us draw some principles to estimate

$$p(h_k|D) = \frac{p(D|h_k) \cdot p(h_k)}{p(D)}$$

- Let us first start with p(h)
  - given no prior knowledge that one hypothesis is more likely than another
    - p(h) can be uniformly distributed

$$\forall_{h \in H} \ p(h) = \frac{1}{|H|}$$

otherwise, estimate the prior base on the observed frequency

## Estimating p(D|h)

- What choice shall we make for P(D|h)?
  - Hypothesis generates data....
  - If data is **discrete**:
  - we use the frequentist approach
    - e.g. I observe 2 out of 10 individuals with blue eyes and brown in shift A and 1 out of 8 in shift B, then
    - $p(\mathbf{x} = [blue\ eyes, brown]|A) = 0.2$  and
    - $p(\mathbf{x} = [blue\ eyes, brown]|B) = 0.125$

#### Bayesian optimal classifier

 What is the most probable classification of the new instance given the training data?

$$h_{MAP} = \arg\max_{h} p(h|\mathbf{x}_{new}) = \arg\max_{h} \frac{p(\mathbf{x}_{new}|h)p(h)}{p(\mathbf{x}_{new})} = \arg\max_{h} p(\mathbf{x}_{new}|h)p(h)$$

... where the hypotheses correspond to our classes

- we ignore the denominator as it does not alter decision
- The Bayesian classifier has as many parameter as:
  - the number of priors minus 1
    - we can deduce one prior from the remaining ones
    - e.g. given  $h_1$ ,  $h_2$  and  $h_3$ ,  $p(h_3) = 1 p(h_2) p(h_1)$
  - the number of parameters associated with the class-conditional distributions,  $p(\mathbf{x}|h)$

#### Bayesian optimal classifier: example

#### Priors

• 
$$p(c=0) = \frac{card(c=0)}{card(\Omega)} = \frac{3}{7}$$
,  $p(c=1) = 1 - p(c=0) = \frac{4}{7}$ 

#### Joint Probability

• 
$$p(v_1 = 0, v_2 = A, v_3 = 0, c = 0) = \frac{card(v_1 = 0, v_2 = A, v_3 = 0, c = 0)}{card(\Omega)} = \frac{1}{7}$$

	$\mathbf{v}_1$	$\mathbf{v}_2$	$\mathbf{v}_3$	class
$x_1$	1	C	1	1
$x_2$	1	С	1	0
$\chi_3$	0	В	1	0
$\chi_4$	0	Α	0	0
$\chi_5$	1	С	1	1
<i>x</i> <sub>6</sub>	0	В	1	1
<i>X</i> <sub>7</sub>	0	Α	0	1

• 
$$p(v_1 = 0, v_2 = A, v_3 = 0 | c = 0) = \frac{1}{3} = \frac{card(v_1 = 0, v_2 = A, v_3 = 0, c = 0)}{card(c = 0)} = \frac{1}{3} = \frac{p(v_1 = 0, v_2 = A, v_3 = 0, c = 0)}{p(c = 0)} = \frac{\frac{1}{7}}{\frac{3}{7}} = \frac{1}{3}$$

Data Joint

• 
$$p(v_1 = 0, v_2 = A, v_3 = 0) = \frac{card(v_1 = 0, v_2 = A, v_3 = 0, c = 0)}{card(\Omega)} = \frac{2}{7}$$

• Data: law of total probability

• 
$$p(v_1 = 0, v_2 = A, v_3 = 0) = p(v_1 = 0, v_2 = A, v_3 = 0, c = 0) + p(v_1 = 0, v_2 = A, v_3 = 0, c = 1) = \frac{1}{7} + \frac{1}{7}$$

Posterior

• 
$$p(c = 0|v_1 = 0, v_2 = A, v_3 = 0) = \frac{p(v_1 = 0, v_2 = A, v_3 = 0|c = 0)p(c = 0)}{p(v_1 = 0, v_2 = A, v_3 = 0)} = \frac{\frac{3}{7} + \frac{1}{7}}{\frac{2}{7}} = \frac{\frac{1}{7}}{\frac{2}{7}} = \frac{1}{2}$$

