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RWTH Lecture Series on Probabilistic Programming 2018

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# Probabilistic Programming Overview Motivation What are Bayesian networks? Conditional independence

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 Motivation

# The importance of Bayesian networks

"Bayesian networks are as important to AI and machine learning

as Boolean circuits are to computer science."

[Stuart Russell (Univ. of California, Berkeley), 2009]

Inference

### Motiva

## Judea Pearl: The father of Bayesian networks





Turing Award 2011: "for fundamental contributions to AI through the development of a calculus for probabilistic and causal reasoning".

Probabilistic Programming       What are Bayesian networks?         Overview       Image: Compare the second	Joost-Pieter Katoen	Probabilistic Programming	5/35
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	1 Motivation		
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# Probabilistic graphical models

### Combine graph theory and probability theory

- Vertices are random variables
- Edges are dependencies between these variables
- Enable usage of graph algorithms
- Graph representation makes (conditional) independence explicit
- Two main types of probabilistic graphical models
  - directed acyclic graphs: Bayesian networks
  - undirected graphs: Markov random fields
- We consider only discrete random variables

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 What are Bayesian networks?

 Bayesian networks

### **Bayesian network**

- A Bayesian network (BN, for short) is a tuple  $B = (V, E, \Theta)$  where
- (V, E) is a directed acyclic graph with finite V in which each v ∈ V represents a random variable with values from finite domain D, and (v, w) ∈ E represents the (causal) dependencies of w on v, and
- ► for each vertex v with k parents, the function  $\Theta_v : D^k \to Dist(D)$  is the conditional probability table of (the random variable represented by) vertex v.

Here,  $w \in V$  is a parent of  $v \in V$  whenever  $(w, v) \in E$ .

The graph structure induces a natural ordering on the parents of a vertex v; the *i*-th entry in a tuple  $\mathbf{d} \in D^k$  of  $\Theta_v$  corresponds to the value assigned to the *i*-th parent of v.

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## Example: Student's mood after an exam



The interpretation of an entry in a vertex' conditional probability table is:  $Pr(v = d \mid parents(v) = \mathbf{d}) = \Theta_v(\mathbf{d})(d)$ , with **d** the values of v's parents

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	D = 0 $D =$	1	D	ifficulty	)	Pre	paration	)	P = 0	P = 1
	0.6 0.4					$\rightarrow$			0.7	0.3
					<					
		G = 0	<i>G</i> = 1			$\checkmark$				
	D=0, P=0	0.95	0.05	(	Grade					
	D = 1, P = 1	0.05	0.95							
	D = 0, P = 1	0.5	0.5							
	D = 1, P = 0	0.6	0.4							
					+			M = 0	M = 1	
				(	Mood		G = 0	0.9	0.1	
							G = 1	0.3	0.7	

How likely does a student end up with a bad mood after getting a bad grade for an easy exam, **given that** she is well prepared?

### **Bayesian network semantics**

### Joint probability function of a Bayesian network

Let  $B = (V, E, \Theta)$  be a BN, and  $W \subseteq V$  be a downward closed set of vertices where  $w \in W$  has value  $\underline{w} \in D$ . The (unique) joint probability function of BN B in which the nodes in W assume values  $\underline{W}$  equals:

$$Pr(W = \underline{W}) = \prod_{w \in W} Pr(w = \underline{w} \mid parents(w) = \underline{parents(w)})$$
$$= \prod_{w \in W} \Theta_w(\underline{parents(w)})(\underline{w}).$$
also called factorisation

The conditional probability distribution of  $W \subseteq V$  given observations on a set  $O \subseteq V$  of vertices is given by  $Pr(W = \underline{W} \mid O = \underline{O}) = \frac{Pr(W = \underline{W} \land O = \underline{O})}{Pr(O = \underline{O})}$ .

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### What are Bayesian networks?

