Probabilistic Reasoning course slides to accompany syllabus 2023-2024

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UU – ICS Master Programmes: Computing Science Artificial Intelligence Data Science



Universiteit Utrecht

Part One

Probabilistic reasoning

- Lecturer: Silja Renooij (s.renooij@uu.nl) Matthijs Vákár (m.i.l.vakar@uu.nl)
- Prerequisites: probability theory & graph theory
- Literature: syllabus, papers, slides & studymanual
- Additional see course website: info: http://www.cs.uu.nl/docs/vakken/prob/

Practical information

Course form:

- lectures
- exercises (formative self assessment) (tip: discuss exercises together)

Grading:

- practical assignments (partially formative; qualitative) (description + deadlines on Blackboard)
- written exam (summative)

Syllabus, Chapter 1:

Introduction

Reasoning under uncertainty

In numerous application areas of knowledge-based decision-support systems we have

- uncertainty concerning the general domain knowledge;
- problem-specific information that is often uncertain, incomplete and even contradictory.

A decision-support system should be capable of dealing with these types of knowledge.

Application of probability theory

Consider a joint probability distribution \Pr on a set of <u>discrete</u> random variables $V = \{V_1, \ldots, V_n\}$. Then, in general:

• representing Pr requires exponential space

consider e.g. n = 2 binary-valued variables, or n = 40; what if they have 5 values each? (and how do you get the numbers?)

- calculating a probability from \Pr by conditioning and marginalisation requires exponential time

consider e.g. computing $Pr(V_1 = true)$ from Pr(V), or $Pr(V_1 = true \mid V_2 = true)$

This cannot be improved without additional knowledge about the probability distribution.

Diagnosis problem: pioneering in the 1960s

Let $H = \{h_1, \ldots, h_n\}, n \ge 1$, be a set of hypotheses, and let $E = \{e_1, \ldots, e_m\}, m \ge 1$, be a set of relevant findings (evidence).

Determine the 'best' diagnosis given findings $e \subseteq E$.

The approach: Compute for each $h \subseteq H$ the probability

$$\Pr(\boldsymbol{h} \mid \boldsymbol{e}) = \frac{\Pr(\boldsymbol{e} \mid \boldsymbol{h}) \Pr(\boldsymbol{h})}{\Pr(\boldsymbol{e})}$$

Drawback: An exponential number of probabilities need to be computed; storage is also exponential.

Pioneering in the 1960s

Determine the diagnosis given findings $e \subseteq E$.

The approach: Assume $h_i \in H$ mutually exclusive, and collectively exhaustive: $\bigcup_{i=1}^{n} \{h_i\} = \Omega$.

Then, compute for each $h_i \in H$:

$$\Pr(h_i \mid \boldsymbol{e}) = \frac{\Pr(\boldsymbol{e} \mid h_i) \Pr(h_i)}{\Pr(\boldsymbol{e})} = \frac{\Pr(\boldsymbol{e} \mid h_i) \Pr(h_i)}{\sum_{k=1}^{n} \Pr(\boldsymbol{e} \mid h_k) \Pr(h_k)}$$

<u>Drawback</u>: We compute only n - 1 probabilities, but computation still requires an exponential number of probabilities.

Pioneering in the 1960s

Determine the diagnosis given findings $e = \{e_p, \ldots, e_q\}, 1 \le p, q \le m.$

The approach: Assume *in addition* that all findings e_1, \ldots, e_m are conditionally independent given $h_i, i = 1, \ldots, n$. Then:

$$\Pr(h_i \mid \boldsymbol{e}) = \frac{\Pr(e_p, \dots, e_q \mid h_i) \Pr(h_i)}{\sum_{k=1}^n \Pr(e_p, \dots, e_q \mid h_k) \Pr(h_k)}$$
$$= \frac{\Pr(e_p \mid h_i) \cdot \dots \cdot \Pr(e_q \mid h_i) \Pr(h_i)}{\sum_{k=1}^n \Pr(e_p \mid h_k) \cdot \dots \cdot \Pr(e_q \mid h_k) \Pr(h_k)}$$

<u>Benefit</u>: Only $m \cdot n$ conditional probabilities and n - 1 prior probabilities are required for the computation.

