#### Sapienza University of Rome

### Master in Artificial Intelligence and Robotics Master in Engineering in Computer Science

# Machine Learning

A.Y. 2020/2021

Prof. L. locchi, F. Patrizi

L. locchi, F. Patrizi

4. Probability and Bayes Networks

1/42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# 4. Probability and Bayes Networks

L. locchi, F. Patrizi

#### Outline

- Uncertainty
- Probability
- Syntax and Semantics
- Inference
- Independence and Bayes' Rule

L. locchi, F. Patrizi

4. Probability and Bayes Networks

3 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Uncertainty

Consider action  $A_t$  = leave for airport t minutes before flight.

Will  $A_t$  get me there on time?

this is a very difficult problem to predict

#### Problems:

- partial observability (road state, other drivers' plans, etc.)
- noisy sensors (traffic reports)
- uncertainty in action outcomes (flat tire, etc.)
- complexity of modelling and predicting traffic

L. locchi, F. Patrizi

4. Probability and Bayes Networks

# Uncertainty

Hence a purely logical approach either

- risks falsehood: "A<sub>25</sub> will get me there on time"
- leads to conclusions that are too weak for decision making: " $A_{25}$  will get me there on time if there's no accident on the bridge and it doesn't rain and my tires remain intact etc etc."
- leads to non-optimal decisions ( $A_{1440}$  might reasonably be said to get me there on time, but I'd have to stay overnight in the airport ...)

L. locchi, F. Patrizi

4. Probability and Bayes Networks

5 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

## **Probability**

Representation of uncertainty with probabilities.

Given the available evidence,  $A_{25}$  will get me at the airport on time with probability 0.04

Given the available evidence,  $A_{60}$  will get me at the airport on time with probability 0.85

Given the available evidence,  $A_{1440}$  will get me at the airport on time with probability 0.999

L. locchi, F. Patrizi

4. Probability and Bayes Networks

# **Probability**

#### Sample space

- $\Omega$  sample space (set of possibilities)
- $\omega \in \Omega$  is a sample point/possible world/atomic event/outcome of a random process/...

Probability space (or probability model)

- Function  $P: \Omega \mapsto \Re$ , such that
  - $0 \le P(\omega) \le 1$
  - $\sum_{\omega \in \Omega} P(\omega) = 1$

Example: rolling a die

$$\Omega = \{1, 2, 3, 4, 5, 6\}$$

$$P(\omega) = \{1/6, 1/6, 1/6, 1/6, 1/6, 1/6\}$$

L. locchi, F. Patrizi

4. Probability and Bayes Networks

7 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

#### **Event**

An event A is any subset of  $\Omega$ 

Probability of an event A is a function assigning to A a value in [0,1]

$$P(A) = \sum_{\{\omega \in A\}} P(\omega)$$

Example 1:  $A_1=$  "die roll < 4",  $A_1=\{1,2,3\}\subset \Omega$ 

$$P(A_1) = P(1) + P(2) + P(3) = 1/6 + 1/6 + 1/6 = 1/2$$

Example 2:  $A_2 =$  "die roll = 4",  $A_2 = \{4\}$ ,  $P(A_2) = 1/6$ 

Example 3:  $A_3 =$  "die roll > 6",  $A_3 = \emptyset$ ,  $P(A_3) = 0$ 

Example 4:  $A_4 =$  "die roll  $\leq 6$ ",  $A_4 = \Omega$ ,  $P(A_4) = 1$ 

L. locchi, F. Patrizi

4. Probability and Bayes Networks

#### Random variables

A random variable (outcome of a random phenomenon) is a function from the sample space  $\Omega$  to some range (e.g., the reals or Booleans)  $X : \Omega \mapsto B$ .

Example:  $Odd : \Omega \mapsto Boolean$ .

X is a variable and a function!

 $X = x_i$ : the random variable X has the value  $x_i \in B$ 

 $X = x_i$  is equivalent to  $\{\omega \in \Omega | X(\omega) = x_i\}$ 

Example:  $Odd = true \equiv \{1, 3, 5\}$ 

L. locchi, F. Patrizi

4. Probability and Bayes Networks

9 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

#### Random variables

P induces a probability distribution for a random variable X:

$$P(X = x_i) = \sum_{\{\omega \in \Omega \mid X(\omega) = x_i\}} P(\omega)$$

Example

$$P(Odd = true) = P(1) + P(3) + P(5) = 1/6 + 1/6 + 1/6 = 1/2$$

# **Propositions**

A proposition is the event (subset of  $\Omega$ ) where an assignment to a random variable holds.