#### Bayesian optimal classifier: example

	$\mathbf{v}_1$	<b>v</b> <sub>2</sub>	<b>v</b> 3	class
$x_1$	1	С	1	1
$x_2$	1	С	1	0
<i>X</i> <sub>3</sub>	0	В	1	0
$\chi_4$	0	Α	0	0
$\chi_{5}$	1	С	1	1
$x_6$	0	В	1	1
<i>x</i> <sub>7</sub>	0	Α	0	1

• We can "classify" new observations in the same way, e.g.  $\mathbf{x}_{\text{new}} = [1, \text{C}, 1]$ , what is the class,  $\mathbf{c} = 0$  or  $\mathbf{c} = 1$ ?

• 
$$p(c = 1, v_1 = 1, v_2 = C, v_3 = 1) = p(v_1 = 1, v_2 = C, v_3 = 1 | c = 1)p(c = 1) = \frac{2}{7}$$

• 
$$p(c = 0, v_1 = 1, v_2 = C, v_3 = 1) = p(v_1 = 1, v_2 = C, v_3 = 1 | c = 0)p(c = 0) = \frac{1}{7}$$

• 
$$p(c = 1, v_1 = 1, v_2 = C, v_3 = 1) > p(c = 0, v_1 = 1, v_2 = C, v_3 = 1)$$

#### **x**<sub>new</sub> is classified with class 1

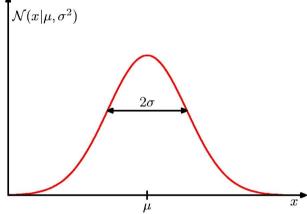
• 
$$p(c = 1 | v_1 = 1, v_2 = C, v_3 = 1) = \frac{p(c=1, v_1=1, v_2=C, v_3=1)}{p(v_1=1, v_2=C, v_3=1)} = \frac{\frac{2}{7}}{\frac{2}{7}} = \frac{2}{3}$$

• 
$$p(c = 0 | v_1 = 1, v_2 = C, v_3 = 1) = \frac{p(c=0, v_1=1, v_2=C, v_3=1)}{p(v_1=1, v_2=C, v_3=1)} = \frac{\frac{7}{7}}{\frac{3}{7}} = \frac{1}{3}$$

• 
$$p(c = 1 | v_1 = 1, v_2 = C, v_3 = 1) + p(c = 1 | v_1 = 1, v_2 = C, v_3 = 0) = 1$$

## Estimating p(D|h)

- If data is **real-valued**:
- We can use Probability Density Function of the Normal distribution
- Is this correct? **No...** 
  - We assume relative probability is real probability
    - However, we do it because it is simple
    - Error for many data points small

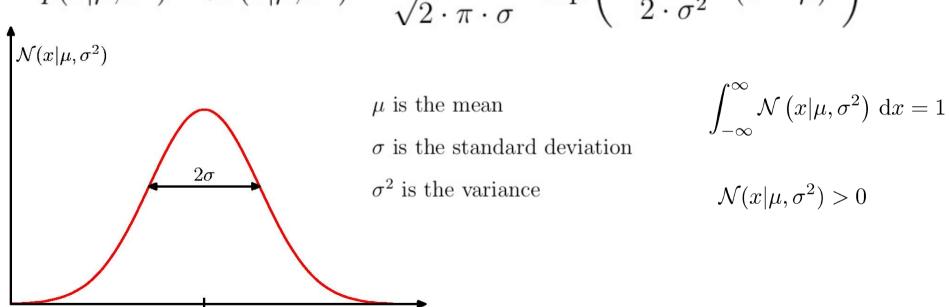


- How do we know that the data is described by Normal distribution?
- This assumption can be wrong!