Example



### What are Bayesian networks?

### The benefits of Bayesian networks

Bayesian networks provide a compact representation of joint distribution functions if the dependencies between the random variables are sparse.

Another advantage of BNs is the explicit representation of conditional independencies.

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Conditional independence

## **Conditional independence**

Two independent events may become dependent given some observation. This is captured by the following notion.

### **Conditional independence**

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Let X, Y, Z be (discrete) random variables. X is conditionally independent of Y given Z, denoted I(X, Z, Y), whenever:

 $Pr(X \land Y \mid Z) = Pr(X \mid Z) \cdot Pr(Y \mid Z)$  or Pr(Z) = 0.

Equivalent formulation:  $Pr(X | Y \land Z) = Pr(X | Z)$  or  $Pr(Y \land Z) = 0$ .

These notions can be easily lifted in a point-wise manner to sets of random variables, e.g.,  $\mathbf{X} = \{X_1, \dots, X_k\}$ .

Examples on the black board.

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Graphoid axioms	[Dawid,	1979],	[Spohn, 1980]
Conditional independence satisfies the following a random variables <b>W</b> , <b>X</b> , <b>Y</b> , <b>Z</b> :	axioms	for di	sjoint sets of
1. $I(X, Z, Y)$ if and only if $I(Y, Z, X)$			Symmetry
2. $I(X, Z, Y \cup W)$ implies $(I(X, Z, Y) \text{ and } I(X, Z))$	Z, W))	D	ecomposition
3. $I(X, Z, Y \cup W)$ implies $I(X, Z \cup Y, W)$			Weak union
4. $(I(\mathbf{X}, \mathbf{Z}, \mathbf{Y}) \text{ and } I(\mathbf{X}, \mathbf{Z} \cup \mathbf{Y}, \mathbf{W}))$ implies $I(\mathbf{X}, \mathbf{X})$	<b>Z</b> , <b>Y</b> ∪	W)	Contraction
5. /(X, Z, Ø)			Triviality

Graphoid axioms of Bayesian networks

Decomposition+Weak union+Contraction together are equivalent to:

 $I(X, Z, Y \cup W)$  if and only if I(X, Z, Y) and  $I(X, Z \cup Y, W)$ .

### Conditional independence

### **Checking conditional independencies**

Deriving the (conditional) independencies is non-trivial. The graphical structure of Bayesian networks enable a simple test. This is based on the concept of d-separation.

loost-Pieter Katoen Probabilistic Programmi obabilistic Programmin Conditional independence Valve types Sequential Divergent Convergent Earthqua Burglary (B) Burglary (B) Earthquake (E) (E) Radio? (R) Radio? (R) Radio (R) Alarm? (A) Alarm (A) Alarr (A) Call? (C) Call? Sequential valve Convergent valve Divergent valve

### Valves

- Consider undirected paths in the underlying DAG G = (V, E) of the BN.
- View every such path as a pipe, and each vertex W on the path as a valve.
- Valves have the status open or closed.
- An undirected path is blocked if at least one valve along the path is closed.
- A value v is open or closed on a path depending on its type on this path:
  - 1. Sequential: when v is a parent of one of its neighbours (on the path) and a child of its other neighbour (on the path)
  - 2. Divergent: when v is a parent of both neighbours
  - 3. Convergent: when v is a child of both neighbours

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### Valve status

A valve v is closed for set **Z** of variables whenever:

- 1. Sequential: if v (is a variable that) occurs in **Z**
- 2. Divergent: if v occurs in **Z**
- 3. Convergent: if neither v nor any of its descendants occurs in **Z**. w is a descendant of v if w is reachable via (directed) edge relation E from v.

### Example

- 1. the sequential valve A is closed iff we know the value of A, otherwise an earthquake E may change our belief in getting a call C.
- 2. the divergent valve *E* is closed iff we know the value of variable *E*, otherwise a radio report on an earthquake may change our belief in the alarm triggering.
- 3. the convergent valve A is closed iff neither the value of variable A nor the value of C are known, otherwise, a burglary may change our belief in an earthquake.