• event  $a \equiv A = true \equiv \{\omega \in \Omega | A(\omega) = true\}$ 

Propositions can be combined using standard logical operators, e.g.:

- event  $\neg a \equiv A = false \equiv \{\omega \in \Omega | A(\omega) = false\}$
- event  $a \wedge b = \text{points } \omega$  where  $A(\omega) = true$  and  $B(\omega) = true$
- event  $\neg a \lor b = \text{points } \omega$  where  $A(\omega) = \text{false or } B(\omega) = \text{true}$

$$P(\neg a \lor b) = \sum_{\{\omega \in \Omega \mid A(\omega) = false \lor B(\omega) = true\}} P(\omega)$$

L. locchi, F. Patrizi

4. Probability and Bayes Networks

11 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Syntax for propositions

- Propositional or Boolean random variables
   e.g., Cavity (do I have a cavity?).
   Cavity = true is a proposition, also written cavity
- Discrete random variables (finite or infinite)
   e.g., Weather is one of < sunny, rain, cloudy, snow >.
   Weather = rain is a proposition
   Values must be exhaustive and mutually exclusive
- Continuous random variables (bounded or unbounded) e.g., Temp = 21.6, Temp < 22.0.
- Arbitrary Boolean combinations of basic propositions e.g.,  $cavity \land Weather = rain \land Temp < 22.0$ .

L. locchi, F. Patrizi

4. Probability and Bayes Networks

# **Prior Probability**

P(h) to denote the initial probability that hypothesis h holds, before we have observed the training data. P(h) is often called the priorprobability of h and may reflect any backgroundknowledge we have about the chance that h is a correct hypothesis. If we have no such prior knowledge, then we might simply assign the same prior probability to each candidate hypothesis.

P(D) to denote the prior probability that training data D will be observed

Prior or unconditional probabilities of propositions correspond to belief prior to arrival of any (new) evidence.

Examples:

$$P(Odd = true) = 0.5$$
  
 $P(Cavity = true) = 0.1$   
 $P(Weather = sunny) = 0.72$ 

L. locchi, F. Patrizi

4. Probability and Bayes Networks

13 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Probability distribution

A *probability distribution* is a function assigning a probability value to all possible assignments of a random variable.

Note: sum of all values must be 1.

Examples:

$$P(Odd) = <0.5, 0.5 >$$
  
 $P(Cavity) = <0.1, 0.9 >$   
 $P(Weather) = <0.72, 0.1, 0.08, 0.1 >$ 

Note: for real valued random variable X, P(X) is a continuous function.

L. locchi, F. Patrizi

4. Probability and Bayes Networks

# Joint probability distribution

Joint probability distribution for a set of random variables gives the probability of every atomic joint event on those random variables (i.e., every sample point in the joint sample space).

Joint probability distribution of the random variables Weather and Cavity:  $P(Weather, Cavity) = a 4 \times 2 \text{ matrix of values:}$ 

Weather =	sunny	rain	cloudy	snow
Cavity = true				
Cavity = false	0.576	0.08	0.064	0.08

Every question about a domain can be answered by the joint distribution because every event is a set of sample points

L. locchi, F. Patrizi

4. Probability and Bayes Networks

15 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

Conditional/Posterior Probability

P(D|h) to denote the probability of observing data D given some world in which hypothesis h holds. More generally, we write P(xly) to denote the probability of x given y. In machine learning problems we are interested in the probability P (h|D) that h holds given the observed training data D. P(h|D) is called the posterior probability of h, because it reflects our confidence that h holds after we have seen the training data D.

N.B: Notice the posterior probability P(h|D) reflects the influence of the training data D, in contrast to the prior probability P(h), which is independent of D.

Belief after the arrival of some evidence.

I know the outcome of a random variable, how does this affect probability of other random variables?

#### Example:

I know that today Weather = sunny, how this information affects the random variable Cavity?

#### Notation:

P(Cavity = true | Weather = sunny): conditional/posterior probability

L. locchi, F. Patrizi

4. Probability and Bayes Networks

# Conditional/Posterior Probability

In general, conditional/posterior probabilities are different from joint probabilities and from prior probabilities.

$$P(Cavity = true | Weather = sunny) \neq$$
  
 $P(Cavity = true, Weather = sunny) \neq$   
 $P(Cavity = true)$ 

L. locchi, F. Patrizi

4. Probability and Bayes Networks

17 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Conditional/Posterior Probability

Consider another Boolean random variable Toothache. Given that I have a toothache, how this affects the event of having a cavity?