GLADYS

GLADYS (GLASGOW DYSPEPSIA SYSTEM) is a system for diagnosing dyspepsia.

The global structure of the system:



D.J. Spiegelhalter, R.P. Knill-Jones (1984). Statistical and knowledge-based approaches to clinical decision-support systems with an application in gastroenterology, Journal of the Royal Statistical Society (Series A), vol. 147, pp. 35-77.

Symptoms and diseases

Context: patients with an Ulcer. Question: which type?

		duodenal ulcer	gastric ulcer
		(n = 248)	(n = 43)
Sex:	male	169	17
	female	79	26
Age:	< 26	43	1
	26 - 40	82	5
	41 - 55	87	19
	> 55	36	18
Daily pain:	yes	21	11
	no	214	27
Effect food	worsens	44	11
on pain:	no effect	82	9
	relieves	104	17
probability		0.85	0.15

The idea

Let \Pr be a joint distribution on the diagnosis search space including hypothesis *h* and observed findings *e*.

The prior odds for h, and posterior odds for h given e, are defined by

$$O(h) = \frac{\Pr(h)}{1 - \Pr(h)} = \frac{\Pr(h)}{\Pr(\neg h)}, \text{ and } O(h \mid \boldsymbol{e}) = \frac{\Pr(h \mid \boldsymbol{e})}{\Pr(\neg h \mid \boldsymbol{e})}$$

Assume that all findings $e_i \in e$ are conditionally independent given h, then

$$O(h \mid \boldsymbol{e}) = \frac{\Pr(\boldsymbol{e} \mid h) \cdot \Pr(h)}{\Pr(\boldsymbol{e} \mid \neg h) \cdot \Pr(\neg h)} = \prod_{i} \frac{\Pr(e_i \mid h)}{\Pr(e_i \mid \neg h)} \cdot O(h)$$

Now consider the following transformation: $10 \cdot \ln O(h \mid e) \dots$

The idea (cntd)

Applying the transformation $10 \cdot \ln$ to

$$O(h \mid \boldsymbol{e}) = \prod_{i} \lambda_{i} \cdot O(h), \text{ where } \lambda_{i} = \frac{\Pr(e_{i} \mid h)}{\Pr(e_{i} \mid \neg h)}$$

results in a score s:

$$s = 10 \cdot \ln O(h \mid e) = 10 \cdot \ln O(h) + \sum_{i} 10 \cdot \ln \lambda_{i} = w_{0} + \sum_{i} w_{i}$$

where w_i is a weight for finding e_i .

The probability $\Pr(h \mid e)$ is now computed from

$$\Pr(h \mid \boldsymbol{e}) = \frac{O(h \mid \boldsymbol{e})}{1 + O(h \mid \boldsymbol{e})} = \frac{e^{\frac{s}{10}}}{1 + e^{\frac{s}{10}}} = \frac{1}{1 + e^{-\frac{s}{10}}}$$

A scoring system

	h: duodenal ulcer (du)	$\neg h$: gastric ulcer (gu)	
	(n = 248)	(n = 43)	
male (m)	169	17	
female (f)	79	26	

Calculation of probabilities, likelihood ratios and weights:

$$\begin{aligned} &\Pr(\mathsf{m} \mid \mathsf{du}) = \frac{169}{248} \sim 0.68, \ \Pr(\mathsf{m} \mid \mathsf{gu}) \sim 0.40 \ \Rightarrow \\ &\lambda_\mathsf{m} = \frac{\Pr(\mathsf{m} \mid \mathsf{du})}{\Pr(\mathsf{m} \mid \mathsf{gu})} = \frac{0.68}{0.40} \sim 1.7 \implies \mathsf{w}_\mathsf{m} = 10 \cdot \ln \lambda_\mathsf{m} \sim 5 \end{aligned}$$

$$\begin{split} &\Pr(f \mid du) = \frac{79}{248} \sim 0.32, \ \Pr(f \mid gu) \sim 0.60 \Rightarrow \\ &\lambda_f = \frac{\Pr(f \mid du)}{\Pr(f \mid gu)} = \frac{0.32}{0.60} \sim 0.53 \implies w_f = 10 \cdot \ln \lambda_f \sim -6 \end{split}$$