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### Probabilistic Programming

### Conditional independence

### **D**-separation

### **D**-separation

Let X, Y, Z be disjoint sets of vertices in the DAG G. X and Y are d-separated by Z in G, denoted  $dsep_G(X, Z, Y)$ , iff every (undirected) path between a vertex in X and a vertex in Y is blocked by some vertex in Z.

A path is **blocked** by **Z** iff at least one vertex on the path is **closed** given **Z**.



Figure 4.9: On the left, R and B are d-separated by E, C. On the right, R and C are not d-separated.

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# A polynomial algorithm for d-separation

Let X, Y, Z be disjoint sets of vertices in the DAG *G*. Apply the following pruning procedure on the DAG *G*:

- 1. Eliminate any leaf vertex v from G with  $v \notin \mathbf{X} \cup \mathbf{Y} \cup \mathbf{Z}$ .
- 2. Repeat this elimination procedure until no more leafs can be eliminated.
- 3. Eliminate all edges emanating vertices in Z.

The remaining DAG is referred to as  $prune_{\mathbf{X},\mathbf{Y},\mathbf{Z}}(G)$ .

### Theorem

Let **X**, **Y**, **Z** be disjoint sets of vertices in the DAG *G*. Then:  $dsep_G(\mathbf{X}, \mathbf{Y}, \mathbf{Z})$  if and only if **X** and **Y** are disconnected in  $prune_{\mathbf{X}, \mathbf{Y}, \mathbf{Z}}(G)$ .

two sets of vertices are disconnected if there is no path between them.

# **D**-separation

D-separation implies independence	[Pearl 1986], [Verma, 1986]
$dsep_G(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ implies $I(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ .	
Proof.	

Left as an exercise. Note that the reverse implication does not hold.  $\hfill\square$ 

As d-separation is defined over all paths, this theorem yields an exponential-time procedure to check (a sufficient condition for) conditional independence.

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# Markov blanket

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The complexity of inference on a Bayesian network is measured in terms of the Markov blanket, an indication of the degree of dependence in the BN.

Conditional independence

### Markov blanket

The Markov blanket for a vertex v in a BN is the set  $\partial v$  of vertices composed of v, v's parents, its children, and its children's other parents.

The average Markov blanket of BN *B* is the average size of the Markov blanket of all its vertices, that is,  $\frac{1}{|V|} \sum_{v \in V} |\partial v|$ .

Every set of nodes in the BN is conditionally independent of v when conditioned on the set  $\partial v$ . That is, for distinct vertices v and w:

 $Pr(v \mid \partial v \land w) = Pr(v \mid \partial v)$  or, equivalently  $I(\{v\}, \{w\}, \partial v)$ 

# Printer troubleshooting in Windows 95



The average Markov blanket of this BN is 5.92, |V| = 76, and |E| = 117

# Some benchmark BN results

Benchmark BNs from www.bnlearn.com

BN	V	<i>E</i>	aMB
hailfinder	56	66	3.54
hepar2	70	123	4.51
win95pts	76	112	5.92
pathfinder	135	200	3.04
andes	223	338	5.61
pigs	441	592	3.92
munin	1041	1397	3.54

### $aMB = average \ Markov \ Blanket \ size$ , a measure of independence in BNs

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Inference

# **Probabilistic inference**

We consider the following probabilistic inference problem: let *B* be a BN with set *V* of vertices and the evidence  $\mathbf{E} \subseteq V$  and the questions  $\mathbf{Q} \subseteq V$ . (Exact) probabilistic inference is to determine the conditional probability

$$Pr(\mathbf{Q} = \mathbf{q} | \mathbf{E} = \mathbf{e}) = \frac{Pr(\mathbf{Q} = \mathbf{q} \land \mathbf{E} = \mathbf{e})}{Pr(\mathbf{E} = \mathbf{e})}$$