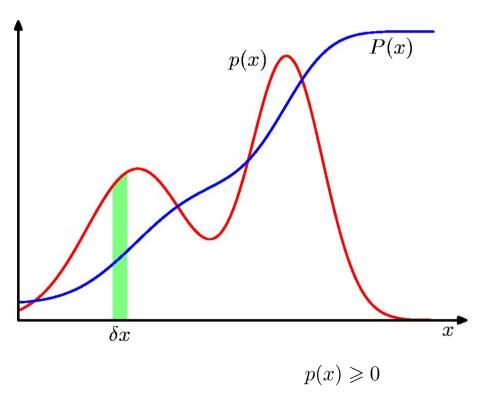
#### Gaussian Distribution

Gaussian distribution or normal is defined by the probability

$$p(x|\mu,\sigma^2) = \mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2 \cdot \pi} \cdot \sigma} \cdot \exp\left(-\frac{1}{2 \cdot \sigma^2} \cdot (x-\mu)^2\right)$$



## Probability Density Function (PDF)



$$p(x \in (a,b)) = \int_{a}^{b} p(x) \, \mathrm{d}x$$

$$P(z) = \int_{-\infty}^{z} p(x) \, \mathrm{d}x$$

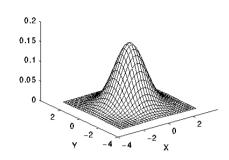
Cumulative distribution function (CDF)

$$\int_{-\infty}^{\infty} p(x) \, \mathrm{d}x = 1$$

## Relative Probability

- Gaussian distribution is a type of continuous probability distribution for a real-valued random variable.
- The Gaussian distribution or normal distribution is defined as PDF (Probability Density Function) that reflects the relative probability.
- The **PDF may give a value greater than one** (small standard deviation).
- It is the area under the curve that represents the probability. However, the PDF reflects the relative probability.
  - Does a continuous probability distribution exist in the real world?

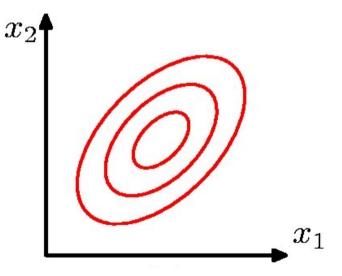
#### Normal Distribution in D dim

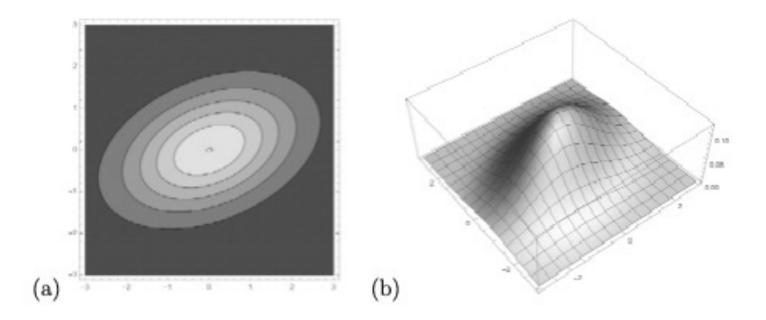


Over D dimensional space

$$p(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2 \cdot \pi)^{D/2}} \cdot \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \cdot \exp\left(-\frac{1}{2} \cdot (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} \cdot (\mathbf{x} - \boldsymbol{\mu})\right)$$
 where

- $\bullet$   $\mu$  is the D dimensional mean vector
- $\Sigma$  is a  $D \times D$  covariance matrix
- $|\Sigma|$  is the determinant of  $\Sigma$





• (a) The Gaussian distribution over 2 dimensional space with  $\mu$  =  $(0, 0)^T$  and the covariance matrix  $\Sigma$ 

$$\Sigma = \left(\begin{array}{cc} 2 & 0.5 \\ 0.5 & 1 \end{array}\right).$$

• (b) Three dimensional plot of the Gaussian.