Example:

$$P(cavity) = 0.2$$
: prior

P(cavity|toothache) = 0.6: posterior

L. locchi, F. Patrizi

# Conditional Probability Distributions

Conditional probability distributions: representation of all the values of conditional probabilities of random variables.

#### Example:

P(Cavity|Toothache) = 2-element vector of 2-element vectors

L. locchi, F. Patrizi

4. Probability and Bayes Networks

19 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Conditional probability

Definition of conditional probability:

$$P(a|b) \equiv \frac{P(a \wedge b)}{P(b)}$$
 if  $P(b) \neq 0$ 

Product rule

$$P(a \wedge b) = P(a|b)P(b) = P(b|a)P(a)$$

A general version holds for whole distributions, e.g., P(Weather, Cavity) = P(Weather|Cavity)P(Cavity)

L. locchi, F. Patrizi

4. Probability and Bayes Networks

## Total probabilities

For a Boolean random variable B

$$P(a) = P(a|b)P(b) + P(a|\neg b)P(\neg b)$$

In general, for a random variable Y accepting mutually exclusive values  $y_i$ 

$$P(X) = \sum_{y_i \in \mathcal{D}(Y)} P(X|Y = y_i) P(Y = y_i)$$

 $\mathcal{D}(Y)$ : set of values for variable Y

L. locchi, F. Patrizi

4. Probability and Bayes Networks

21 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

#### Chain Rule

Chain rule is derived by successive application of product rule:

$$P(X_{1}, X_{2}) = P(X_{1})P(X_{2}|X_{1})$$

$$P(X_{1}, ..., X_{n}) = P(X_{1}, ..., X_{n-1})P(X_{n}|X_{1}, ..., X_{n-1})$$

$$= P(X_{1}, ..., X_{n-2})P(X_{n-1}|X_{1}, ..., X_{n-2})P(X_{n}|X_{1}, ..., X_{n-1})$$

$$= ...$$

$$= \prod_{i=1}^{n} P(X_{i}|X_{1}, ..., X_{i-1})$$

L. locchi, F. Patrizi

# Inference by Enumeration

Start with the joint distribution:

	toothache		¬ toothache	
	catch ¬ catch		catch	¬ catch
cavity	.108	.012	.072	.008
¬ cavity	.016	.064	.144	.576

For any proposition  $\phi$ , sum the atomic events where it is true:

$$P(\phi) = \sum_{\omega:\omega \models \phi} P(\omega)$$

L. locchi, F. Patrizi

4. Probability and Bayes Networks

23 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Inference by Enumeration

Start with the joint distribution:

	toothache		¬ toothache	
	catch	¬ catch	catch	¬ catch
cavity	.108	.012	.072	.008
¬ cavity	.016	.064	.144	.576

For any proposition  $\phi$ , sum the atomic events where it is true:

$$P(\phi) = \sum_{\omega:\omega \models \phi} P(\omega)$$

$$P(toothache) = 0.108 + 0.012 + 0.016 + 0.064 = 0.2$$

# Inference by Enumeration

Start with the joint distribution:

	toothache		¬ toothache	
	catch ¬ catch		catch	¬ catch
cavity	.108	.012	.072	.008
¬ cavity	.016	.064	.144	.576

For any proposition  $\phi$ , sum the atomic events where it is true:

$$P(\phi) = \sum_{\omega:\omega\models\phi} P(\omega)$$

$$P(cavity \lor toothache) = 0.108 + 0.012 + 0.072 + 0.008 + 0.016 + 0.064 = 0.28$$

L. locchi, F. Patrizi

4. Probability and Bayes Networks

25 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Inference by Enumeration

Start with the joint distribution:

	toothache		¬ toothache	
	catch	¬ catch	catch	¬ catch
cavity	.108	.012	.072	.008
¬ cavity	.016	.064	.144	.576

Can also compute conditional probabilities:

$$P(\neg cavity | toothache) = \frac{P(\neg cavity \land toothache)}{P(toothache)}$$
$$= \frac{0.016 + 0.064}{0.108 + 0.012 + 0.016 + 0.064} = 0.4$$

#### Normalization

Start with the joint distribution:

	toothache		¬ toothache		
	catch	¬ catch		catch	¬ catch
cavity	.108	.012		.072	.008
¬ cavity	.016	.064		.144	.576

Denominator can be viewed as a normalization constant  $\alpha$ 

 $P(Cavity|toothache) = \alpha P(Cavity, toothache)$ =  $\alpha [P(Cavity, toothache, catch) + P(Cavity, toothache, \neg catch)]$ =  $\alpha [\langle 0.108, 0.016 \rangle + \langle 0.012, 0.064 \rangle]$ =  $\alpha \langle 0.12, 0.08 \rangle = \langle 0.6, 0.4 \rangle$ 