Symptoms and their weights

		duodenal ulcer	gastric ulcer	weight
		(n = 248)	(n = 43)	
Sex:	male	169	17	5
	female	79	26	-6
Age:	< 26	43	1	18
	26 - 40	82	5	10
	41 - 55	87	19	-2
	> 55	36	18	-10
Daily pain:	yes	21	11	-12
	no	214	27	3
Effect food	worsens	44	11	-4
on pain:	no effect	82	9	4
	relieves	104	17	0
prior		0.85	0.15	17

An example diagnosis

A 30 year old woman reports to the clinic. She has pain in the abdominal area, but not on a daily basis; the pain worsens as soon as she eats.

Calculation of the score:

•	the initial score:	+17
•	the patient is female:	- 6
•	her age is 30:	+10
•	she is in pain, but not every day:	+ 3
•	food intake worsens the pain:	- 4
		+20

Given that the patient has one of the two diseases, duodenal ulcer and gastric ulcer, she has with probability

$$(1 + e^{-\frac{20}{10}})^{-1} \approx 1.14^{-1} \approx 0.88$$

a duodenal ulcer and a gastric ulcer with probability 0.12.

Reviewing 'Idiot's Bayes'

The naive Bayes approach is

- mathematically correct, and
- computationally easy.

However

- underlying assumptions usually unacceptable;
- and, at the time, for larger applications
 - number of hypotheses often large → undoable to compute each Pr(h_i | e);
 - often not enough information for reliable probability assessments.

History: diagnosis in the 1970s



The most likely hypothesis given observed findings is determined as follows:

- prune the search space using heuristic rules;
- approximate the missing probabilities required, for example with:

 $\Pr(e_i \wedge e_j) = \min\{\Pr(e_i), \Pr(e_j)\};\$

• select the hypothesis with the highest probability.

Reviewing the quasi-probabilistic models

The quasi-probabilistic models are

- computationally easy, and
- easy to use,

even for larger applications.

However, these models are

- mathematically incorrect, and
- even as an approximation model not convincing.

The rehabilitation of probability theory in the 1980s

J. Pearl introduces what we now call probabilistic graphical models (PGMs) :

- a graphical model to represent the knowledge in a complex multi-variate domain
 - graph encodes probabilistic independences
 - joint probability distribution is factorized into smaller functions
- knowledge representation is separated from reasoning
 ⇒ allows generic algorithms for
 - inference (computing probabilities)
 - learning
 - . . .

The Probabilistic Graphical Model framework

Probabilistic Graphical Model: a compact representation of a joint probability distribution \Pr over a set of random variables, comprised of:

- qualitative knowledge of Pr: a graph representation of the independences between the variables involved;
- quantitative knowledge of Pr: functions that capture part of Pr 'locally' per group of variables.

Algorithms associated with the framework are often tailored to

- the type of graphical model: directed or undirected
- the type of random variables: discrete and/or continuous

Probabilistic Graphical Models

J. Pearl introduced PGMs based on

- undirected graphs: Markov networks (Markov Random Fields)
 - · Gibbs random field: joint distribution is strictly positive
 - Ising/Potts model (Physics): pairwise MRF with discrete variables
 - Applications in image processing, computer vision, ...
- directed (acyclic) graphs: Bayesian networks (BNs)
 - Naive Bayes: restricted topology, discrete or continuous (Gaussian) variables
 - Hidden Markov model (HMM): 'Dynamic' BN with restricted topology, discrete variables
 - Particle/Kalman Filter: HMM with continuous/Gaussian variables
 - Applications in medicine, biology, genetics, speech recognition, spamfiltering,...

Focus on Bayesian networks

PGMs are considered to be interpretable models. When used as a modelling tool, directed models are often preferred.

Judea Pearl introduced several algorithms for inferring 'beliefs' from those represented in a Bayesian network:

- first for trees and polytrees (singly connected graphs)
- then for multiply-connected graphs
- for the latter, the algorithm by Steffen Lauritzen & David Spiegelhalter was the first to find wide-spread use.