#### Covariance Matrix

• A position  $c_{ij} = \Sigma_{ij}$  of this matrix measures the tendency of two features,  $x_i$  and  $x_j$ , to vary in the same direction, for N features indexed by k

$$c_{ij} = \frac{\sum_{k=1}^{N} (x_{k,i} - \overline{x_i}) \cdot (x_{k,j} - \overline{x_j})}{N - 1}$$

- with  $\overline{x_i}$  and  $\overline{x_i}$  being the arithmetic mean of the two variables of the sample
- Covariances are symmetric;  $c_{ij} = c_{ji}$  and, so, the resulting covariance matrix  $\Sigma$  is symmetric and positive-definite

$$\Sigma = \left( egin{array}{cccc} c_{11} & c_{12} & \cdots & c_{1m} \\ c_{21} & c_{22} & \cdots & c_{2m} \\ dots & dots & \ddots & dots \\ c_{m1} & c_{m2} & \cdots & c_{mm} \end{array} 
ight)$$

#### Multivariate Gaussian: example

Approximate a multivariate Gaussian distribution using the following points:  $\{(-2,2)^T, (-1,3)^T, (0,1)^T, (-2,1)^T\}$ 

• 
$$\mu = \frac{1}{4} \left( \begin{bmatrix} -2 \\ 2 \end{bmatrix} + \begin{bmatrix} -1 \\ 3 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \begin{bmatrix} -2 \\ 1 \end{bmatrix} \right) = \begin{bmatrix} -1.25 \\ 1.75 \end{bmatrix}$$

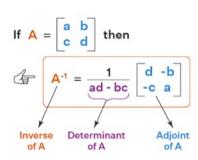
• 
$$c_{12} = c_{21} = \frac{(-2+1.25)(2-1.75)+(-1+1.25)(3-1.75)+(0+1.25)(1-175)+(-2+1.25)(1-1.75)}{3} = -0.83$$

• 
$$c_{11} = \frac{(-2+1.25)^2 + (-1+1.25)^2 + (0+1.25)^2 + (-2+1.25)^2}{3} = 0.92$$

• 
$$c_{22} = \frac{(2-1.75)^2 + (3-1.75)^2 + (1-175)^2 + (1-1.75)^2}{3} = 0.92$$

• 
$$\Sigma = \begin{pmatrix} c_{11} & c_{21} \\ c_{12} & c_{22} \end{pmatrix} = \begin{pmatrix} 0.92 & -0.083 \\ -0.083 & 0.92 \end{pmatrix}$$
.

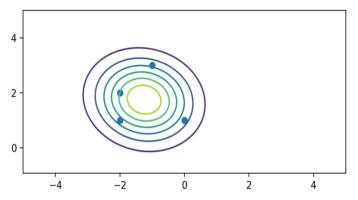
• 
$$\Sigma^{-1} = \begin{pmatrix} 1.1 & 0.1 \\ 0.1 & 1.1 \end{pmatrix}$$
. Det $(\Sigma) = |\Sigma| = 0.833$ Type equation here.



$$N(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{2/2}\sqrt{0.083}} exp\left(-\frac{1}{2} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} - \begin{bmatrix} -1.25 \\ 1.75 \end{pmatrix}^T \begin{bmatrix} 1.1 & 0.1 \\ 0.1 & 1.1 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} - \begin{bmatrix} -1.25 \\ 1.75 \end{bmatrix} \right)$$

#### Multivariate Gaussian: example

- What is the shape of the previous 2-dimensional Gaussian?
  - fixing  $\mu$  and  $\Sigma$  inspection...



What is the probability of observing (0,0)?