We consider:

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### Decision variants of probabilistic inference

The decision variant of probabilistic inference is: for a given probability  $p \in \mathbb{Q} \cap [0, 1)$ :

	does $Pr(\mathbf{Q} = \mathbf{q} \mid$	$\mathbf{E} = \mathbf{e} >$	р?	Т	1	
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**•** special case:  $Pr(\mathbf{E} = \mathbf{e}) > p$ ? **STI** 

 $^{1}TI = Threshold$  Inference and STI = Simple TI.

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Inference

# Example



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# The complexity class PP

PP (Probabilistic Polynomial-Time) is the class of decision problems solvable by a probabilistic Turing machine<sup>2</sup> in polynomial time with an error probability < 1/2. Formally, a language *L* is in PP iff there is a probabilistic TM *M* such that:

- 1. *M* runs in polynomial time on all inputs
- 2. For all  $w \in L$ , *M* outputs 1 with probability larger than 1/2
- 3. For all  $w \notin L$ , *M* outputs 1 with probability at most 1/2.
- A PP-problem can be solved to any fixed degree of accuracy by running a randomised polynomial-time algorithm a sufficient (but bounded) number of times.

Remark: if all choices are binary and the probability of each transition is 1/2, then the majority of the runs accept input w iff  $w \in L$ . This majority, however, is not fixed and may (exponentially) depend on the input, e.g., a problem in PP may accept "yes"-instances with size |w| with probability  $1/2 + \frac{1}{2|w|}$ . This makes problems in PP intractable in general.

 $^2\mathsf{A}$  probabilistic TM is a non-deterministic TM which chooses between the available transitions at each point according to some probability distribution.

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# Complexity of probabilistic inference

Decision variants of probabilistic inference	
For a given probability $p \in \mathbb{Q} \cap [0, 1)$ :	
$\blacktriangleright \text{ does } Pr(\mathbf{Q} = \mathbf{q} \mid \mathbf{E} = \mathbf{e}) > p?$	TI
▶ special case: $Pr(\mathbf{E} = \mathbf{e}) > p$ ?	STI

### Complexity of probabilistic inference [Cooper, 1990]

The decision problems TI and STI are PP-complete.

### Proof.

- 1. Hardness: by a reduction of MAJSAT to STI (since STI is a special case of TI, MAJSAT is reducible to TI).
- Membership: To show TI is in PP, a polynomial-time algorithm is provided that can guess a solution to TI while guaranteeing that the guess is correct with probability exceeding <sup>1</sup>/<sub>2</sub>.

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# The complexity class PP



 $NP \subseteq PP$  (as SAT lies in PP) and  $coNP \subseteq PP$  (as PP is closed under complement). PP is contained in PSPACE (as there is a polynomial-space algorithm for MAJSAT).

PP is comparable to the class #P — the counting variant of NP — the class of function problems "compute f(x)" where f is the number of accepting runs of an NTM running in polynomial time.

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# The decision problems SAT and MAJSAT

### The decision problems SAT and MAJSAT

Let  $\alpha$  be a propositional logical formula (in conjunctive normal form, CNF) over a finite set **X** of Boolean variables.

- 1. Does there exist a valuation over **X** such that  $\alpha$  holds? SAT
- 2. Does the majority of the assignments to **X** make  $\alpha$  hold? MAJSAT

# Known facts [Cook, 1971] and [??]

- **1**. The SAT problem is NP-complete.
- 2. The MAJSAT problem is PP-complete.

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# Showing hardness of STI

By reducing MAJSAT to STI. As STI is a special case of TI, MAJSAT can also be reduced to TI.

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# Showing membership

To show TI is in PP, a polynomial-time algorithm is provided that can guess a solution to TI while guaranteeing that the guess is correct with probability exceeding 1/2.