Also see "Inference in Bayesian Networks: a Historical Perspective", by Adnan Darwiche

An example: Classical Swine Fever (CSF)

The classical swine fever network is a decision-support system for the early detection of classical swine fever (varkenspest).

- early detection of CSF is important, but hard;
- the network has been developed in cooperation with 2 veterinarians of the Central Veterinary Institute of Wageningen UR;
- part of european EPIZONE project;
- veterinarians all over the country collected data with PDAs

The Classical swine fever network: initial graphical structure



The Classical swine fever network: probability tables



 $\Pr(Appetite \mid BodyTemp \land Malaise)$

Classical swine fever: prior probabilities



Classical swine fever: diagnostic reasoning



Classical swine fever: prognostic reasoning



A Bayesian network: necessary ingredients

Definition:

A Bayesian network is a pair $\mathcal{B} = (G, \Gamma)$ such that

- *G* is an *acyclic directed graph* with nodes representing a set of *random variables V*;
- $\Gamma = \{\gamma_{V_i} \mid V_i \in V\}$ is a set of *assessment functions*.

Property:

$$\Pr(\boldsymbol{V}) = \prod_{V_i \in \boldsymbol{V}} \gamma_{V_i}(V_i \mid \boldsymbol{\rho}(V_i))$$

defines a *joint probability distribution* \Pr on V such that G is a *directed I-map* for the *independence relation* I_{\Pr} of \Pr .

About this course ...

The following subjects will be addressed in this course:

- the syntactics and semantics of PGMs;
- for BNs and probabilistic models in general (latter through Probabilistic Programming):
 - algorithms for probabilistic inference (exact and approximate);
 - methods for constructing a probabilistic model for a domain of application;
- methods for evaluating a discrete Bayesian network's performance and behaviour;
- (methods for controlling and explaining reasoning).

Syllabus, Chapter 2:

Preliminaries

(Discrete) Random variables

Let $V = \{V_1, \ldots, V_n\}$, $n \ge 1$, be a set of random variables. Each variable $V_i \in V$ can take on one of $m \ge 2$ values.

For ease of exposition we mostly consider 'binary' variables:

- $V_i = true$, denoted by v_i ;
- $V_i = false$, denoted by $\neg v_i$ (or by $\overline{v_i}$).

The set V spans a Boolean Algebra of logical propositions \mathcal{V} :

- T(rue), F(alse) $\in \mathcal{V}$;
- for all variables $V_i \in V$ we have that $v_i \in \mathcal{V}$;
- for all $x \in \mathcal{V}$ we have that $\neg x \in \mathcal{V}$;
- for all $x, y \in \mathcal{V}$ we have that $x \wedge y \in \mathcal{V}$ and $x \vee y \in \mathcal{V}$.

The elements of \mathcal{V} obey the usual rules of propositional logic.

The joint probability distribution

Definition:

Let $\mathcal V$ be the Boolean Algebra of propositions spanned by a set of random variables $\bm V.$ Let $\Pr:\mathcal V\to[0,1]$ be a function such that

- Pr is positive: for each $x \in \mathcal{V}$ we have that $Pr(x) \ge 0$ and, more specifically, $Pr(\mathsf{F}) = 0$;
- \Pr is normed: $\Pr(\mathsf{T}) = 1$;
- Pr is additive: we have, for each $x, y \in \mathcal{V}$ with $x \wedge y \equiv \mathsf{F}$, that $\Pr(x \lor y) = \Pr(x) + \Pr(y)$.

The function \Pr is a joint probability distribution on V; the function value $\Pr(x)$ is the probability of x.

Independence of propositions

Definition: Let \mathcal{V} be the Boolean Algebra of propositions spanned by a set of random variables V. Let Pr be a joint probability distribution on V.