• 
$$N\left(\begin{bmatrix}0\\0\end{bmatrix} \mid \mu, \Sigma\right) = \frac{1}{2\pi\sqrt{0.083}} exp\left(-\frac{1}{2}\left(\begin{bmatrix}0\\0\end{bmatrix} - \begin{bmatrix}-1.25\\1.75\end{bmatrix}\right)^T \begin{bmatrix}1.1 & 0.1\\0.1 & 1.1\end{bmatrix}\left(\begin{bmatrix}0\\0\end{bmatrix} - \begin{bmatrix}-1.25\\1.75\end{bmatrix}\right)\right) = 0.0145$$

#### Bayesian optimal classifier: example

- Consider a population of 100 individuals
  - 30 individuals have phenotype A, 30 have B, and remaining ones have C
  - the expression of three genes (variables) are characterized by the following 3-dimensional Gaussians

$$N_{A}\left(\mu_{A} = \begin{bmatrix} 0.375 \\ 0.875 \\ 0.25 \end{bmatrix}, \Sigma_{A} = \begin{bmatrix} 3.41 & 1.34 & 2.6 \\ 1.34 & 2.125 & 1.18 \\ 2.6 & 1.18 & 2.8 \end{bmatrix}\right), N_{B}\left(\mu_{B} = \begin{bmatrix} 0.5 \\ 0.125 \\ 0.875 \end{bmatrix}, \Sigma_{B} = \begin{bmatrix} 0.286 & 0.07 & -0.07 \\ 0.07 & 0.125 & 0.018 \\ -0.07 & 0.018 & 0.125 \end{bmatrix}\right), N_{C}\left(\mu_{C} = \begin{bmatrix} 0 \\ -0.125 \\ 0.125 \end{bmatrix}, \Sigma_{C} = \begin{bmatrix} 1.7 & 1.14 & 1 \\ 1.14 & 1.55 & 0.73 \\ 1 & 0.73 & 0.98 \end{bmatrix}\right)$$

$$p(A) = \frac{30}{100}, p(B) = \frac{30}{100}, p(C) = \frac{40}{100}, \text{ prior, called mixture parameters}$$

**classify** observations  $\mathbf{x}_1 = [0, 1.1, -0.8]$ 

$$p(\mathbf{x}_{1}|N_{A})=0.019. \quad p(\mathbf{x}_{1}|N_{B})=5.4E-14. \quad p(\mathbf{x}_{1}|N_{C})=0.0088$$

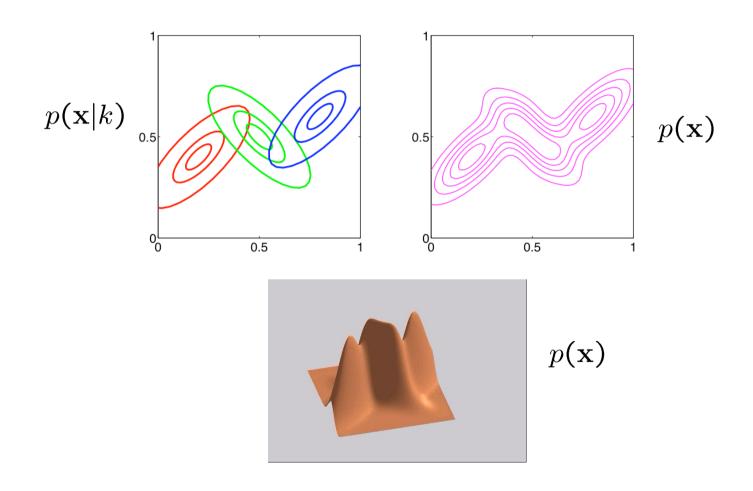
$$p(\mathbf{x}_{1},N_{A})=p(A)p(\mathbf{x}_{1}|N_{A}), \quad p(x,N_{B})=p(B)p(\mathbf{x}_{1}|N_{B}), \quad p(\mathbf{x}_{1},N_{C})=p(C)p(\mathbf{x}_{1}|N_{C})$$

$$p(\mathbf{x}_{1})=p(\mathbf{x}_{1},N_{A})+p(x,N_{B})+p(\mathbf{x}_{1},N_{C})$$

• 
$$p(A|\mathbf{x}_1) = \frac{p(A)p(\mathbf{x}_1|N_A)}{p(\mathbf{x}_1)} = \frac{0.0057}{0.0057 + 0 + 0.0035} = 0.619565, p(B|\mathbf{x}_1) = \frac{p(B)p(\mathbf{x}_1|N_B)}{p(\mathbf{x}_1)} = \frac{0}{0.0057 + 0 + 0.0035} = 0,$$
  