General idea: compute distribution on query variable by fixing evidence variables and summing over hidden variables

L. locchi, F. Patrizi

4. Probability and Bayes Networks

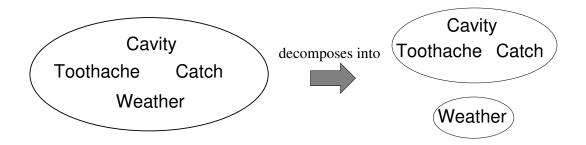
27 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Independence

A and B are independent iff

$$P(A|B) = P(A)$$
 or  $P(B|A) = P(B)$  or  $P(A,B) = P(A)P(B)$ 



$$P(Toothache, Catch, Cavity, Weather) = P(Toothache, Catch, Cavity)P(Weather)$$

# Independence

P(Toothache, Catch, Cavity, Weather) has 32 entries P(Toothache, Catch, Cavity) and P(Weather) have 8 + 4 = 12 entries

Example: n independent biased coins, reduced size from  $2^n$  to n

Absolute independence powerful, but rare.

Complex systems have hundreds of variables, none of which are independent.

L. locchi, F. Patrizi

4. Probability and Bayes Networks

29 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Conditional independence

- P(Toothache, Cavity, Catch) has  $2^3 1 = 7$  independent entries
- If I have a cavity, the probability that the probe catches in it does not depend on whether I have a toothache:
  - (1) P(catch|toothache, cavity) = P(catch|cavity)
- The same independence holds if I haven't got a cavity:
  - (2)  $P(catch|toothache, \neg cavity) = P(catch|\neg cavity)$
- Catch is conditionally independent of Toothache given Cavity: P(Catch|Toothache, Cavity) = P(Catch|Cavity)
- Equivalent statements:

```
P(Toothache|Catch, Cavity) = P(Toothache|Cavity)

P(Toothache, Catch|Cavity) = P(Toothache|Cavity)P(Catch|Cavity)
```

Thus representation of P(Toothache, Catch|Cavity) is simplified

L. locchi, F. Patrizi

4. Probability and Bayes Networks

# Conditional independence

General formulation:

X conditionally independent from Y given Z iff P(X|Y,Z) = P(X|Z)

$$P(X, Y|Z) = P(X|Y, Z)P(Y|Z) = P(X|Z)P(Y|Z)$$

$$P(Y_1, ..., Y_n | Z) = P(Y_1 | Y_2, ..., Y_n, Z) P(Y_2 | Y_3 ..., Y_n, Z) ... P(Y_n | Z)$$

 $Y_i$  conditionally independent from  $Y_j$  given Z

$$P(Y_1,\ldots,Y_n|Z)=P(Y_1|Z)P(Y_2|Z)\cdots P(Y_n|Z)$$

L. locchi, F. Patrizi

4. Probability and Bayes Networks

31 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

## Conditional independence

Chain rule + Conditional independence

$$P(X,Y,Z) = P(X|Y,Z)P(Y,Z) = P(X|Y,Z)P(Y|Z)P(Z)$$
  
=  $P(X|Z)P(Y|Z)P(Z)$ 

P(Toothache, Catch, Cavity)

- = P(Toothache|Catch, Cavity)P(Catch, Cavity)
- = P(Toothache|Catch, Cavity)P(Catch|Cavity)P(Cavity)
- = P(Toothache|Cavity)P(Catch|Cavity)P(Cavity)
- 2+2+1=5 independent numbers (instead of  $2^3-1$ )

In most cases, the use of conditional independence reduces the size of the representation of the joint distribution from exponential in n to linear in n.

L. locchi, F. Patrizi

# Bayes' Rule

• Product rule  $P(a \land b) = P(a|b)P(b) = P(b|a)P(a)$ 

$$\Rightarrow$$
 Bayes' rule  $P(a|b) = \frac{P(b|a)P(a)}{P(b)}$ 

or in distribution form

$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)} = \alpha P(X|Y)P(Y)$$

Useful for assessing diagnostic probability from causal probability:

$$P(Cause|Effect) = \frac{P(Effect|Cause)P(Cause)}{P(Effect)}$$

L. locchi, F. Patrizi

4. Probability and Bayes Networks

33 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Bayes' Rule and conditional independence

Bayes rule

$$P(Z|Y_1,\ldots,Y_n) = \alpha P(Y_1,\ldots,Y_n|Z) P(Z)$$

 $Y_i, \ldots Y_n$  conditionally independent each other given Z

$$P(Z|Y_1,\ldots,Y_n) = \alpha P(Y_1|Z) \cdots P(Y_n|Z) P(Z)$$

Effects conditionally independent each other given a cause.

$$P(Cause|Effect_1, ..., Effect_n) = \alpha P(Cause) \prod_i P(Effect_i|Cause)$$

Total number of parameters is *linear* in n

L. locchi, F. Patrizi

4. Probability and Bayes Networks

# Bayesian networks



A simple, graphical notation for conditional independence assertions and hence for compact specification of full joint distributions.