Propositions $x, y \in \mathcal{V}$ are called independent in \Pr if

 $\Pr(x \land y) = \Pr(x) \cdot \Pr(y)$

Propositions $x, y \in \mathcal{V}$ are called conditionally independent given the proposition $z \in \mathcal{V}$ if we have that

 $\Pr(x \land y \mid z) = \Pr(x \mid z) \cdot \Pr(y \mid z)$

The two notions of independence (1)

Consider two propositions x, y ∈ V such that x and y are independent ¹:



x

$$Pr(x) = \frac{1}{2}; Pr(y) = \frac{1}{4};$$

$$Pr(x \land y) = \frac{1}{8}$$

$$= Pr(x) \cdot Pr(y)$$

Can $z \in \mathcal{V}$ exist such that x and y are dependent given z?

• Yes:



$$\begin{aligned} \Pr(x \mid z) &> 0; \Pr(y \mid z) > 0; \\ \Pr(x \land y \mid z) &= 0 \\ &\neq & \Pr(x \mid z) \cdot \Pr(y \mid z) \end{aligned}$$

¹The square has area 1, representing the total probability mass.

The two notions of independence (2)

• Consider two propositions $x, y \in \mathcal{V}$ such that x and y are dependent:



$$Pr(x) = \frac{1}{2}; Pr(y) = \frac{1}{5};$$

$$Pr(x \land y) = \frac{1}{7}$$

$$> Pr(x) \cdot Pr(y)$$

Can $z \in \mathcal{V}$ exist such that x and y are conditionally independent given z?



$$Pr(x \mid z) = \frac{4}{5}; Pr(y \mid z) = \frac{1}{2};$$

$$Pr(x \land y \mid z) = \frac{4}{10}$$

$$= Pr(x \mid z) \cdot Pr(y \mid z)$$

Configurations

Let \mathcal{V} be spanned by random variables V and let $W \subseteq V$.

- proposition $w \in V$ is called a configuration of W iff it is a conjunction of value assignments to the variables from W;
- *c*_{*W*} is used to denote an arbitrary configuration of *W*;
- W also indicates all possible configurations to the set W (notation abuse!): W is then considered to be a template for all possible configurations c_W;
- if $W = \emptyset$, then by convention $c_W = c_{\emptyset} = \mathsf{T}$.

Example: Let $W = \{V_1, V_3, V_7\}$, with $W = V_1 \land V_3 \land V_7$ the associated configuration template. Some configurations c_W captured by this template are:

$$V_1 = true \land V_3 = true \land V_7 = false$$
$$v_1 \land \neg v_3 \land v_7$$
$$\neg v_1 \land v_3 \land \neg v_7$$

Conventions and notation

	set (bold faced)	singleton
variables/templates (capital)	V	V
values/configurations	$c_{oldsymbol{V}}, oldsymbol{v}$	c_V , v

- conjunctions are often left implicit: e.g. $v_1 v_2$ denotes $v_1 \wedge v_2$;
- note the following differences (!)

probabilities: $Pr(c_V), Pr(c_V), Pr(v), Pr(v), Pr(v \mid c_E)$ distributions: $Pr(V), Pr(V), Pr(V \mid e)$ distribution sets: Pr(V | E), Pr(V | E)

Independence of variables

<u>Definition</u>: Let V be a set of random variables and let $X, Y, Z \subseteq V$. Let Pr be a joint distribution on V.

 $oldsymbol{X}$ is called conditionally independent of $oldsymbol{Y}$ given $oldsymbol{Z}$ in \Pr , if

 $\Pr(\boldsymbol{X} \mid \boldsymbol{Y} \land \boldsymbol{Z}) = \Pr(\boldsymbol{X} \mid \boldsymbol{Z})$

If this holds for $Z = \emptyset$ then X is (marginally) independent of Y.

Remarks:

- Note the template notation: equation should hold for all c_X , c_Y and c_Z !
- $\Pr(\mathbf{X} \mid \mathbf{Y} \land \mathbf{Z}) = \Pr(\mathbf{X} \mid \mathbf{Z}) \Rightarrow$ $\Pr(\mathbf{X} \land \mathbf{Y} \mid \mathbf{Z}) = \Pr(\mathbf{X} \mid \mathbf{Z}) \cdot \Pr(\mathbf{Y} \mid \mathbf{Z})$

(See syllabus exercise 2.6)