•  $p(C|\mathbf{x}_1) = \frac{p(C)p(\mathbf{x}_1|N_C)}{p(\mathbf{x}_1)} = \frac{0.0035}{0.0057 + 0 + 0.0035} = 0.380435$ 

 $\mathbf{x}_1$  is classified with phenotype A

# Example: Mixture of 3 Gaussians k



### Bayes optimal classifier

#### Advantages

- when data distributions are well-approximated, provides highly accurate results
- priors can be easily neglected to not bias posteriors

#### Disadvantages

- requires a good amount of data to estimate joint distributions
  - impracticable in the presence of high-dimensional data
- can be computationally **expensive** 
  - discrete data: need to compute the posterior probability for every hypothesis
  - numeric data: need to approximate distributions
    - e.g. fitting multivariate Gaussians can be expensive due covariance matrix inversion

#### Joint distribution

- A joint distribution for toothache, cavity, catch, *dentist's probe catches in my tooth*  $\otimes$ 
  - we need to know the conditional probabilities of the conjunction of toothache and cavity
  - what can a dentist conclude if the probe catches in the aching tooth?

$$P(cavity \mid toothache \land catch) = \frac{P(toothache \land catch \mid cavity)P(cavity)}{P(toothache \land cavity)}$$

#### Problem?

• For n possible variables there are  $2^n$  possible combinations

	toothache		no toothache	
	catch	no catch	catch	no catch
cavity	0.108	0.012	0.072	0.008
no cavity	0.016	0.064	0.144	0.576

## Conditional independence

 Once we know that the patient has cavity we do not expect the probability of the probe catching to depend on the presence of toothache

```
• independence P(catch | cavity \land toothache) = P(catch | cavity)

P(toothache | cavity \land catch) = P(toothache | cavity)
```

 The decomposition of large probabilistic domains into weakly connected subsets via conditional independence is one of the most important developments in the recent history of AI

```
P(a \land b) = P(a)P(b)

P(toothache, catch, cavity, Weather = cloudy) = P(a \mid b) = P(a)

= P(Weather = cloudy)P(toothache, catch, cavity) P(b \mid a) = P(b)
```

## Naive Bayes Classifier

 Along with decision trees, neural networks, nearest neighbor, one of the most practical learning methods

- When to use:
  - Moderate or large training set available
  - Attributes that describe instances are conditionally independent given classification
- Successful applications:
  - Diagnosis
  - Classifying text documents

## Naive Bayes Classifier

- Assume target function  $f: X \rightarrow V$ , where each instance x described by attributes  $a_1, a_2 \dots a_n$
- Most probable value of f(x) is:

$$v_{MAP} = \arg \max_{v_j \in V} P(v_j | a_1, a_2 \dots a_n)$$

$$v_{MAP} = \arg \max_{v_j \in V} \frac{P(a_1, a_2 \dots a_n | v_j) P(v_j)}{P(a_1, a_2 \dots a_n)}$$

$$= \arg \max_{v_j \in V} P(a_1, a_2 \dots a_n | v_j) P(v_j)$$

 $V_{NB}$ 

• Naive Bayes assumption:

$$P(a_1, a_2 \dots a_n | v_j) = \prod_i P(a_i | v_j)$$

• which gives

Naive Bayes classifier: 
$$v_{NB} = \arg \max_{v_j \in V} P(v_j) \prod_i P(a_i | v_j)$$

## Naive Bayes Algorithm

- For each target value  $v_i$
- $\hat{P}(v_j)$  estimate  $P(v_j)$
- For each attribute value  $a_i$  of each attribute a
- $\hat{P}(a_i|v_j)$  **\lefthi** estimate  $P(a_i|v_j)$

$$v_{NB} = \arg\max_{v_j \in V} \hat{P}(v_j) \prod_{a_i \in x} \hat{P}(a_i | v_j)$$