L. locchi, F. Patrizi

4. Probability and Bayes Networks

35 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Bayesian networks



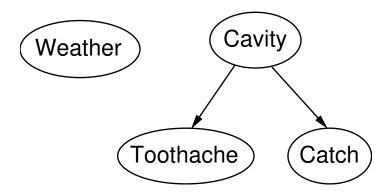
#### Syntax:

- a set of nodes, one per variable
- ullet a directed, acyclic graph (link pprox "directly influences")
- a conditional distribution for each node given its parents:  $P(X_i|\text{Parents}(X_i))$

In the simplest case, conditional distribution represented as a *conditional* probability table (CPT) giving the distribution over  $X_i$  for each combination of parent values.

# Dentist BN Example

Topology of network encodes conditional independence assertions:



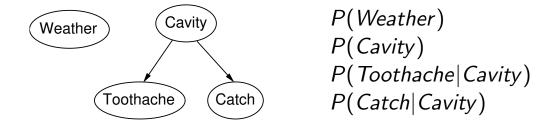
Weather is independent of the other variables

Toothache and Catch are conditionally independent given Cavity

L. Iocchi, F. Patrizi
4. Probability and Bayes Networks
37 / 42
Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Dentist BN Example

BN model given by the set of CPT  $P(X_i|\text{Parents}(X_i))$  for each variable  $X_i$ 



All the joint probabilities can be computed from this model. How many independent values?

# Burglar BN Example

I'm at work, neighbor John calls to say my alarm is ringing, but neighbor Mary doesn't call. Sometimes the alarm is set off by minor earthquakes. Is there a burglar?

Variables: Burglar, Earthquake, Alarm, JohnCalls, MaryCalls Network topology reflects "causal" knowledge:

- A burglar can set the alarm
- An earthquake can set the alarm
- The alarm can cause Mary to call
- The alarm can cause John to call

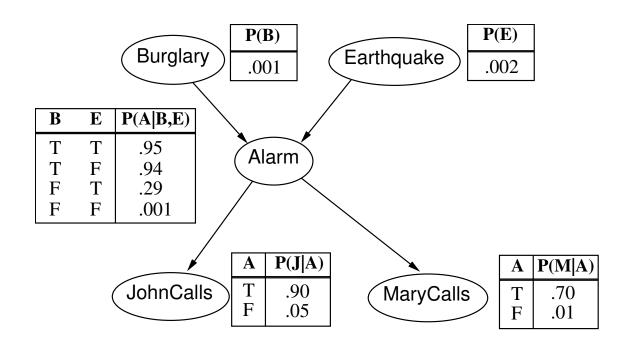
L. locchi, F. Patrizi

4. Probability and Bayes Networks

39 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Burglar BN Example



## Compactness

A CPT for Boolean variable  $X_i$  with k Boolean parents has  $2^k$  rows for the combinations of parent values



Each row requires one number p for  $X_i = true$  (the number for  $X_i = false$  is just 1 - p)

If each variable has no more than k parents, the complete network requires  $O(n \cdot 2^k)$  numbers

I.e., grows linearly with n, vs.  $O(2^n)$  for the full joint distribution For burglary net, 1+1+4+2+2=10 numbers (vs.  $2^5-1=31$ )

L. locchi, F. Patrizi

4. Probability and Bayes Networks

41 / 42

Sapienza University of Rome, Italy - Machine Learning (2020/2021)

# Computing joint probabilities

All joint probabilities computed with the chain rule:

$$P(x_1,\ldots,x_n)=\prod_{i=1}^n P(x_i|\mathrm{Parents}(X_i))$$



e.g., 
$$P(j \land m \land a \land \neg b \land \neg e)$$

= 
$$P(j|a)P(m|a)P(a|\neg b, \neg e)P(\neg b)P(\neg e)$$
  
=  $0.9 \times 0.7 \times 0.001 \times 0.999 \times 0.998$ 

 $\approx$  0.00063