## Training dataset

Class:

C1:buys\_computer='yes' C2:buys\_computer='no'

Data sample:

X =
(age<=30,
Income=medium,
Student=yes
Credit\_rating=Fair)</pre>

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
3040	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
3140	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
3140	medium	no	excellent	yes
3140	high	yes	fair	yes
>40	medium	no	excellent	no

#### Naïve Bayesian Classifier: Example

• Compute P(X|C<sub>i</sub>) for each class

```
P(age="<30" | buys_computer="yes") = 2/9=0.222
P(age="<30" | buys_computer="no") = 3/5 = 0.6
P(income="medium" | buys_computer="yes")= 4/9 = 0.444
P(income="medium" | buys_computer="no") = 2/5 = 0.4
P(student="yes" | buys_computer="yes)= 6/9 = 0.667
P(student="yes" | buys_computer="no")= 1/5=0.2
P(credit_rating="fair" | buys_computer="yes")=6/9=0.667
P(credit_rating="fair" | buys_computer="no")=2/5=0.4
```

P(buys\_computer=,,yes")=9/14 P(buys\_computer=,,no")=5/14

• X=(age<=30 ,income =medium, student=yes,credit\_rating=fair)

 $P(X|C_1)$ :  $P(X|buys\_computer="yes")= 0.222 \times 0.444 \times 0.667 \times 0.0.667 = 0.044$ 

 $P(X|C_2)$ :  $P(X|buys\_computer="no")= 0.6 \times 0.4 \times 0.2 \times 0.4 = 0.019$ 

 $P(X|C_1)*P(C_1):$   $P(X|buys\_computer="yes")*P(buys\_computer="yes")=0.028$   $P(X|C_2)*P(C_2):$   $P(X|buys\_computer="no")*P(buys\_computer="no")=0.007$ 

**X** belongs to class "buys\_computer=yes"  $P(C_1 | X) = 0.028/(0.028+0.007)$ 

#### Estimating probabilities in small samples

- We have estimated probabilities by the times the event is observed,  $n_c$ , over total opportunities, n
  - ullet poor estimates when  $n_c$  is very small
  - **problem**: what if none of the training instances with target value  $v_j$  have attribute value  $a_i$ ?  $\rightarrow n_c$  is 0!
- when  $n_c$  is very small:  $\hat{P}(a_i|v_j) = \frac{n_c + mp}{n+m}$   $v_{NB} =_{v_j \in V} P(v_j) \prod_i \hat{P}(a_i|v_j)$ 
  - n is number of training examples for which  $v = v_i$
  - $n_c$  number of examples for which  $v=v_i$  and a=ai
  - *p* is the prior estimate
  - m is the weight given to prior (i.e. number of "virtual" examples)

### Naïve Bayes: comments

#### Advantages

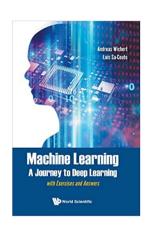
- easy to implement, good results obtained in most of the cases
- The decomposition of large probabilistic domains into weakly connected subsets via conditional independence is one of the most important developments in the recent history of AI
- Conditional independence assumption is often violated
- ...but it works surprisingly well anyway

### Naïve Bayes: comments

#### Disadvantages

- Assumption: class conditional independence, therefore loss of accuracy
- Practically, dependencies exist among variables
- E.g., hospitals: patients: Profile: age, family history etc Symptoms: fever, cough etc., Disease: lung cancer, diabetes etc
- Dependencies among these cannot be modeled by Naïve Bayesian Classifier
- How to deal with these dependencies?
  - Bayesian Belief Networks

#### Literature



- Machine Learning A Journey to Deep Learning, A.
   Wichert, Luis Sa-Couto, World Scientific, 2021
  - Chapter 2